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METASTABILITY OF THE ABC MODEL IN THE ZERO-TEMPERATURE LIMIT AND OF REVERSIBLE RANDOM WALKS IN POTENTIAL FIELDS

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Abstract

In this thesis we study the phenomenon of metastability in two specific contexts.

In the first part of the text, we consider the zero-temperature limit of the ABC Model. The ABC model is a conservative stochastic dynamics consisting of three species of particles, labeled A, B, C, on a discrete ring $\{-N, \dots, N\}$ (one particle per site). The system evolves by nearest neighbor transpositions: $AB \to BA$, $BC \to CB$, $CA \to AC$ with rate q and $BA \to AB$, $CB \to BC$, $AC \to CA$ with rate 1. We investigate a strongly asymmetric regime, the zero-temperature limit, where $q = e^{-\beta}$, $\beta \uparrow \infty$. The main result asserts that the particles almost always form three pure domains (one of each species) and that, as the system size N grows with β, this segregated shape evolves (in a proper time-scale) as a Brownian motion on the circle, which may have a drift.

In the second part, we consider reversible random walks in potential fields. More precisely, let Ξ be an open and bounded subset of $\mathbb{R}^d$ and let $F : \Xi \to \mathbb{R}$ be a twice continuously differential function. Denote by Ξ_N the discretization of Ξ, $\Xi_N = \Xi \cap (N^{-1}\mathbb{Z}^d)$, and denote by $\{X_N(t) : t \geq 0\}$ the continuous-time, nearest-neighbor, random walk on Ξ_N which jumps from $\boldsymbol{x}$ to $\boldsymbol{y}$ at rate $e^{-(1/2)N[F(\boldsymbol{y})-F(\boldsymbol{x})]}$. We examine the metastable behavior of $\{X_N(t) : t \geq 0\}$ among the wells of the potential F. Our main result states that, in an appropriate time-scale, the evolution of the random walk on Ξ_N can be described by a random walk in a weighted graph, in which the vertices represent the wells of the force field and the edges represent the saddle points.

Keywords: Metastability, Tunneling, Scaling limits, ABC Model, Brownian motion, Reversible random walks, Exit points

Resumo

Nesta tese estudamos o fenômeno de metaestabilidade em dois contextos específicos.

Na primeira parte do texto, consideramos o limite de temperatura zero do Modelo ABC. O modelo é um dinâmica markoviana conservativa que consiste em três tipos de partículas, rotuladas A, B, C, em um círculo discreto $\{-N, \dots, N\}$ (uma partícula por sítio). O sistema evolui através de transposições de partículas vizinhas mais próximas: $AB \to BA$, $BC \to CB$, $CA \to AC$ com taxa q e $BA \to AB$, $CB \to BC$, $AC \to CA$ com taxa 1. Nós investigamos um regime fortemente assimétrico, o limite de temperatura zero, onde $q = e^{-\beta}$, $\beta \uparrow \infty$. O principal resultado afirma que as partículas formam quase sempre três domínos puros (um de cada espécie) e que quando o tamanho do sistema, N, cresce com β, essa forma segregada evolui (em uma escala de tempo apropriada) como um movimento browniano no círculo, o qual pode ter um drift.

Na segunda parte, consideramos passeios aleatórios reversíveis em campos potenciais. Mais precisamente, seja Ξ um aberto limitado de $\mathbb{R}^d$, e $F : \Xi \to \mathbb{R}$ uma função suave. Seja $\Xi_N = \Xi \cap (N^{-1}\mathbb{Z}^d)$, e denote por $\{X_N(t) : t \geq 0\}$ o passeio aleatório a tempo contínuo em Ξ_N que pula de um ponto $\boldsymbol{x}$ para um ponto vizinho $\boldsymbol{y}$ à taxa $e^{-(1/2)N[F(\boldsymbol{y})-F(\boldsymbol{x})]}$. Nós examinamos o comportamento metaestável de $\{X_N(t) : t \geq 0\}$ entre os vales do potencial F, no limite $N \uparrow \infty$. Nosso principal resultado estabelece que em apropriadas escalas de tempo a evolução do passeio aleatório em Ξ_N pode ser descrita por um passeio aleatório em um grafo ponderado em que cada vértice representa um vale do potencial F e cada aresta representa um ponto de sela.

Palavras-chave: Metaestabilidade, Tunelamento, Limites de escala, Modelo ABC, Movimento Browniano, Passeios aleatórios reversíveis, Pontos de saída.

Contents

Introdução

Esta tese é baseada em nossos trabalhos [37] e [34], nos quais analisamos o fenômeno de *metaestabilidade* em dois diferentes contextos.

Metaestabilidade

De maneira informal, dizemos que um processo possui comportamento metaestável quando ele fica por um tempo longo em um estado antes de uma transição rápida para outro estado estável. Basicamente, metaestabilidade se refere à existência de duas ou mais escalas de tempo segundo as quais o processo mostra diferentes comportamentos. Na menor escala, a dinâmica alcança rapidamente um aparente equilíbrio e permanece restrita a um subconjunto do espaço de estados. Entretanto, quando o processo é visto em uma escala de tempo maior, observam-se eventuais transições entre estes estados de pseudo-equilíbrio, ou uma transição para um estado ainda mais estável.

Como fenômeno físico, metaestabilidade está presente em grande variedade de situações na natureza. Um exemplo clássico é a tardia transição de um líquido super-congelado para o estado sólido. Outros exemplos ocorrem na formação de grandes biomoléculas, como as proteínas; em reações químicas; em sistemas magnéticos de magnetização oposta a um campo externo; e até mesmo em transições entre aparentes equilíbrios no mercado de ações. O papel da matemática consiste em formular modelos microscópicos para as dinâmicas de interesse e provar o comportamento metaestável nesses modelos, o que pode contribuir no entendimento das características essenciais por trás da universalidade desse fenômeno. Em tais propostas de modelagem a metaestabilidade costuma ser atribuída à presença de algum tipo de aleatoriedade na dinâmica básica.

O inovador trabalho de Kramers [32] em 1940, com objetivo de descrever uma reação química, introduz um dos primeiros modelos matemáticos para metaestabilidade ao analisar o movimento de uma partícula em um potencial unidimensional de duplo-vale sob influência de um ruído gaussiano. Matematicamente, uma primeira formulação rigorosa de estados metaestáveis surge com os trabalhos de Lebowitz e Penrose [35] em 1971 no contexto da teoria de van der Waals-Maxwell da transição líquido-vapor.

Subsequentemente, Cassandro, Galves, Olivieri e Vares [21] em 1984 introduziram a abordagem de *análise de caminhos*, baseada em técnicas de grandes desvios nas trajetórias da dinâmica, no espírito da teoria de Freidlin and Wentzell [28] para pertubações aleatórias de sistemas dinâmicos. Em muitos diferentes contextos, estas ideias permitiram provar que o tempo de saída de um conjunto metaestável tem distribuição exponencial; obter estimativas para o valor esperado desse tempo; descrever as trajetórias típicas de escape e calcular a distribuição do ponto de saída de um conjunto metaestável. Para uma excelente revisão dessas técnicas e mais referências, indicamos o recente livro de Olivieri e Vares [40].

Em [15, 16], Bovier, Eckhoff, Gayrard e Klein iniciam uma abordagem de metaestabilidade via *teoria do potencial* baseada em cálculos de capacidades para redes elétricas associadas a cadeias de Markov reversíveis, no sentido de [23]. Os autores estabelecem também relações entre pequenos autovalores do gerador associado à dinâmica e tempos médios de saída de domínios. Essa abordagem fornece menos informação a respeito das trajetórias típicas, porém permite obter estimativas mais precisas para os tempos médios de saída de conjuntos metaestáveis [19], exibindo precisamente o pré-fator (a menos de erro multiplicativo convergindo para 1), em comparação à abordagem por análise de caminhos, onde as estimativas dos tempos médios de saída se dão por equivalência logarítmica. Para uma revisão dessas técnicas referimos a [13, 14].

Em [3, 6] Beltrán e Landim introduzem o que mais tarde se chamou de abordagem *martingal* para metaestabilidade [7]. Uma das ideias-chave aqui é observar o traço do processo nos conjuntos metaestáveis. Esse procedimento consiste em ignorar pedaços das trajetórias que são negligenciáveis nas escalas temporais de interesse. Tal método não se limita ao caso reversível, embora seja bem mais simples nesse caso. As ferramentas de teoria do potencial também costumam ser úteis nessa abordagem, já que é possível expressar as probabilidades de salto do processo traço, entre outras formas, por meio de capacidades. Assim como na abordagem via teoria do potencial, este método permite examinar modelos em que a razão entre as taxas de salto não é exponencial no parâmetro de escala, modelos onde se tem barreira energética logarítmica [4]. Nessa teoria, as informações sobre os tempos de transições entre os conjuntos metaestáveis são codificadas por um teorema que expressa a convergência da dinâmica (propriamente reescalada), em uma topologia introduzida em [33], para uma cadeia de Markov limite com simplificado espaço de estados. Esse resultado é, portanto, especialmente interessante no caso de diversos conjuntos metaestáveis em competição em uma mesma escala de tempo. Sob certas condições gerais em termos de capacidades e da medida estacionária, em [3] a referida convergência é demonstrada com uso da caracterização de processos de Markov via martingais.

As diferentes abordagens fornecem uma gama de ferramentas, mas descrições completas baseiam-se na análise específica de cada modelo. Geralmente é relevante a estrutura geométrica do espaço de configurações, o perfil energético associado e a caracterização das chamadas configurações de sela, o que pode facilitar o cálculo preciso das quantidades de interesse via princípios variacionais. Muitas técnicas são consideravelmente mais simples ou somente aplicáveis na presença de reversibilidade.

Nesta tese analisamos metaestabilidade em dois modelos diferentes. Em ambos os modelos, nosso objetivo é caracterizar as dinâmicas markovianas limites no sentido de [3, 33] de modo a obter uma descrição simples para o comportamento dos processos em grandes escalas de tempo. No Capítulo 1, analisamos o limite de temperatura zero do modelo ABC, um sistema de partículas conservativo que, com exceção de um caso especial, não é reversível. No Capítulo 2, analisamos passeios aleatórios reversíveis em discretizações de subconjuntos limitados de $\mathbb{R}^d$ para os quais a medida estacionária é descrita por um potencial de multi-vales F. No que segue, apresentamos brevemente os modelos e os principais resultados de cada parte deste trabalho.

Modelo ABC no limite de temperatura zero

Na primeira parte desta tese são apresentados resultados sobre o comportamento metaestável do sistema de partículas conhecido como *modelo ABC*. Introduzido por Evans et al. [26, 27], o modelo é uma dinâmica conservativa que consiste em três tipos de partículas, rotuladas A, B e C, em um círculo discreto $\{-N, \dots, N\}$ (uma partícula por sítio). A dinâmica markoviana evolui através de transposições entre partículas vizinhas: $AB \to BA$, $BC \to CB$, $CA \to AC$ com taxa q e $BA \to AB$, $CB \to BC$, $AC \to CA$ com taxa 1.

O comportamento assintótico do processo tem sido bastante estudado no regime *fracamente assimétrico*, $q = e^{-\beta/N}$, introduzido por Clincy et al. [22] (ver também [2, 9, 12, 8]), quando o tamanho do sistema, N, vai para infinito e β é um parâmetro fixo que faz o papel do inverso da temperatura, a qual podemos interpretar como o grau de desordem do sistema. Aqui investigamos um regime *fortemente assimétrico*, o limite de temperatura zero, em que $q = e^{-\beta}$, $\beta \uparrow \infty$. Neste regime, mostra-se que as partículas segregam-se formando quase sempre três domínios puros, um de cada espécie, localizados na ordem cíclica ABC.

Quando o número de partículas de cada tipo, N_A, N_B e N_C, é fixo (i.e. não varia com β) observamos um fenômeno de metaestabilidade, que revela um interessante (e, à primeira vista, surpreendente) comportamento assintótico não local. A saber, para N_A, N_B, N_C constantes, quando $\beta \uparrow \infty$ a dinâmica do modelo ABC na escala de tempo $e^{\min\{N_A,N_B,N_C\}\beta}$ converge[1] para um processo de Markov que evolui nas $N_A + N_B + N_C$ configurações segregadas, o qual salta de uma configuração para outra qualquer a uma taxa estritamente positiva. As taxas de salto do processo markoviano limite podem ser expressas em termos de probabilidades de absorção de uma dinâmica extremamente mais simples (ver Figura 1.1). No Capítulo 1 este resultado é apresentado de maneira precisa (Teorema 1.2.5) em termos do já mencionado processo traço que é um objeto central em nossa análise do modelo ABC.

Nosso principal resultado no estudo do modelo ABC, Teorema 1.2.2, considera o limite quando o número de partículas cresce com β. Neste caso, sob certas condições no modo com que N_A, N_B e $N_C \uparrow \infty$ com β, na escala de tempo $N^2 e^{\min\{N_A,N_B,N_C\}\beta}$ quando $\beta \uparrow \infty$, a evolução do centro de massa das partículas de tipo A (por exemplo) converge para um movimento browniano no círculo. Sem assumir densidade positiva de cada tipo de partícula, encontramos um interessante caso em que o movimento browniano limite tem um drift.

Uma diferença significativa entre o modelo ABC e outros processos onde resultados semelhantes foram demonstrados (ver, por exemplo, [5, 31]) é que, com exceção do caso $N_A = N_B = N_C$, o processo ABC é não reversível e sua medida invariante não é explicitamente conhecida. Para o nosso conhecimento, esta é a primeira descrição precisa do limite de temperatura zero para um processo desse tipo.

Passeios aleatórios reversíveis em campos potenciais

Na segunda parte desta tese, estudamos o comportamento metaestável de passeios aleatórios reversíveis em campos potenciais. Este é um problema antigo cuja origem pode remeter pelo menos ao trabalho de Kramers [32]. O problema foi considerado por Freidlin e Wentsell [28] e por Galves, Olivieri e Vares [29] no contexto de pequenas pertubações aleatórias de sistemas dinâmicos, e, mais recentemente, por Bovier, Eckhoff, Gayrard e Klein em uma série de artigos [15, 16, 17, 18] através da abordagem de metaestabilidade via teoria do potencial.

Analisamos passeios aleatórios em discretizaçõces de um subconjunto de $\mathbb{R}^d$ ao qual é associado um perfil energético F com diversos mínimos locais. Mais precisamente, seja Ξ um aberto limitado de $\mathbb{R}^d$, e $F : \Xi \to \mathbb{R}$ uma função suave. Seja $\Xi_N = \Xi \cap (N^{-1}\mathbb{Z}^d)$, e denote por $\{X_N(t) : t \geq 0\}$ o passeio aleatório a tempo contínuo em Ξ_N que pula de um ponto $\boldsymbol{x}$ para um ponto vizinho $\boldsymbol{y}$ à taxa $e^{-(1/2)N[F(\boldsymbol{y})-F(\boldsymbol{x})]}$. Nós examinamos o comportamento metaestável de $\{X_N(t) : t \geq 0\}$ entre os vales do potencial F, no limite $N \uparrow \infty$.

Assumimos que o potencial F tem um número finito de pontos críticos. Nos mínimos locais exigimos que a matriz hessiana de F tenha autovalores estritamente

[1] A convergência ocorre em uma topologia apropriada introduzida em [33], mais fraca que a de Skohorod.

positivos; nos pontos de sela exigimos exatamente um autovalor estritamente negativo, os demais sendo estritamente positivos. Sob estas condições nosso principal resultado, Teorema 2.2.4, estabelece que em apropriadas escalas de tempo a evolução do passeio aleatório em Ξ_N pode ser descrita por um passeio aleatório em um grafo ponderado em que cada vértice representa um vale do potencial F (i.e, vizinhança de um mínimo local) e cada aresta representa um ponto de sela. Em cada escala de tempo considerada, a dinâmica assintótica pode ter pontos abosorventes, correspondendo a vales mais profundos. Quanto aos pontos transientes, as respectivas taxas de salto dependem apenas do comportamento do potencial em vizinhanças dos mínimos e das selas relevantes. Tais taxas são explicitadas em termos do determinante e do autovalor negativo (no caso das selas) da matriz hessiana de F nesses pontos.

Nossa análise ganha especial interesse no caso em que existem vários vales com mesma profundidade em um mesmo nível energético. Esse cenário, que não havia sido considerado anteriormente, permite o acontecimento de situações mais ricas, uma vez que a dinâmica limite, no sentido de [33], em cada escala de tempo, não se limita necessariamente a apenas um salto possível de um estado transiente para um estado absorvente.

Nosso segundo principal resultado nesse contexto, Teorema 2.2.7, considera o problema dos pontos de saída de um vale. Seja $\boldsymbol{x}$ um mínimo local do potencial F e $\{\boldsymbol{z}_1, \dots, \boldsymbol{z}_k\}$ as mais baixas selas de F separando $\boldsymbol{x}$ de outros mínimos locais. No Teorema 2.2.7 obtemos as probabilidades assintóticas de que o passeio aleatório $\{X_N(t) : t \geq 0\}$ saia do vale contendo o mínimo $\boldsymbol{x}$ atravessando vizinhanças mesoscópicas das selas $\boldsymbol{z}_i$.

CHAPTER 1

Zero-temperature limit of the ABC model

ABSTRACT. We consider the ABC model on a ring in a strongly asymmetric regime. The main result asserts that the particles almost always form three pure domains (one of each species) and that this segregated shape evolves, in a proper time scale, as a Brownian motion on the circle, which may have a drift. This is, to our knowledge, the first proof of a zero-temperature limit for a non-reversible dynamics whose invariant measure is not explicitly known.

1.1 Introduction

The *ABC model*, introduced by Evans et al. [26, 27], is a stochastic conservative dynamics consisting of three species of particles, labeled A, B, C, on a discrete ring $\{-N, \ldots, N\}$ (one particle per site). The system evolves by nearest neighbor transpositions: $AB \to BA$, $BC \to CB$, $CA \to AC$ with rate q and $BA \to AB$, $CB \to BC$, $AC \to CA$ with rate 1.

The asymptotic behavior of the process (and of its variations) has been widely studied in the *weakly asymmetric* regime $q = e^{-\beta/N}$, introduced by Clincy et al. [22], when the system size N goes to infinity and β is a fixed control parameter which plays the role of the inverse temperature. In this regime, an interesting phase transition phenomenon arises as β is tuned.

We investigate here a *strongly asymmetric* regime, the zero-temperature limit, where $q = e^{-\beta}$, $\beta \uparrow \infty$. We consider two types of asymptotics: In Theorem 1.2.5 we examine the behavior of the process in the case where the number of particles of each species, N_A, N_B and N_C, is fixed and $\beta \uparrow \infty$; in Theorem 1.2.2, N_A, N_B and N_C increase with β.

We show in Lemma 1.2.1 that the particles almost always form three pure domains, one of each species, located clockwise in the cyclic-order ABC. For fixed volume, we show that, in the time scale $e^{\min\{N_A,N_B,N_C\}\beta}$, as $\beta \uparrow \infty$, the process converges to a Markov chain that evolves among these $2N+1$ segregated configurations, jumping from any configuration to any other at positive rates. These jump rates can be expressed in terms of some absorption probabilities of a much simpler dynamics.

When N grows with β, with some restrictions on the speed of this growth, we prove in Theorem 1.2.2 that, in the time scale $N^2 e^{\min\{N_A,N_B,N_C\}\beta}$, the center of mass of the particles of type A (for example) moves as a Brownian motion on the circle. Without assuming positive proportion of each type of particle, we identify an interesting degenerated case in which the limit Brownian motion has a drift.

Our method for proving Theorem 1.2.2 involves the analysis of the trace process in the set of the segregated configurations, the process which neglects the time spent in other configurations.

Results of the same nature (the description of the dynamics among the ground states in finite volume and the convergence to a Brownian motion on a large torus) were obtained for the Kawasaki dynamics for the Ising lattice gas at low temperature in two dimensions by Beltrán, Gois and Landim [5, 31]. Many techniques used in our analysis of the ABC model come from these papers. We emphasize that, in comparison with the Kawasaki dynamics, a significant difference is that, with the exception of the case $N_A = N_B = N_C$, the ABC process is non-reversible and its invariant measure is not explicitly known.

In this strongly asymmetric regime we are dealing, the model fits the assumptions considered by Olivieri and Scoppola in [39]. In principle, the general procedure proposed by them, consisting in the analysis of successive time-scales, e^{β}, $e^{2\beta}, \dots$, could be applied here, especially if we were interested in understanding the mechanism of nucleation of the process starting from an arbitrary configuration. However, the analysis based on this iterative scheme would become quite complicated in the ABC model due to the combinatorial complexity of the evolution among the metastable configurations which would appear in each scale. Our analysis, which relies on a precise understanding of the microscopic dynamics when the process is close to one of the segregated configurations, leads to a very accurate understanding of the limiting process in the time-scale required for transitions among the most stable configurations.

1.2 Notations and results

1.2.1 The ABC Process

Given an integer N, let $\Lambda_N = \{-N, \dots, N\}$ be the one-dimensional discrete ring of size $2N+1$. A configuration in $\widetilde{\Omega}^N := \{A, B, C\}^{\Lambda_N}$ is denoted by $\omega = \{\omega(k) : k \in \Lambda_N\}$, where $\omega(k) = \alpha$ if site k is occupied by a particle of type $\alpha \in \{A, B, C\}$. We make the convention that $\alpha+1, \alpha+2, \dots$ denote the particle types that are successors to α in the cyclic-order ABC.

For $i, j \in \Lambda_N$ and $\omega \in \widetilde{\Omega}^N$ we denote by $\sigma^{i,j}\omega$ the configuration obtained from ω by exchanging the particles at the sites i and j:

$$(\sigma^{i,j}\omega)(k) = \begin{cases} \omega(k) & \text{if } k \notin \{i, j\}, \\ \omega(j) & \text{if } k = i, \\ \omega(i) & \text{if } k = j. \end{cases}$$

We consider the continuous-time Markov chain $\{\eta^\beta(t) : t \geq 0\}$ on the state space $\widetilde{\Omega}^N$ whose generator L_β acts on functions $f : \widetilde{\Omega}^N \to \mathbb{R}$ as

$$(L_\beta f)(\omega) = \sum_{k \in \Lambda_N} c_k^\beta(\omega)[f(\sigma^{k,k+1}\omega) - f(\omega)]$$

where, for $\beta \geq 0$, the jump rates c_k^β are given by

$$c_k^\beta(\omega) = \begin{cases} e^{-\beta} & \text{if } (\omega(k), \omega(k+1)) \in \{(A,B), (B,C), (C,A)\}, \\ 1 & \text{otherwise.} \end{cases}$$

Almost always we omit the index β and denote $\eta^\beta(t)$ just by $\eta(t)$.

As the system evolves by nearest neighbor transpositions, the number of particles of each species is conserved. Therefore, given three integers N_α, $\alpha \in \{A, B, C\}$, such that $N_A + N_B + N_C = 2N+1$, we have a well defined process on the component $\Omega^{N_A, N_B, N_C} = \{\omega \in \widetilde{\Omega}^N : \sum_{k \in \Lambda_N} \mathbf{1}\{\omega(k) = \alpha\} = N_\alpha, \, \alpha \in \{A, B, C\}\}$, which is clearly irreducible and then admits a unique invariant measure. To shorten notation, let us suppose that we have fixed N_A, N_B, and N_C as functions of N and then we write simply Ω^N instead of Ω^{N_A, N_B, N_C}.

The invariant measure $\mu_\beta = \mu_{\beta,N}$ is in general not explicit known. However, in the special case of equal densities $N_A = N_B = N_C$, as shown in [26, 27], the process is reversible with respect to the Gibbs measure μ_β, given by

$$\mu_\beta(\omega) = \frac{1}{Z_\beta} e^{-\beta \mathbb{H}(\omega)},$$

where Z_β is the normalizing partition function and $\mathbb{H}$ is a non-local Hamiltonian, which may be written as

$$\mathbb{H}(\omega) = \frac{1}{2N+1} \sum_{k\in\Lambda_N} \sum_{i=1}^{2N} i\mathbf{1}\big\{(\omega(k), \omega(k+i)) \in \{(A,B),(B,C),(C,A)\}\big\}. \quad (1.2.1)$$

A simple computation relying on the equal densities constraint shows that nearest neighbor transpositions of type $(\alpha, \alpha{+}1) \to (\alpha{+}1, \alpha)$ increase the energy $\mathbb{H}$ by 1 unit, while the opposite kind of transposition decreases $\mathbb{H}$ by 1 unit. The reversibility of the process in this special case follows from this observation.

The configurations in which the particles form three pure regions, one of each species, located clockwise in the cyclic-order ABC deserve a special notation. Define $\omega_0^N \in \Omega^N$ as

$$\omega_0^N(j) = \begin{cases} A & \text{if } 0 \le j \le N_A - 1, \\ B & \text{if } N_A \le j \le N_A + N_B - 1, \\ C & \text{otherwise,} \end{cases}$$

and, for each $k \in \Lambda_N$, define $\omega_k^N = \Theta^k \omega_0^N$, where $\Theta^k : \Omega^N \to \Omega^N$ stands for the shift operator $(\Theta^k\omega)(i) = \omega(i-k)$. By convention we omit the index N in the notation, and we write simply ω_k instead of ω_k^N. Denote by Ω_0^N the set of these configurations:

$$\Omega_0^N = \{\omega_k : k \in \Lambda_N\}.$$

We remark that, in the equal densities case, Ω_0^N corresponds to the set of ground states of the energy $\mathbb{H}$.

For each $\omega \in \Omega^N$ denote by $\mathbf{P}_\omega^\beta$ the probability measure induced by the Markov process $\{\eta(t) : t \ge 0\}$ starting from ω on the Skorohod space $D([0,\infty), \Omega^N)$ of càdlàg paths. Expectation with respect to $\mathbf{P}_\omega^\beta$ is represented by $\mathbf{E}_\omega^\beta$.

1.2.2 Main results

We analyze in this article the asymptotic evolution, as $\beta \uparrow \infty$, of the Markov process $\{\eta(t) : t \ge 0\}$, where also the number of particles may depend on β. For simplicity, we omit this dependence in the notation.

From now on, we use the notation

$$M = \min\{N_A, N_B, N_C\}.$$

If the process starts from some $\omega_k \in \Omega_0^N$, at least M jumps of rate $e^{-\beta}$ are needed in order to visit another configuration in Ω_0^N. This suggests that, for fixed N, the interesting time scale to consider is $e^{M\beta}$. In Section 1.9 we show that, in the time scale $N^2 e^{M\beta}$, if N does not increase too fast with β, the process spends a negligible time outside Ω_0^N:

Lemma 1.2.1. *Let* $M^* = \max\{N_A, N_B, N_C\}$. *Assume that*

$$\lim_{\beta\to\infty} N^3 4^{M^*} e^{-\beta} = 0 \tag{1.2.2}$$

Then, for every $k \in \Lambda_N$, $t \geq 0$

$$\lim_{\beta\to\infty} \mathbf{E}^{\beta}_{\omega_k}\left[\int_0^t \mathbf{1}\{\eta(sN^2e^{M\beta}) \notin \Omega_0^N\}ds\right] = 0. \tag{1.2.3}$$

Our main result, Theorem 1.2.2, characterizes the motion of this segregated shape in the time-scale $N^2e^{M\beta}$ when the system size grows with β. We express the result in terms of the convergence of the evolution of a macroscopic variable associated to the configurations: the center of mass of the particles of type A. In order to define this center of mass we need to introduce some other notations. For any configurations $\xi, \zeta \in \Omega^N$, by a path from ξ to ζ we mean a sequence of configurations $\gamma = (\xi = \xi_0, \xi_1, \ldots, \xi_n = \zeta)$ such that ξ_k can be obtained from ξ_{k-1} by a simple nearest neighbor transposition. We define $\text{dist}(\xi, \zeta)$ as the smallest n such that there exists a path from ξ to ζ of length n. For any n, and $k \in \Lambda_N$, define

$$\Delta_k^n = \{\omega \in \Omega^N : \text{dist}(\omega, \omega_k) = n\}. \tag{1.2.4}$$

Due to the periodic boundary conditions, for many configurations the centers of mass of the particles of type α, $\alpha \in \{A, B, C\}$, are not well defined. However, the proof of Lemma 1.2.1 in fact shows that, under (1.2.2), for any $t \geq 0$

$$\lim_{\beta\to\infty} \mathbf{P}^{\beta}_{\omega_0}\left[\eta(s) \notin \Xi^N \text{ for some } 0 \leq s \leq tN^2e^{M\beta}\right] = 0, \tag{1.2.5}$$

where Ξ^N is a subset of configurations such that $\Xi^N \subseteq \Gamma^N := \bigcup_{k\in\Lambda_N} \Gamma_k^N$, where

$$\Gamma_k^N = \left(\bigcup_{n=0}^{M} \Delta_k^n\right) \cup \bigcup_{i_1,i_2,i_3,i_4\in\Lambda_N} \{\sigma^{i_1,i_2}\sigma^{i_3,i_4}\omega_k\}.$$

Note that the configurations in Γ_k^N that are not at distance M or less from ω_k differ from ω_k by at most two transpositions, not necessarily nearest-neighbor. In Γ^N, the center of mass can be defined unambiguously. Suppose, for example, that $N_A = M$. For $\omega \in \Gamma_0^N$, define the center of mass (of the particles of type A) of the configuration ω, denoted by $\mathcal{C}(\omega)$, as

$$\mathcal{C}(\omega) = \frac{1}{N}\sum_{k\in\Lambda_N} \frac{k\mathbf{1}\{\omega(k) = A\}}{N_A}.$$

Then, for a configuration $\xi \in \Gamma_k^N$, $k \in \Lambda_N$, take $\omega \in \Gamma_0^N$ such that $\xi = \Theta^k\omega$, and define $\mathcal{C}(\xi) = \mathcal{C}(\omega) + k/N \mod [-1, 1]$. Just for completeness, for $\xi \notin \Gamma^N$ define $\mathcal{C}(\xi) = 0$. Actually, by (1.2.5) this latter definition is not relevant.

Let

$$d := |\{\alpha \in \{A, B, C\} : N_\alpha = M\}|. \tag{1.2.6}$$

Note that d may vary with β, but we omit this dependence to simplify the notation. Define

$$\theta_\beta := \frac{1}{2d} e^{M\beta} N^2. \tag{1.2.7}$$

Our main result is the following theorem.

Theorem 1.2.2. *Assume that $\eta(0) = \omega_0$ and that $N \uparrow \infty$ as $\beta \uparrow \infty$ in such a way that $N_A < N_B \leq N_C$, with $N_A \uparrow \infty$, $N_A/N \to r_A \geq 0$,*

$$\lim_{\beta\to\infty} \left(\frac{1}{3}\right)^{N_B} N_C = b \in [0, \infty) \tag{1.2.8}$$

and

$$\lim_{\beta\to\infty} (N^5 4^{N_A} + N^3 4^{N_C}) e^{-\beta} = 0. \tag{1.2.9}$$

Then, as $\beta \uparrow \infty$, the process $\{\mathcal{C}(\eta(t\theta_\beta)) : t \geq 0\}$ converges in the uniform topology to the diffusion

$$\{(1/2)r_A - (3/2)bt + B_t : t \geq 0\} \tag{1.2.10}$$

on the circle $[-1, 1]$, where $\{B_t : t \geq 0\}$ is a Brownian motion with infinitesimal variance equal to 1. If $b = 0$ in (1.2.8), we may replace the assumption $N_A < N_B$ by $N_A \leq N_B$.

Remark 1.2.3. *In Theorem 1.2.2, if N_B increases not so slowly, in the sense that $b = 0$ in (1.2.8), then the limit is a Brownian motion without drift. This is the case when we have positive proportion of each type of particle:*

$$\lim_{\beta\to\infty} \frac{N_\alpha}{N} > 0, \quad \alpha \in \{A, B, C\}. \tag{1.2.11}$$

On the other hand, if N_B increases even more slowly, in the sense that $b = \infty$ in (1.2.8), then we have to look at the process in another time scale. Suppose, for example, that we can find some $u \in (1, 2)$ such that

$$\lim_{\beta\to\infty} \left(\frac{1}{3}\right)^{N_B} N_C^{u-1} = c \in (0, \infty). \tag{1.2.12}$$

In this case, replacing (1.2.8) by (1.2.12), we can prove that, as $\beta \uparrow \infty$, the process $\{\mathcal{C}(\eta(tN^u e^{N_A\beta})) : t \geq 0\}$ converges to a deterministic linear function $\{\mu t : t \geq 0\}$ on the circle $[-1, 1]$, where μ is a constant which depends on c. This will become clear with the proofs given in Section 1.8.

Remark 1.2.4. *In Lemma 1.2.1, the restriction* (1.2.2) *is not optimal. It comes from our crude estimation of* $\mu_\beta(\Xi^N)$ *in the general densities case, where the invariant measure is not explicitly known. By repeating the steps that lead to* (1.9.16), *we see that assertion* (1.2.3) *also hods if*

$$\lim_{\beta\to\infty} \mu_\beta(\Omega^N \setminus \Omega_0^N) = 0. \tag{1.2.13}$$

In the special case of equal densities, where the invariant measure is explicitly known, we can verify (1.2.13) *without any assumption that controls the growth of* N. *Details are given in Section 1.9.*

1.2.3 Results for the trace process in Ω_0^N

Now we present some results that are preliminary steps in our method to prove Theorem 1.2.2, but which are interesting by themselves.

Denote by $\{\eta_0(t) : t \geq 0\}$ the trace of the process $\{\eta(t) : t \geq 0\}$ on the set Ω_0^N, i.e, the Markov chain obtained from $\{\eta(t) : t \geq 0\}$ by neglecting the time spent outside Ω_0^N. More precisely, we define $\{\eta_0(t) : t \geq 0\}$ by

$$\mathcal{T}_t = \int_0^t \mathbf{1}\left\{\eta(s) \in \Omega_0^N\right\} ds; \quad \mathcal{S}_t = \sup\{s \geq 0 : \mathcal{T}_s \leq t\}; \quad \eta_0(t) = \eta\left(\mathcal{S}_t\right). \tag{1.2.14}$$

We refer to [3] for important elementary properties of the trace process.

To prove Theorem 1.2.2 we first analyze the trace process $\{\eta_0(t) : t \geq 0\}$. For finite volume we obtain the following result which reveals an interesting non-local asymptotic behavior.

Theorem 1.2.5. *For* N_A, N_B *and* N_C *constant greater than or equal to* 3, *as* $\beta \uparrow \infty$ *the speeded up process* $\{\eta_0(e^{M\beta}t) : t \geq 0\}$ *converges to a Markov process on* Ω_0^N *which jumps from* ω_i *to* ω_j *at a strictly positive rate* $r(i,j)$.

The proof of this theorem, as well as the expression for $r(i,j)$, is given in Section 1.6. This theorem is complemented with Lemma 1.2.1, which says that we are not losing much just looking at the trace process in Ω_0^N. The rates $r(i,j)$, which depend also on N_A, N_B and N_C, can be expressed in terms of some absorption probabilities of a simple Markov dynamics, the one described by Figure 1.1 in the next section.

Remark 1.2.6. *It is possible to reformulate Theorem 1.2.5, without referring to the trace process, by asserting the convergence of the (time re-scaled) original process* $\{\eta(e^{M\beta}t) : t \geq 0\}$ *in a topology introduced in [33], weaker than the Skorohod one.*

Denote by $R_0^\beta(\omega_i,\omega_j)$ the jump rates of the trace process $\{\eta_0(t) : t \geq 0\}$. By translation invariance, it is clear that

$$R_0^\beta(\omega_i,\omega_j) = R_0^\beta(\omega_0,\omega_{j-i}) =: r_\beta(j-i). \tag{1.2.15}$$

Let $\mathbf{X}(\omega_k) = k$, $k \in \Lambda_N$, so that if $X(t) = \mathbf{X}(\eta_0(t))$ then $\{X(t) : t \geq 0\}$ is a random walk on Λ_N which jumps from i to j at rate $r_\beta(j-i)$.

The next result refers to the case where N goes to infinity as a function of β. We start considering the degenerated case where N_A and N_B are constants and only N_C goes to infinity. We have a ballistic behavior in this situation.

Theorem 1.2.7. *Assume that $3 \leq N_A < N_B$ are constants and that $N_C \uparrow \infty$ as $\beta \uparrow \infty$ in such a way that*

$$\lim_{\beta \to \infty} N_C^5 \beta e^{-\beta} = 0. \tag{1.2.16}$$

If $\eta(0) = \omega_0$, then, as $\beta \uparrow \infty$, the process $\{X(tNe^{N_A\beta})/N : t \geq 0\}$ converges in the uniform topology to a linear function $\{v(N_A, N_B)t : t \geq 0\}$ on the circle $[-1, 1]$.

The condition $N_A < N_B$ is crucial for the ballistic behavior. If N_A and N_B are constant but $N_A = N_B$, then the process $\{X(t) : t \geq 0\}$ is symmetric. In this case, scaling time by $N^2 e^{M\beta}$ we can prove the convergence to a Brownian motion if $N_C^6 \beta e^{-\beta} \downarrow 0$. In the case $N_A \neq N_B$, the velocity $v(N_A, N_B)$, which is an antisymmetric function of N_A and N_B, is negative when $N_A < N_B$. It can be expressed in terms of some absorption probabilities for a random walk in a simple graph, which can be explicitly computed in terms of N_A and N_B. The analysis of the asymptotic dependence of $v(N_A, N_B)$ on N_A and N_B, which is presented in Lemma 1.7.4 helps us to find the specific scenario, (1.2.8), for the convergence to a Brownian motion with drift.

The proof of Theorem 1.2.7 is given in Section 1.8, where we also state and prove the version of Theorem 1.2.2 referring to the trace process (Theorem 1.8.1).

1.3 Sketch of the proofs

Our main result, Theorem 1.2.2, is a consequence of the corresponding Theorem 1.8.1 and the fact, to be proved in Section 1.10, that (assuming $\eta(0) = \omega_0$) the process $\{\mathcal{C}(\eta(t\theta_\beta)) : t \geq 0\}$ is close to the trace process $\{X(t\theta_\beta)/N + r_A/2 : t \geq 0\}$ in the Skohorod space $D([0, \infty), [-1, 1])$.

The main idea to analyze the trace of the process $\{\eta(t) : t \geq 0\}$ on Ω_0^N is to consider first the trace on a larger set Ω_1^N. Now we will see why such a set Ω_1^N comes naturally.

To fix ideas, suppose that $3 \leq N_A \leq N_B \leq N_C$ are constants[1]. Suppose that the process starts from the configuration $\omega_k \in \Omega_0^N$. Note that, in order to visit any other configuration in Ω_0^N, at least N_A jumps of rate $e^{-\beta}$ are needed. The most simple trajectory that we can imagine between ω_k and another configuration in Ω_0^N occurs

[1]An interactive picture of the possible configurations of the ABC model, which can help in the visualization of the trajectories, can be found at http://tube.geogebra.org/student/m98277.

when the whole block of particles of type A is crossed, for example, by a particle of type C walking clockwise (and for this, N_A jumps of rate $e^{-\beta}$ are needed) and then this detached particle of type C can continue moving in clockwise direction inside the domain of particles of type B (now performing rate 1 jumps) until, after crossing all the particles of type B, it meets the other particles of type C. This way, we arrive at the configuration ω_{k-1}. In an analogous way, we find a path from ω_k to ω_{k+1}. This reveals that the correct time scale to analyze the trace process on Ω_0^N is $e^{N_A\beta}$.

At first glance, it appears that these trajectories we described are the only ones possible in the time scale $e^{N_A\beta}$ and that the asymptotic dynamics will be restricted to jumps from ω_k to ω_{k+1} or ω_{k-1}. So, Theorem 1.2.5 is somewhat surprising. The truth is that, for any j, there exists a trajectory from ω_k, which is possible in the time scale $e^{N_A\beta}$, such that the next visited configuration in Ω_0^N is ω_j. The explanation is the following. Starting from ω_k, in a time of order $e^{N_A\beta}$ it is possible that we have a meeting of a particle of type C and a particle of type B inside the domain of particles of type A. Once these two particles meet, they can interchange their positions performing a rate 1 jump. This way, we fall in a metastable configuration from which all possible jumps have rate $e^{-\beta}$. This configuration is very similar to ω_k except for the pair BC inside the block of As. For this configuration, transposition of nearest neighbor particles that are far from this pair BC, which may occur at the frontiers between two different domains, are reverted with high probability in the next jump of the chain. So, let us focus in what can happen with this pair BC.

After a time of order e^{β}, this pair can disappear if BC turns to CB and then, with rate 1 jumps, the particles C and B return to their original positions in the configuration ω_k. But also, in a time of order e^{β}, the pair BC can move inside the domain of particles of type A. For example, with a rate $e^{-\beta}$ jump, the particle C can move to the right, in such a way that $ABCAA$ becomes $ABACA$. Now, with a rate 1 jump, the particle B moves to the right and we obtain $AABCA$. Clearly, the pair BC can also move to the left. This way, we can move the pair BC until, for example, near to the right end of the block of particles of type A, and we arrive at a configuration that is almost ω_k except for the appearance of a block $AABCABB$ in the frontier of the regions of particles A and B. From this configuration, the pair CA can turn to AC and after N_B jumps of rate 1 we arrive at ω_{k-1}. But also, by the same reason as before, instead of becomes AC, in times of order e^{β} the pair CA can move inside the domain of particles of type B until eventually the process may arrive at a configuration that is almost ω_{k-1} except for a block $BBCABCC$ in the frontier of regions of particles of types B and C. At this point, after a time of order e^{β}, the pair AB can turn to BA and then, after N_C jumps of rate 1, the process can arrive at ω_{k-2}. This shows how, in time scale $e^{M\beta}$, it is possible to find a path starting from ω_k such that the next visited configuration in Ω_0^N is ω_{k-2}. Clearly, we could continue moving a pair of particles in order to arrive at any configuration in Ω_0^N.

The class of the metastable configurations which appears in the above described paths will be called Ω_1^N, and it will be precisely defined in Section 1.4. As the above discussion indicates, starting from a configuration in Ω_0^N, after a time of order $e^{N_A\beta}$, we can visit a configuration $\omega \in \Omega_1^N$ where we will stay for a time of order e^{β}. Starting from $\omega \in \Omega_1^N$, in time scale e^{β}, essentially, what we see is a Markov chain $\{\widehat{\eta}_1(e^{\beta}t) : t \geq 0\}$ in Ω_1^N for which the configurations in Ω_0^N are absorbing states. The structure of this dynamics reveals to be pretty simple, as shown in Figure 1.1.

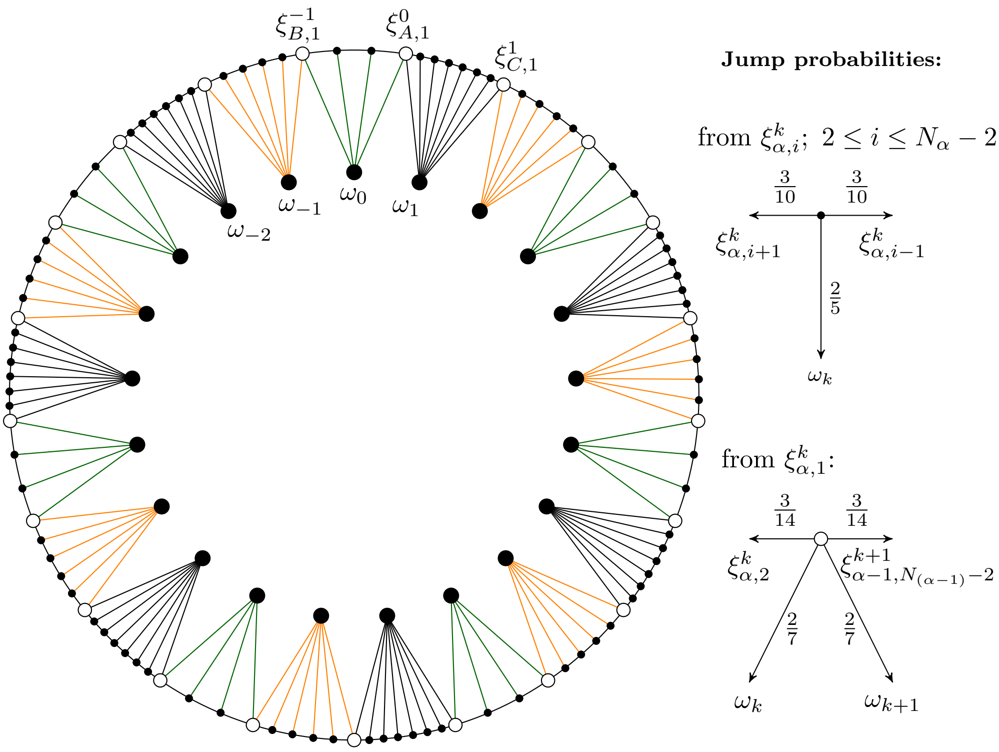

Figure 1.1: Graph structure of the ideal dynamics $\{\widehat{\eta}_1(t) : t \geq 0\}$ related to the process. The picture illustrates the case $N_A = 5$, $N_B = 7$ and $N_C = 9$. The inner vertices represent the configurations in Ω_0^N, absorbing states for this dynamics. The outer vertices represent the metastable configurations in $\Omega_N^1 \setminus \Omega_N^0$, which will be precisely defined in the next section. The arrows on the right completely describe the corresponding discrete-time jump chain.

The dynamics described in Figure 1.1 indicates that the trace on Ω_0^N is not a symmetric process and that this asymmetry can be balanced depending on the relative quantities of each type of particle. This behavior is at the origin of the drift which appears in Theorem 1.2.2.

We have, therefore, a strategy to analyze the trace of $\{\eta(t) : t \geq 0\}$ on Ω_0^N. At first, we consider the trace on Ω_1^N. This will be the subject of Section 1.5.

Essentially, we have to answer the following question: starting from a configuration ω in Ω_1^N, what is the distribution of the next visited configuration in Ω_1^N? We split this question into two, depending if ω belongs to Ω_0^N or not. In the first case, we will see an interesting "uniformity" for this distribution, in a sense to be clarified at Proposition 1.5.5. At this point the error terms in our estimates increase exponentially in N, and here is where some constraints referring to the growth of N arise. In the second case, we observe that the process is well approximated by the asymptotic Markov chain $\{\widehat{\eta}_1(t) : t \geq 0\}$.

To pass from the trace on Ω_1^N to the trace on Ω_0^N, we have to look at the absorptions probabilities on Ω_0^N for the chain $\{\widehat{\eta}_1(t) : t \geq 0\}$ starting from $\Omega_1^N \setminus \Omega_0^N$. In Section 1.6, we present (approximations of) the jump rates $r_\beta(k)$, $k \in \Lambda_N$, defined on (1.2.15), as functions of these absorption probabilities, which are estimated in Section 1.7 allowing us to prove, in Section 1.8, the results for the trace process on Ω_0^N in the case where $N \uparrow \infty$ with β.

All the above discussion also suggests what are the typical configurations that may appear between two consecutive visits to the set Ω_0^N. In Section 1.9 we will estimate the measure μ_β of these configurations and this will allow us to prove that the process spends a negligible time outside Ω_0^N.

1.4 The subset of configurations Ω_1^N

In this section we define the set of configurations Ω_1^N establishing notation that identifies each one of its elements. Throughout the text, even when not explicitly mentioned, we are assuming that $M \geq 3$.

1.4.1 The configurations $\zeta_{\alpha,i}^k$

For $k \in \Lambda_N$, $\alpha \in \{A, B, C\}$ and $0 \leq i \leq N_\alpha$, denote by $\zeta_{\alpha,i}^k$ the configuration at distance N_α from ω_k, obtained from $\omega_k \in \Omega_0^N$ by a meeting of two distinct particles of types different from α in the block of particles of type α. The index i indicates the position of this meeting. More precisely, let f_α be the position of the first particle of type α in the configuration ω_0, i.e,

$$f_\alpha = N_A \mathbf{1}\{\alpha \in \{B, C\}\} + N_B \mathbf{1}\{\alpha = C\}.$$

Then,

$$\zeta_{\alpha,i}^k = \Theta^k \sigma^{f_{(\alpha+1)}, f_\alpha + i} \sigma^{f_\alpha - 1, f_\alpha - 1 + i} \omega_0.$$

Note that the extreme case $i = 0$ (respectively $i = N_\alpha$) indicates that a particle of type $\alpha+1$ (respectively $\alpha-1$) has crossed the whole block of particles of type α until meeting a particle of type $\alpha - 1$ (respectively $\alpha + 1$). As illustrated in Figure 1.2, with this notation, $\zeta^k_{\alpha,N_\alpha} = \zeta^{k-1}_{\alpha+1,0}$, and these are the only configurations of this type with double representation.

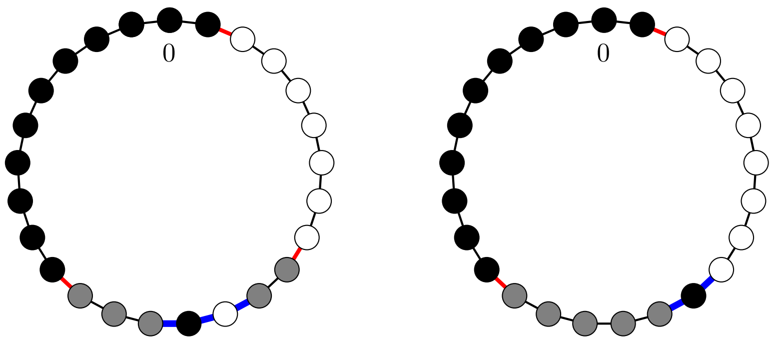

Figure 1.2: The configurations $\zeta^2_{B,2}$ and $\zeta^2_{B,0} = \zeta^3_{A,8}$ for $N_A = 8, N_B = 5, N_C = 12$. The white, gray and black circles represent respectively particles of type A, B and C. We use blue (respectively red) edges to indicate transpositions that occur at rate 1 (respectively $e^{-\beta}$).

For $k \in \Lambda_N$ and $\alpha \in \{A, B, C\}$, we denote by $\mathcal{F}^{N,k}_\alpha$ the corresponding set of such configurations:

$$\mathcal{F}^{N,k}_\alpha = \{\zeta^k_{\alpha,i} : 0 \leq i \leq N_\alpha\}. \tag{1.4.1}$$

We will see in Section 1.5 that, if the process starts from ω_k, as $\beta \uparrow \infty$, the configurations in the set $\bigcup_{\alpha:N_\alpha=M} \mathcal{F}^{N,k}_\alpha$ are those that can be reached in a time of order $e^{M\beta}$ that allow the process to escape from the basin of attraction of the configuration ω_k.

1.4.2 The configurations $\xi^k_{\alpha,i}$

For $k \in \Lambda_N$, $\alpha \in \{A, B, C\}$ and $1 \leq i \leq N_\alpha - 1$ we denote by $\xi^k_{\alpha,i}$ the configuration obtained from $\zeta^k_{\alpha,i}$ by interchanging the positions of the two distinct particles that have met in the block of particles of type α. More precisely:

$$\xi^k_{\alpha,i} = \Theta^k \sigma^{f_\alpha+i-1, f_\alpha+i} \zeta^0_{\alpha,i}.$$

Note that the jump leading $\zeta^k_{\alpha,i}$ to $\xi^k_{\alpha,i}$ has rate 1.

Again, as illustrated in Figure 1.3, it happens that some of these configurations have double representations, namely $\xi^k_{\alpha,N_\alpha-1} = \xi^{k-1}_{\alpha+1,1}$.

We denote by $\mathcal{G}^N$ the space of such configurations:

$$\mathcal{G}^{N,k}_\alpha = \{\xi^k_{\alpha,i} : 1 \leq i \leq N_\alpha - 1\}, \qquad \mathcal{G}^N = \bigcup_{k\in\Lambda_N} \bigcup_{\alpha\in\{A,B,C\}} \mathcal{G}^{N,k}_\alpha. \tag{1.4.2}$$

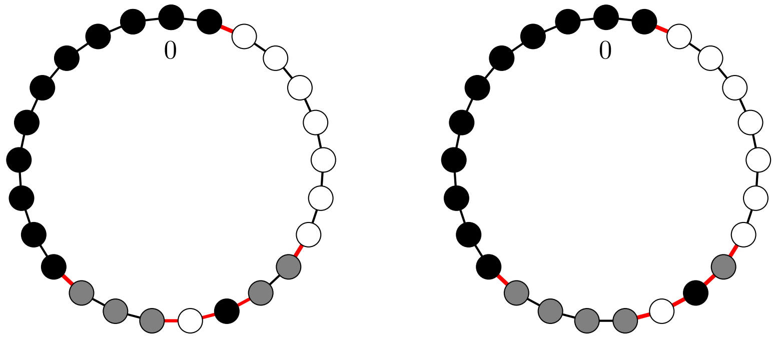

Figure 1.3: The configurations $\xi^2_{B,2}$ and $\xi^2_{B,1} = \xi^3_{A,7}$ for $N_A = 8$, $N_B = 5$, $N_C = 12$. The white, gray and black circles represent respectively particles of type A, B and C.

From a configuration in $\mathcal{G}^N$, each possible jump has rate $e^{-\beta}$. In the particular case of equal densities these configurations are local minima of the energy $\mathbb{H}$ defined in (1.2.1). In the next section we analyze the trace of the ABC model on the set

$$\Omega_1^N := \Omega_0^N \cup \mathcal{G}^N.$$

1.5 Trace of $\{\eta(t) : t \geq 0\}$ on Ω_1^N

For a configuration $\omega_k \in \Omega_0^N$, denote by $V(\omega_k)$ the set of configurations that can be obtained from ω_k after a sequence of nearest neighbor transpositions of type $(\alpha, \alpha+1) \to (\alpha+1, \alpha)$, i.e, rate $e^{-\beta}$ jumps. In other words, $V(\omega_k)$ is the set of configurations from which we can arrive at ω_k just performing rate 1 jumps. Recall the definition of Δ_k^n in (1.2.4) and note that $\bigcup_{n=0}^{M} \Delta_k^n \subset V(\omega_k)$. For $\omega \in \Omega^N$, denote by $R(\omega)$ and $B(\omega)$ the sets of configurations that can be obtained from ω by a simple nearest neighbor transposition of types $(\alpha, \alpha+1) \to (\alpha+1, \alpha)$ and $(\alpha+1, \alpha) \to (\alpha, \alpha+1)$, respectively. Note that, if $\omega \in \Delta_k^n$, for $1 \leq n \leq M-1$, then

$$R(\omega) \subseteq \Delta_k^{n+1}, \quad B(\omega) \subseteq \Delta_k^{n-1}. \tag{1.5.1}$$

Now, define $B_k^*(\omega) = B(\omega) \cap V(\omega_k)$ and $D_k^*(\omega) = B(\omega) \setminus V(\omega_k)$. In words, for a configuration $\omega \in V(\omega_k)$, the set $D_k^*(\omega)$ is formed by the configurations that are not in $V(\omega_k)$ which can be reached from ω after a rate 1 jump. The configurations $\omega \in \bigcup_{\alpha: N_\alpha = M} \mathcal{F}_\alpha^{N,k}$ are those in $\bigcup_{n=0}^{M} \Delta_k^n$ for which $D_k^*(\omega) \neq \emptyset$. We can see in Figure 1.2 that, for example, $|R(\zeta^2_{B,2})| = 3$, $|B_k^*(\zeta^2_{B,2})| = 2$ and $D_k^*(\zeta^2_{B,2}) = \{\xi^2_{B,2}\}$.

In the graph representation of a configuration, call an edge *blue*, *red*, or *black* if, respectively, the particles it links exchange their positions at rate 1, $e^{-\beta}$ or are of the same type. With this convention, $|R(\omega)|$ and $|B(\omega)|$ are the numbers of red and blue edges of the configuration ω and $V(\omega_k)$ is the set of configurations obtained from ω_k by a sequence of transpositions performed only in red edges. A configuration

$\omega \in V(\omega_k)$ can have two kinds of blue edges (call them blue$_1$ and blue$_2$), whose transposition leads to configurations in $B_k^*(\omega)$ and $D_k^*(\omega)$ respectively.

Lemma 1.5.1. *Let $k \in \Lambda_N$ and $\omega \in V(\omega_k)$ then*

$$|R(\omega)| \leq |B_k^*(\omega)| + 3. \tag{1.5.2}$$

Proof. For $\omega = \omega_k$, equality holds in (1.5.2), because the configuration ω_k has three red edges and no blue edges. Therefore, to conclude the proof by induction, we just have to check that if (1.5.2) holds for a configuration $\omega \in V(\omega_k)$, then it remains true after a transposition in a red edge $(l, l+1)$ of ω.

Observe that the transposition in the edge $(l, l+1)$ only changes the color of the three adjacent edges $(l-1, l)$, $(l, l+1)$ and $(l+1, l+2)$. After this transposition, the initially red edge $(l, l+1)$ becomes a blue$_1$ edge. For the other two edges, it is easy to check that black becomes red, blue becomes black, and red becomes blue. And then, by checking all the possible cases we see that

$$|R(\sigma^{l,l+1}\omega)| - |B_k^*(\sigma^{l,l+1}\omega)| \leq |R(\omega)| - |B_k^*(\omega)|,$$

which completes the prove. □

For any subset $\Pi \subset \Omega^N$, denote by H_Π and H_Π^+, respectively, the hitting time and the first return to Π:

$$\begin{aligned} H_\Pi &= \inf\left\{t > 0 : \eta(t) \in \Pi\right\}, \\ H_\Pi^+ &= \inf\left\{t > 0 : \eta(t) \in \Pi\,,\, \eta(s) \neq \eta(0) \text{ for some } 0 < s < t\right\}. \end{aligned}$$

Corollary 1.5.2. *For any $\beta > \log 4$, and $k \in \Lambda_N$*

$$\mathbf{P}_{\omega_k}^\beta \left[H_{\Delta_k^M} < H_{\omega_k}^+\right] \leq \left(4e^{-\beta}\right)^{M-1}, \tag{1.5.3}$$

and, for each $\omega \in \Delta_k^{M-1}$

$$\mathbf{P}_\omega^\beta \left[H_{\Delta_k^M} < H_{\omega_k}\right] \leq 4e^{-\beta}. \tag{1.5.4}$$

Proof. By the observation (1.5.1), if the current state of the process is a configuration $\omega \in \Delta_k^n$, $1 \leq n \leq M-1$, the next visited configuration belongs to Δ_k^{n+1} with probability

$$p_\beta(\omega) = \frac{|R(\omega)|e^{-\beta}}{|B(\omega)| + |R(\omega)|e^{-\beta}}, \tag{1.5.5}$$

and to Δ_k^{n-1} with probability $1 - p_\beta(\omega)$. By Lemma 1.5.1,

$$p_\beta(\omega) \leq \frac{4e^{-\beta}}{1 + 4e^{-\beta}} =: p_\beta. \tag{1.5.6}$$

Consider the random walk on $\{0, 1, \dots, M\}$ that jumps from $n \in \{1, \dots, M-1\}$ to $n+1$ with probability p_β and to $n-1$ with probability $1-p_\beta$. We know that, starting from n, this walk reaches M before 0 with probability

$$p_\beta(n, M) = \frac{\left(e^\beta/4\right)^n - 1}{\left(e^\beta/4\right)^M - 1}.$$

A simple coupling argument allows us to dominate the probabilities appearing in (1.5.3) and (1.5.4) respectively by $p_\beta(1, M)$ and $p_\beta(M-1, M)$, from which we get the corresponding bounds. □

Recall the definition of the set $\mathcal{F}_\alpha^{N,k}$ given in (1.4.1). For each $\omega \in \Delta_k^M$, $k \in \Lambda_N$, consider the probability measure $\Phi^N(\omega, \cdot)$ defined on Ω_1^N in the following way:
If $\omega \notin \bigcup_{\alpha: N_\alpha = M} \mathcal{F}_\alpha^{N,k}$,

$$\Phi^N(\omega, \{\omega_k\}) = 1;$$

If α is such that $N_\alpha = M$,

$$\Phi^N(\zeta_{\alpha,0}^k, \{\omega_k\}) = \Phi^N(\zeta_{\alpha,0}^k, \{\omega_{k+1}\}) = \Phi^N(\zeta_{\alpha,M}^k, \{\omega_k\}) = \Phi^N(\zeta_{\alpha,M}^k, \{\omega_{k-1}\}) = \frac{1}{2};$$

and, for $1 \le i \le M-1$,

$$\Phi^N(\zeta_{\alpha,i}^k, \Pi) = \begin{cases} \frac{1}{3} & \text{if } \Pi = \{\xi_{\alpha,i}^k\}, \\ \frac{2}{3} & \text{if } \Pi = \{\omega_k\}. \end{cases}$$

Throughout the paper we adopt the convention that $C_0 < \infty$ is a constant independent of N_A, N_B, N_C and β whose value may change from line to line.

Lemma 1.5.3. *There exists a constant C_0 such that, for all $\beta > 0$, $k \in \Lambda_N$, and $\omega \in \Delta_k^M$,*

$$\left| \mathbf{P}_\omega^\beta \left[\eta(H_{\Omega_1^N}) \in \Pi \right] - \Phi^N(\omega, \Pi) \right| \le C_0 N e^{-\beta}, \ \Pi \subset \Omega_1^N.$$

Proof. We examine each case separately. Suppose the process starts from a configuration $\omega \in \Delta_k^M \setminus \bigcup_{\alpha: N_\alpha = M} \mathcal{F}_\alpha^{N,k}$. In this case $D_k^*(\omega) = \emptyset$ and $B(\omega) \subseteq \Delta_k^{M-1}$, and then, as in the previous proof, starting from ω, the next visited configuration belongs to Δ_k^{M-1} with high probability $1 - p_\beta(\omega) \ge 1 - p_\beta$, for $p_\beta(\omega)$ and p_β given in (1.5.5) and (1.5.6). Now observe that from Δ_k^{M-1} to reach a configuration in $\Omega_1^N \setminus \{\omega_k\}$ the process has to cross Δ_k^M. So, conditioning in the first jump and using the second part of Corollary 1.5.2 we get that $\mathbf{P}_\omega^\beta \left[H_{\Omega_1^N} \neq H_{\omega_k} \right] \le C_0 e^{-\beta}$.

Now suppose the process starts from $\zeta_{\alpha,i}^k$ for $1 \le i \le N_\alpha - 1$, $N_\alpha = M$. As illustrated in Figure 1.2, from $\zeta_{\alpha,i}^k$ there are three possible rate $e^{-\beta}$ jumps and three possible rate 1 jumps, one of these leading to $\xi_{\alpha,i}^k$ and the others two leading to Δ_k^{M-1}. So, as before, we obtain the corresponding hitting probability conditioning in the first jump and using the second part of Corollary 1.5.2.

Finally, suppose the process starts from $\zeta^k_{\alpha,0}$. As illustrated in Figure 1.2, from this configuration there are two possible rate $e^{-\beta}$ jumps and two possible rate 1 jumps, one of these leading to $B^*_k(\zeta^k_{\alpha,0}) \subset \Delta^{M-1}_k$ and the other leading to $D^*_k(\zeta^k_{\alpha,0}) \subset V(\omega_{k+1})$, from which we can reach ω_{k+1} (before any other configuration in Ω^N_1) performing $N_{(\alpha-1)} - 1 < 2N$ jumps that have high probability $1/(1+4e^{-\beta})$. This is done by movements of the detached particle of type $\alpha+1$ in counterclockwise direction inside the domain of particles of type $\alpha-1$ until it meets the other particles of type $\alpha+1$. Therefore

$$\begin{aligned} \mathbf{P}^\beta_{\zeta^k_{\alpha,0}}\left[\eta\left(H_{\Omega^N_1}\right) = \omega_{k\pm1}\right] &\geq \frac{1}{2+2e^{-\beta}}\left(\frac{1}{1+4e^{-\beta}}\right)^{2N} \\ &= \frac{1}{2} + \mathcal{O}(Ne^{-\beta}). \end{aligned}$$

The argument for the case in which the process starts from $\zeta^k_{\alpha,M}$ is analogous. □

Actually, for many configurations $\omega \in \Delta^M_k$ we could have obtained a better estimation of the hitting distribution in Ω^N_1, considering from ω how many rate $e^{-\beta}$ jumps are necessary in order to avoid that the first visited configuration in Ω^N_1 will be ω_k. However, to take advantage of such more precise information a much more complex analysis would be needed in the proof of Proposition 1.5.5 below.

Denote by $\{\eta_1(t) : t \geq 0\}$ the trace of the process $\{\eta(t) : t \geq 0\}$ on Ω^N_1. It is defined as in (1.2.14) with Ω^N_0 changed by Ω^N_1. Surprisingly, as we will see in Proposition 1.5.5, for this process the jump rates from ω_k to any configuration in $\bigcup_{\alpha:N_\alpha=M}\mathcal{G}^{N,k}_\alpha$ are, asymptotically, the same. This is due to the remarkable fact (somewhat hidden in the next proof) that, as $\beta\uparrow\infty$, the position i of the meeting of the two different detached particles is asymptotically distributed in $\{0,1,\dots,M\}$ as $\left(\frac{1}{2M},\frac{1}{M},\dots,\frac{1}{M},\frac{1}{2M}\right)$.

The proof of the next lemma is based on a combinatorial identity that was first obtained by computing, in two different ways, some hitting probabilities for a simplified dynamics related the ABC model (two biased random walks). However, in Section 1.11 a completely elementary proof for this identity is presented.

Later we will assume stronger restrictions in the way that $N\uparrow\infty$ as $\beta\uparrow\infty$, but for now, inspired in the estimate obtained in Lemma 1.5.3, it is already natural to assume that

$$\lim_{\beta\to\infty} Ne^{-\beta} = 0. \tag{1.5.7}$$

Lemma 1.5.4. *Assume* (1.5.7). *There exist constants C_0 and β_0 such that for all $\beta > \beta_0$, $k \in \Lambda_N$, and $\alpha \in \{A,B,C\}$ such that $N_\alpha = M$,*

$$\left|\mathbf{P}^\beta_{\omega_k}\left[H_{\Delta^M_k} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}\right] - q_i e^{-(M-1)\beta}\right| \leq C_0 M\left(4e^{-\beta}\right)^M, \tag{1.5.8}$$

where

$$q_i = \begin{cases} \frac{2}{3} & \text{if } 1 \le i \le M-1, \\ \frac{1}{3} & \text{if } i = 0 \text{ or } M. \end{cases}$$

Proof. Let us decompose the event $[H_{\Delta_k^M} = H_{\zeta_{\alpha,i}^k} < H_{\omega_k}^+]$ in the number of jumps to go from ω_k to $\zeta_{\alpha,i}^k$. Denote by τ_l the instant of the l-th jump of the chain $\{\eta(t) : t \ge 0\}$. By the observation (1.5.1), in each step of a path corresponding to this event, the distance to ω_k either increases or decreases by 1 unit. So

$$\mathbf{P}_{\omega_k}^{\beta}\left[H_{\Delta_k^M} = H_{\zeta_{\alpha,i}^k} < H_{\omega_k}^+\right] = \sum_{l=0}^{\infty} \mathbf{P}_{\omega_k}^{\beta}\left[\tau_{M+2l} = H_{\Delta_k^M} = H_{\zeta_{\alpha,i}^k} < H_{\omega_k}^+\right]. \qquad (1.5.9)$$

A path from ω_k to Δ_k^M of size $M+2l$ should increase the distance to ω_k in $M+l$ steps and decrease in l steps. As already observed in the proof of Corollary 1.5.2, from any configuration $\omega \in \cup_{n=1}^{M-1} \Delta_k^n$, the probability that the distance to ω_k increases in the next jump of the chain is bounded by $4e^{-\beta}$. Now, observe that the number of possible evolutions of the distance to ω_k along a path from ω_k to Δ_k^M of size $M+2l$ is bounded by $\binom{M+2l}{l}$. Decomposing the event $[\tau_{M+2l} = H_{\Delta_k^M} < H_{\omega_k}^+]$ in these possible profiles and then applying inductively the strong Markov property for each term, we obtain

$$\mathbf{P}_{\omega_k}^{\beta}\left[\tau_{M+2l} = H_{\Delta_k^M} < H_{\omega_k}^+\right] \le \binom{M+2l}{l}\left[4e^{-\beta}\right]^{M+l-1}.$$

Using, for $1 \le l \le M$, the bound $\binom{M+2l}{l} \le (M+2l)^l \le (3M)^l$, and, for $l > M$, the universal bound $\binom{M+2l}{l} \le 2^{M+2l}$, we obtain that

$$\sum_{l=1}^{\infty} \mathbf{P}_{\omega_k}^{\beta}\left[\tau_{M+2l} = H_{\Delta_k^M} = H_{\zeta_{\alpha,i}^k} < H_{\omega_k}^+\right] \le C_0[4e^{-\beta}]^M \left(M\sum_{l=1}^{M}[12Me^{-\beta}]^{l-1} + 2^M \sum_{l=M}^{\infty}[16e^{-\beta}]^{l-1}\right) \le C_0 M(4e^{-\beta})^M, \qquad (1.5.10)$$

for β large enough, in view of (1.5.7).

Let us focus now in the term corresponding to $l = 0$, which computes the probability of the trajectories from ω_k to $\zeta_{\alpha,i}^k$ with exactly M jumps. Consider first the case $1 \le i \le M-1$. Without loss of generality, let us suppose that $\alpha = B$. The configuration $\zeta_{B,i}^k$ is obtained from ω_k when a particle of type A meets a particle of type C in the region of particles of type B, in such a way that the particle A has done i jumps, and the particle C has done $M-i$ jumps. For $j \in \{1,\dots,i\}$ denote by $\mathcal{A}_j$ the event in which the first j jumps are made by the particle A and the $(j+1)$-th jump is made by the particle C. For $r \in \{1,\dots,M-i\}$, define $\mathcal{C}_r$ in a analogous way. Then

$$\mathbf{P}^{\beta}_{\omega_k}\left[\tau_M = H_{\Delta_k^M} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}\right] = \sum_{j=1}^{i}\mathbf{P}^{\beta}_{\omega_k}\left[\tau_M = H_{\Delta_k^M} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}, \mathcal{A}_j\right] + \sum_{r=1}^{M-i}\mathbf{P}^{\beta}_{\omega_k}\left[\tau_M = H_{\Delta_k^M} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}, \mathcal{C}_r\right].$$

Now note that there are $\binom{M-j-1}{i-j}$ possible paths of size M corresponding to the event $[\tau_M = H_{\Delta_k^M} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}, \mathcal{A}_j]$. In each of these paths, the first jump has probability $1/3$, the next j jumps have probability $e^{-\beta}/(1+4e^{-\beta})$ and the next $M-j-1$ jumps have probability $e^{-\beta}/(2+5e^{-\beta})$. Figure 1.4 illustrates this situation in a particular example.

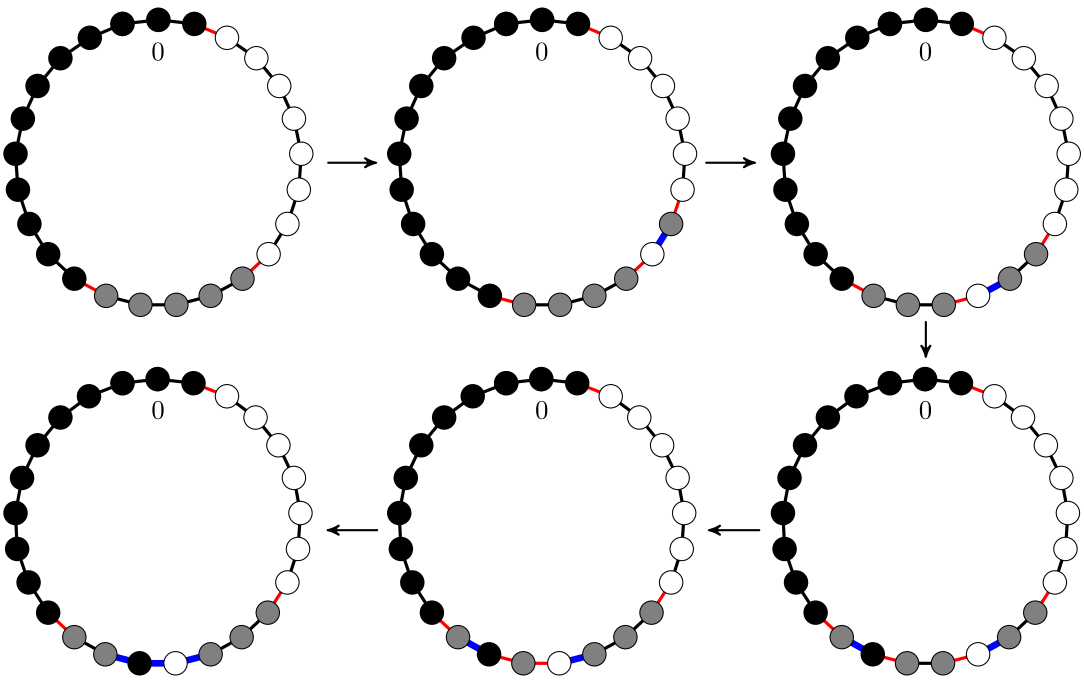

Figure 1.4: One of the two paths from ω_2 to $\xi^2_{B,3}$ that correspond to the event $\mathcal{A}_2$. In this example, $N_A = 8$, $N_B = 5$, $N_C = 12$. The white, gray and black circles represent respectively particles of type A, B and C.

Doing the same analysis for the trajectories corresponding to the events $\mathcal{C}_r$, we conclude that

$$\begin{aligned}
\mathbf{P}^{\beta}_{\omega_k}&\left[\tau_M = H_{\Delta_k^M} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}\right] \\
&= \sum_{j=1}^{i}\binom{M-j-1}{i-j}\frac{1}{3}\left(\frac{e^{-\beta}}{1+4e^{-\beta}}\right)^{j}\left(\frac{e^{-\beta}}{2+5e^{-\beta}}\right)^{M-j-1} \\
&\quad+\sum_{r=1}^{M-i}\binom{M-r-1}{M-i-r}\frac{1}{3}\left(\frac{e^{-\beta}}{1+4e^{-\beta}}\right)^{r}\left(\frac{e^{-\beta}}{2+5e^{-\beta}}\right)^{M-r-1}.
\end{aligned}$$

This can be rewritten as

$$\begin{aligned}
&\frac{1}{3}e^{-(M-1)\beta}\left(1+\mathcal{O}(Me^{-\beta})\right) \\
&\quad\times\left[\sum_{j=1}^{i}\binom{M-j-1}{i-j}\left(\frac{1}{2}\right)^{M-j-1}+\sum_{r=1}^{M-i}\binom{M-r-1}{M-i-r}\left(\frac{1}{2}\right)^{M-r-1}\right].
\end{aligned}$$

And then, by Lemma 1.11.1, for $i \in \{1, \dots, M-1\}$

$$\mathbf{P}^{\beta}_{\omega_k}\left[\tau_M = H_{\Delta_k^M} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}\right] = \frac{2}{3}e^{-(M-1)\beta} + \mathcal{O}(Me^{-M\beta}). \tag{1.5.11}$$

In the cases $i = 0$ or $i = M$, there is a unique path of size M from ω_k to $\zeta^k_{\alpha,i}$, which has probability equal to

$$\frac{1}{3}\left(\frac{e^{-\beta}}{1+4e^{-\beta}}\right)^{M-1}.$$

Therefore, for $i = 0$ or $i = M$

$$\mathbf{P}^{\beta}_{\omega_k}\left[\tau_M = H_{\Delta_k^M} = H_{\zeta^k_{\alpha,i}} < H^+_{\omega_k}\right] = \frac{1}{3}e^{-(M-1)\beta} + \mathcal{O}(Me^{-M\beta}). \tag{1.5.12}$$

Using (1.5.9), (1.5.10), (1.5.11) and (1.5.12) we obtain (1.5.8). □

Recall the definitions of d in (1.2.6) and of $\mathcal{G}^{N,k}_{\alpha}$ in (1.4.2) and let $R^{\beta}_1(\cdot,\cdot)$ denote the jump rates of $\{\eta_1(t) : t \geq 0\}$, the trace process on Ω^N_1.

Proposition 1.5.5. *Assume* (1.5.7). *There exist finite constants C_0 and β_0 such that for all $\beta > \beta_0$, $k \in \Lambda_N$ and $\xi \in \Omega^N_1$,*

$$\left|R^{\beta}_1(\omega_k,\xi) - \mathbf{R}_1(\omega_k,\xi)e^{-M\beta}\right| \leq C_0 N 4^M e^{-(M+1)\beta}, \tag{1.5.13}$$

where

$$\mathbf{R}_1(\omega_k,\xi) = \begin{cases} \frac{d}{2} & \text{if } \xi \in \{\omega_{k-1},\omega_{k+1}\}, \\ \frac{2}{3} & \text{if } \xi \in \bigcup_{\alpha:N_\alpha=M}\mathcal{G}^{N,k}_{\alpha}, \\ 0 & \text{if } \xi \notin \bigcup_{\alpha:N_\alpha=M}\mathcal{G}^{N,k}_{\alpha}\cup\{\omega_{k-1},\omega_{k+1}\}. \end{cases}$$

Proof. By [3, Proposition 6.1], for every $\omega, \xi \in \Omega_1^N$,

$$R_1^\beta(\omega, \xi) = \lambda_\beta(\omega)\mathbf{P}_\omega^\beta\left[H_{\Omega_1^N}^+ = H_\xi\right], \tag{1.5.14}$$

where $\lambda_\beta(\omega)$ is the total jump rate from ω for the original chain $\{\eta(t) : t \geq 0\}$. A crucial observation is that, starting from ω_k, to reach any other configuration in Ω_1^N the process has to cross Δ_k^M. Thus, for every $\xi \in \Omega_1^N$, $\xi \neq \omega_k$, on the event $\{H_{\Omega_1^N}^+ = H_\xi\}$ we have that $H_{\Delta_k^M} < H_{\Omega_1^N}^+$, and then by the strong Markov property,

$$\mathbf{P}_{\omega_k}^\beta\left[H_{\Omega_1^N}^+ = H_\xi\right] = \sum_{\omega\in\Delta_k^M}\mathbf{P}_{\omega_k}^\beta\left[H_{\Delta_k^M} = H_\omega < H_{\omega_k}^+\right]\mathbf{P}_\omega^\beta\left[H_{\Omega_1^N} = H_\xi\right]. \tag{1.5.15}$$

If $\xi \notin \bigcup_{\alpha:N_\alpha=M}\mathcal{G}_\alpha^{N,k} \cup \{\omega_{k-1}, \omega_{k+1}\}$ then, by Lemma 1.5.3,

$$\mathbf{P}_\omega^\beta\left[H_{\Omega_1^N} = H_\xi\right] \leq C_0 N e^{-\beta},$$

for every $\omega \in \Delta_k^M$. So

$$\begin{aligned}\mathbf{P}_{\omega_k}^\beta\left[H_{\Omega_1^N}^+ = H_\xi\right] &\leq C_0 N e^{-\beta}\sum_{\omega\in\Delta_k^M}\mathbf{P}_{\omega_k}^\beta\left[H_{\Delta_k^M} = H_\omega < H_{\omega_k}^+\right]\\ &= C_0 N e^{-\beta}\mathbf{P}_{\omega_k}^\beta\left[H_{\Delta_k^M} < H_{\omega_k}^+\right] \leq C_0 N\left(4e^{-\beta}\right)^M\end{aligned}$$

by the first part of Corollary 1.5.2. So, by (1.5.14) and the fact that $\lambda_\beta(\omega_k) = 3e^{-\beta}$ we get (1.5.13) for $\xi \notin \bigcup_{\alpha:N_\alpha=M}\mathcal{G}_\alpha^{N,k} \cup \{\omega_{k-1}, \omega_{k+1}\}$.

Now let us consider the case $\xi = \xi_{\alpha,i}^k$ for $N_\alpha = M$, $1 \leq i \leq M-1$. By Lemma 1.5.3, for every $\omega \in \Delta_k^M$

$$\mathbf{P}_\omega^\beta\left[H_{\Omega_1^N} = H_{\xi_{\alpha,i}^k}\right] = \frac{1}{3}\mathbf{1}\left\{\omega = \zeta_{\alpha,i}^k\right\} + \mathcal{O}\left(Ne^{-\beta}\right).$$

Therefore, by (1.5.14), (1.5.15), and the first part of Corollary 1.5.2,

$$R_1^\beta\left(\omega_k, \xi_{\alpha,i}^k\right) = e^{-\beta}\mathbf{P}_{\omega_k}^\beta\left[H_{\Delta_k^M} = H_{\zeta_{\alpha,i}^k} < H_{\omega_k}^+\right] + \mathcal{O}\left(N(4e^{-\beta})^{M+1}\right).$$

And then, by Lemma 1.5.4,

$$R_1^\beta\left(\omega_k, \xi_{\alpha,i}^k\right) = \frac{2}{3}e^{-M\beta} + \mathcal{O}\left(N(4e^{-\beta})^{M+1}\right).$$

Let us make the same argument for the case $\xi = \omega_{k+1}$. By Lemma 1.5.3, for every $\omega \in \Delta_k^M$

$$\mathbf{P}_\omega^\beta\left[H_{\Omega_1^N} = H_{\omega_{k+1}}\right] = \frac{1}{2}\mathbf{1}\left\{\omega \in \{\zeta_{\alpha,0}^k : N_\alpha = M\}\right\} + \mathcal{O}\left(Ne^{-\beta}\right).$$

Again, using (1.5.14), (1.5.15), and the first part of Corollary 1.5.2, we obtain that

$$R_1^\beta(\omega_k, \omega_{k+1}) = \frac{3e^{-\beta}}{2} \sum_{\alpha: N_\alpha = M} \mathbf{P}^\beta_{\omega_k}\left[H_{\Delta_k^M} = H_{\zeta^k_{\alpha,0}} < H^+_{\omega_k}\right] + \mathcal{O}\left(N(4e^{-\beta})^{M+1}\right).$$

And therefore, by Lemma 1.5.4,

$$R_1^\beta(\omega_k, \omega_{k+1}) = \frac{d}{2} e^{-M\beta} + \mathcal{O}\left(N(4e^{-\beta})^{M+1}\right).$$

The case $\xi = \omega_{k-1}$ is analogous. □

The proposition we just proved estimates the jump rates of the trace process $\{\eta_1(t) : t \geq 0\}$ from the configurations in Ω_0^N. Now we want to estimate the jump rates from the configurations in $\mathcal{G}^N$. Arguing as in this last proof, for each configuration in $\mathcal{G}^N$ as initial distribution, we will need to compute the distribution of the process in the first return to Ω_1^N. If we allow errors of order $Ne^{-\beta}$, these hitting probabilities are easily obtained.

From any configuration $\xi^k_{\alpha,i} \in \mathcal{G}^N$, as illustrated in Figure 1.3, there are six possibilities for the first jump. Each of these six configurations is associated to one of the six red edges of the configuration $\xi^k_{\alpha,i}$. This association provides a way to label these configurations. We will denote these configurations by $\xi^{k,j}_{\alpha,i}$, for $j = 1, \dots, 6$. We do this in such a way that, if we enumerate the red edges of $\xi^k_{\alpha,i}$ as $r_1, \dots, r_6$ clockwise, then $\xi^{k,j}_{\alpha,i}$ is the configuration obtained from $\xi^k_{\alpha,i}$ after a transposition in r_j. To fix a initial point for the enumeration of the red edges, we impose that this is done in such a way that $\xi^{k,2}_{\alpha,i} = \zeta^k_{\alpha,i}$. Note that, with this convention we have that $\xi^{k,j}_{\alpha,N_\alpha-1} = \xi^{k-1,j+1}_{\alpha+1,1}$ and, for $1 \leq i \leq N_\alpha - 2$, $\xi^{k,3}_{\alpha,i} = \xi^{k,1}_{\alpha,i+1}$. See Figures 1.5 and 1.6 for an example.

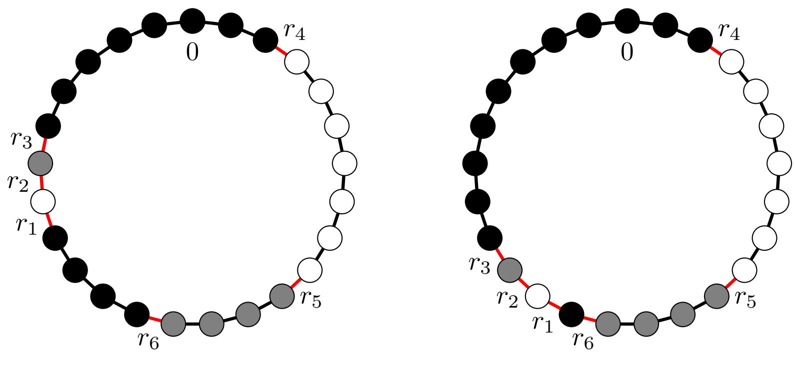

Figure 1.5: The configurations $\xi^2_{C,4}$ and $\xi^2_{C,1}$ with the corresponding labels of the red edges. In this example $N_A = 8$, $N_B = 5$, $N_C = 12$. The white, gray and black circles represents respectively particles of types A, B and C.

For each $\omega \in R(\xi^k_{\alpha,i})$, $k \in \Lambda_N$, $\alpha \in \{A, B, C\}$, $1 \leq i \leq N_\alpha - 1$, consider the probability measure $\Phi^N(\omega, \cdot)$ defined on Ω_1^N in the following way:

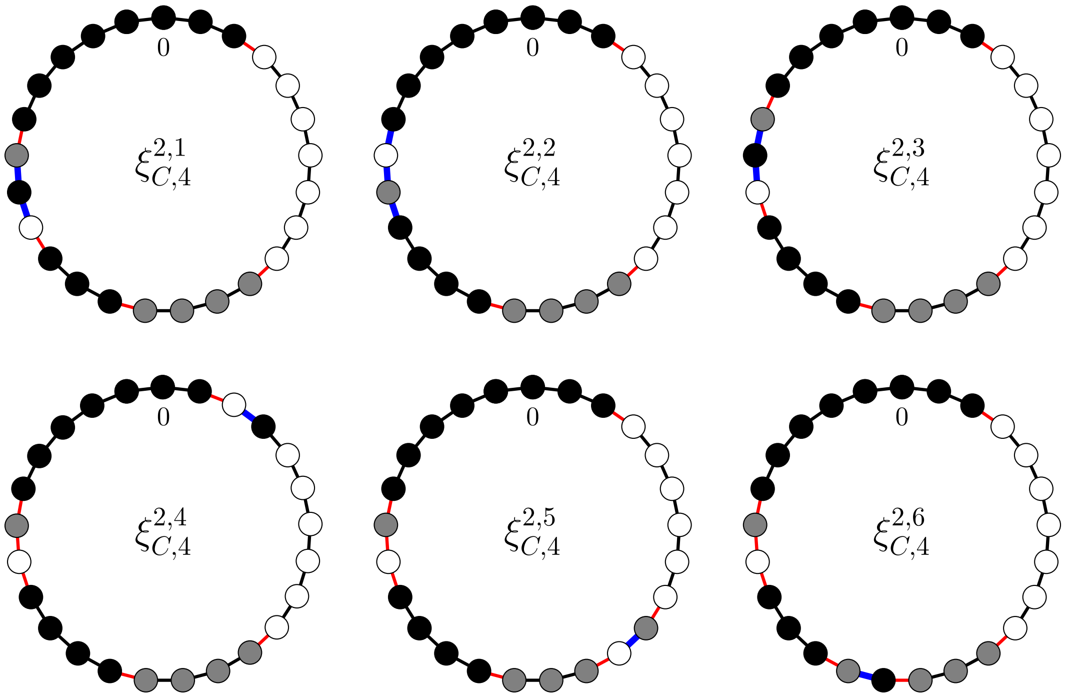

Figure 1.6: The six configurations that can be reached after one jump from the configuration $\xi^2_{C,4}$, which is illustrated in Figure 1.5.

(i) If $2 \le i \le N_\alpha - 2$,

$$\Phi^N\left(\xi^{k,j}_{\alpha,i}, \{\xi^k_{\alpha,i}\}\right) = 1, \text{ for } j = 4,5,6;$$

$$\Phi^N\left(\xi^{k,j}_{\alpha,i}, \Pi\right) = \begin{cases} \frac{1}{2} & \text{if } \Pi = \{\xi^k_{\alpha,i}\}, \\ \frac{1}{2} & \text{if } \Pi = \{\xi^k_{\alpha,i-2+j}\} \end{cases}, \text{ for } j = 1,3;$$

and

$$\Phi^N\left(\xi^{k,2}_{\alpha,i}, \Pi\right) = \begin{cases} \frac{1}{3} & \text{if } \Pi = \{\xi^k_{\alpha,i}\}, \\ \frac{2}{3} & \text{if } \Pi = \{\omega_k\}. \end{cases}$$

(ii) And if $i = 1$,

$$\Phi^N\left(\xi^{k,j}_{\alpha,1}, \Pi\right) = \begin{cases} \frac{1}{3} & \text{if } \Pi = \{\xi^k_{\alpha,1}\}, \\ \frac{2}{3} & \text{if } \Pi = \{\omega_{k+2-j}\} \end{cases}, \text{ for } j = 1,2;$$

$$\Phi^N\left(\xi^{k,3}_{\alpha,1}, \Pi\right) = \begin{cases} \frac{1}{2} & \text{if } \Pi = \{\xi^k_{\alpha,1}\}, \\ \frac{1}{2} & \text{if } \Pi = \{\xi^k_{\alpha,2}\} \end{cases}, \quad \Phi^N\left(\xi^{k,6}_{\alpha,1}, \Pi\right) = \begin{cases} \frac{1}{2} & \text{if } \Pi = \{\xi^k_{\alpha,1}\}, \\ \frac{1}{2} & \text{if } \Pi = \{\xi^{k+1}_{\alpha-1,N_{\alpha-1}-2}\} \end{cases}$$

and

$$\Phi^N\left(\xi^{k,j}_{\alpha,1}, \{\xi^k_{\alpha,i}\}\right) = 1, \text{ for } j = 4,5.$$

Lemma 1.5.6. *There exists a constant C_0, such that, for any $\beta > 0$, $k \in \Lambda_N$, $\alpha \in \{A, B, C\}$, $1 \le i \le N_\alpha - 1$ and $\omega \in R(\xi^k_{\alpha,i})$*

$$\left| \mathbf{P}^\beta_\omega \left[\eta(H_{\Omega^N_1}) \in \Pi \right] - \Phi^N(\omega, \Pi) \right| \le C_0 N e^{-\beta}. \tag{1.5.16}$$

Proof. We present the proof for the case $2 \le i \le N_\alpha - 2$, the extreme case $i = 1$ is similar and the verification is left to the reader.

As observed in the proof of Lemma 1.5.1, a transposition in one of the red edges of $\xi^k_{\alpha,i}$ only changes the color of this edge, which always becomes a blue edge, and of the two that are adjacent to it, for which black becomes red, and red becomes blue.

In the configuration $\xi^k_{\alpha,i}$, for $2 \le i \le N_\alpha - 2$, as illustrated in Figure 1.5, the edges adjacent to r_4, r_5 and r_6 are all black. Then, by the above observation, as illustrated in Figure 1.6, for $j = 4, 5, 6$, we have that $|R(\xi^{k,j}_{\alpha,i})| = 7$ and $B(\xi^{k,j}_{\alpha,i}) = \{\xi^k_{\alpha,i}\}$. Therefore, if τ_1 is the instant of the first jump of the chain, for $j = 4, 5, 6$,

$$\mathbf{P}^\beta_{\xi^{k,j}_{\alpha,i}} \left[H_{\Omega^N_1} = H_{\xi^k_{\alpha,i}} \right] \ge \mathbf{P}^\beta_{\xi^{k,j}_{\alpha,i}} \left[\eta(\tau_1) = \xi^k_{\alpha,i} \right] = \frac{1}{1 + 7e^{-\beta}} = 1 + \mathcal{O}(e^{-\beta}).$$

This proves (1.5.16) for $\omega = \xi^{k,j}_{\alpha,i}$, $j = 4, 5, 6$.

Doing the same kind of analysis for the edge r_1 of the configuration $\xi^k_{\alpha,i}$, we note that $|R(\xi^{k,1}_{\alpha,i})| = 5$ and $|B(\xi^{k,1}_{\alpha,i})| = 2$. In fact, we can see that

$$B(\xi^{k,1}_{\alpha,i}) = \left\{ \xi^k_{\alpha,i}, \xi^k_{\alpha,i-1} \right\}.$$

Therefore, for $l = i - 1, i$

$$\mathbf{P}^\beta_{\xi^{k,1}_{\alpha,i}} \left[H_{\Omega^N_1} = H_{\xi^k_{\alpha,l}} \right] \ge \mathbf{P}^\beta_{\xi^{k,1}_{\alpha,i}} \left[\eta(\tau_1) = \xi^k_{\alpha,l} \right] = \frac{1}{2 + 5e^{-\beta}} = \frac{1}{2} + \mathcal{O}(e^{-\beta}).$$

This proves (1.5.16) for $\omega = \xi^{k,1}_{\alpha,i}$, and the proof for $\omega = \xi^{k,3}_{\alpha,i}$ is analogous.

Now let us consider the case $\omega = \xi^{k,2}_{\alpha,i} = \zeta^k_{\alpha,i} \in V(\omega_k) \cap \Delta^{N_\alpha}_k$. The case $N_\alpha = M$ was already considered in Lemma 1.5.3. In that proof a better approximation (error of order $e^{-\beta}$ instead of $Ne^{-\beta}$) was given using the second part of Corollary 1.5.2. In the general case we need to argue differently. We have that $|B(\zeta^k_{\alpha,i})| = |R(\zeta^k_{\alpha,i})| = 3$. One of the three configurations in $B(\zeta^k_{\alpha,i})$ is $\xi^k_{\alpha,i}$. So

$$\mathbf{P}^\beta_{\zeta^k_{\alpha,i}} \left[H_{\Omega^N_1} = H_{\xi^k_{\alpha,i}} \right] \ge \mathbf{P}^\beta_{\zeta^k_{\alpha,i}} \left[\eta(\tau_1) = \xi^k_{\alpha,i} \right] = \frac{1}{3 + 3e^{-\beta}} = \frac{1}{3} + \mathcal{O}\left(e^{-\beta}\right). \tag{1.5.17}$$

From the other two configurations in $B(\zeta^k_{\alpha_i})$, the configuration ω_k is the only one in Ω^N_1 that can be reached after a sequence of rate 1 jumps. Moreover, starting from some of the two configurations in $B(\zeta^k_{\alpha,i}) \setminus \{\xi^k_{\alpha,i}\} = B^*_k(\zeta^k_{\alpha,i})$, if the next $N_\alpha - 1$ jumps of the chain correspond to transpositions in blue edges of the configurations, then, after these jumps, the process will ultimately fall in ω_k. This gives

$$\mathbf{P}^\beta_{\zeta^k_{\alpha,i}} \left[H_{\Omega^N_1} = H_{\omega_k} \right] \ge \frac{1}{3 + 3e^{-\beta}} \sum_{\omega \in B^*_k(\zeta^k_{\alpha,i})} \mathbf{P}^\beta_\omega \left[\bigcap_{l=1}^{N_\alpha - 1} \{\eta(\tau_l) \in B(\eta(\tau_{l-1}))\} \right]. \tag{1.5.18}$$

In this situation, transpositions in blue edges corresponds to movements of the detached particle of type $\alpha+1$ in clockwise direction inside the domain of particles of type α or movements of the detached particle of type $\alpha-1$ in counterclockwise direction. Therefore, any configuration ω that can be reached from $B_k^*(\zeta_{\alpha,i}^k)$ after a sequence of transposition in blue edges belongs to $V(\omega_k)$. In fact, to arrive in ω_k, we just need to keep moving the detached particles in the correct direction until they meet the corresponding region of particles of their type. So the inequality of Lemma 1.5.1 holds for these configurations. And then, applying inductively the strong Markov property in (1.5.18) we see that

$$\mathbf{P}^{\beta}_{\zeta^k_{\alpha,i}}\left[H_{\Omega_1^N}=H_{\omega_k}\right]\geq\frac{2}{3+3e^{-\beta}}\left(\frac{1}{1+4e^{-\beta}}\right)^{N_\alpha-1}=\frac{2}{3}+\mathcal{O}\left(Ne^{-\beta}\right). \tag{1.5.19}$$

Inequalities (1.5.17) and (1.5.19) prove (1.5.16) for the case $\omega=\xi_{\alpha,i}^{k,2}$. This concludes the proof of the lemma. □

Proposition 1.5.7. *There exists a finite constant C_0 such that for any $\beta>0$, $k\in\Lambda_N$, $\alpha\in\{A,B,C\}$ and $\omega\in\Omega_1^N$,*

$$\left|R_1^\beta(\xi^k_{\alpha,i},\omega)-\mathbf{R}_1(\xi^k_{\alpha,i},\omega)e^{-\beta}\right|\leq C_0Ne^{-2\beta},$$

where, for $2\leq i\leq N_\alpha-2$

$$\mathbf{R}_1(\xi^k_{\alpha,i},\omega)=\begin{cases}\frac{1}{2} & \text{if } \omega\in\{\xi^k_{\alpha,i-1},\xi^k_{\alpha,i+1}\},\\ \frac{2}{3} & \text{if } \omega=\omega_k,\\ 0 & \text{if } \omega\notin\{\xi^k_{\alpha,i-1},\xi^k_{\alpha,i+1},\omega_k\}.\end{cases}$$

and for $i=1$ (recall that $\xi^k_{\alpha,1}=\xi^{k+1}_{\alpha-1,N_{(\alpha-1)}-1}$),

$$\mathbf{R}_1(\xi^k_{\alpha,1},\omega)=\begin{cases}\frac{1}{2} & \text{if } \omega\in\{\xi^k_{\alpha,2},\xi^{k+1}_{\alpha-1,N_{(\alpha-1)}-2}\},\\ \frac{2}{3} & \text{if } \omega\in\{\omega_k,\omega_{k+1}\},\\ 0 & \text{if } \omega\notin\{\xi^k_{\alpha,2},\xi^{k+1}_{\alpha-1,N_{(\alpha-1)}-2},\omega_k,\omega_{k+1}\}.\end{cases}$$

Proof. By (1.5.14),

$$R_1^\beta(\xi^k_{\alpha,i},\omega)=\lambda_\beta(\xi^k_{\alpha,i})\mathbf{P}^\beta_{\xi^k_{\alpha,i}}\left[H^+_{\Omega_1^N}=H_\omega\right]=6e^{-\beta}\mathbf{P}^\beta_{\xi^k_{\alpha,i}}\left[H^+_{\Omega_1^N}=H_\omega\right].$$

Now, conditioning in the first jump, and using Lemma 1.5.6 we get

$$R_1^\beta(\xi^k_{\alpha,i},\omega)=e^{-\beta}\sum_{j=1}^{6}\mathbf{P}^\beta_{\xi^{k,j}_{\alpha,i}}\left[H^+_{\Omega_1^N}=H_\omega\right]=\mathbf{R}_1(\xi^k_{\alpha,i},\omega)e^{-\beta}+\mathcal{O}\left(Ne^{-2\beta}\right),$$

as desired. □

1.6 Trace of $\{\eta(t) : t \geq 0\}$ on Ω_0^N

Knowing the jump rates for the trace process $\{\eta_1(t) : t \geq 0\}$ on the set Ω_1^N, we can obtain the jump rates for the trace process on the set Ω_0^N computing, for each configuration $\omega \in \mathcal{G}^N$, the distribution of the first visited configuration in Ω_0^N for the process $\{\eta_1(t) : t \geq 0\}$ starting from ω. We start replacing the original process $\{\eta_1(t) : t \geq 0\}$ by an ideal process $\{\widehat{\eta}_1(t) : t \geq 0\}$ for which these absorption probabilities are more easily obtained.

For α such that $N_\alpha = M$, define

$$\mathcal{G}_\alpha^N = \{\xi_{\gamma,j}^k : j = 1, \dots, N_\gamma - 1; \quad \gamma + k = \alpha\}.$$

To understand why we defined $\mathcal{G}_\alpha^N$ this way note that, starting from some $\xi_{\alpha,i}^0$, the configurations $\xi_{\gamma,j}^k$ in $\mathcal{G}^N$ which may be visited by the process after times of order e^β are those such that $\gamma + k = \alpha$. On the set $\Omega_0^N \cup \mathcal{G}_\alpha^N$ consider the continuous-time Markov chain $\{\widehat{\eta}_1(t) : t \geq 0\}$ with absorbing states Ω_0^N that jumps from $\xi_{\gamma,i}^k$ to ω with the ideal rates

$$\widehat{R}_1^\beta(\xi_{\gamma,i}^k, \omega) := \mathbf{R}_1(\xi_{\gamma,i}^k, \omega) e^{-\beta}$$

given in Proposition 1.5.7. Note that the corresponding discrete-time jump chain depends only on N_A, N_B and N_C, and not directly on β. Figure 1.1 presents the graph structure of this simple dynamics.

For α such that $N_\alpha = M$, $1 \leq i \leq M-1$ and $k \in \Lambda_N$, denote by $p_\alpha^N(i,k)$ the probability for the chain $\{\widehat{\eta}_1(t) : t \geq 0\}$ of, starting from $\xi_{\alpha,i}^0$ being absorbed in ω_k.

Lemma 1.6.1. *There exists a constant C_0 such that, for any $\beta > 0$, $k \in \Lambda_N$, α such that $N_\alpha = M$, and $1 \leq i \leq M-1$*

$$\left| \mathbf{P}_{\xi_{\alpha,i}^0}^\beta \left[H_{\Omega_0^N} = H_{\omega_k} \right] - p_\alpha^N(i,k) \right| \leq C_0 N^3 \beta e^{-\beta}. \tag{1.6.1}$$

Proof. By Proposition 1.5.7, there exists a constant C_0 such that

$$\max_{\xi \in \mathcal{G}_\alpha^N \cup \Omega_0^N} \sum_{\omega \in \mathcal{G}_\alpha^N \cup \Omega_0^N} \left| R_1^\beta(\xi, \omega) - \widehat{R}_1^\beta(\xi, \omega) \right| \leq C_0 N^3 e^{-2\beta}.$$

Therefore, for all $1 \leq i \leq M$, there exists a coupling $\overline{\mathbf{P}}^\beta$ of the two processes such that $\eta_1(0) = \widehat{\eta}_1(0) = \xi_{\alpha,i}^0$, $\overline{\mathbf{P}}^\beta$-a.s, and such that for all $t > 0$,

$$\overline{\mathbf{P}}^\beta \left[T_{cp} \leq t \right] \leq P \left[\mathcal{E}(C_0 N^3 e^{-2\beta}) \leq t \right], \tag{1.6.2}$$

where $T_{cp} = \inf\{t > 0 : \eta_1(t) \neq \widehat{\eta}_1(t)\}$ and $\mathcal{E}(C_0 N^3 e^{-2\beta})$ is a mean $(C_0 N^3 e^{-2\beta})^{-1}$ exponential random variable. To prove (1.6.1) it is sufficient to prove that

$$\overline{\mathbf{P}}^\beta \left[\eta_1(H_{\Omega_0^N}^{\eta_1}) \neq \widehat{\eta}_1(H_{\Omega_0^N}^{\widehat{\eta}_1}) \right] \leq \widetilde{C} N^3 \beta e^{-\beta},$$

for some universal constant $\widetilde{C}$, where $H^{\eta_1}_{\Omega_0^N}$ and $H^{\widehat{\eta}_1}_{\Omega_0^N}$ are the hitting times of Ω_0^N for this two processes. Let $T_\beta = \frac{3}{2}\beta e^{\beta}$.

$$\begin{aligned}\overline{\mathbf{P}}^\beta\left[\eta_1(H^{\eta_1}_{\Omega_0^N}) \neq \widehat{\eta}_1(H^{\widehat{\eta}_1}_{\Omega_0^N})\right] &= \overline{\mathbf{P}}^\beta\left[\eta_1(H^{\eta_1}_{\Omega_0^N}) \neq \widehat{\eta}_1(H^{\widehat{\eta}_1}_{\Omega_0^N}),\ H^{\widehat{\eta}_1}_{\Omega_0^N} \leq T_\beta\right] \\ &\quad + \overline{\mathbf{P}}^\beta\left[\eta_1(H^{\eta_1}_{\Omega_0^N}) \neq \widehat{\eta}_1(H^{\widehat{\eta}_1}_{\Omega_0^N}),\ H^{\widehat{\eta}_1}_{\Omega_0^N} > T_\beta\right] \\ &\leq \overline{\mathbf{P}}^\beta\left[T_{cp} \leq T_\beta\right] + \overline{\mathbf{P}}^\beta\left[H^{\widehat{\eta}_1}_{\Omega_0^N} > T_\beta\right]. \end{aligned} \tag{1.6.3}$$

By the definition of the process $\{\widehat{\eta}_1(t) : t \geq 0\}$, the absorption time $H^{\widehat{\eta}_1}_{\Omega_0^N}$ is stochastically dominated by a mean $\left(\frac{2}{3}e^{-\beta}\right)^{-1}$ exponential random variable. Using this fact and (1.6.2) in (1.6.3), we obtain that

$$\begin{aligned}\overline{\mathbf{P}}^\beta\left[\eta_1(H^{\eta_1}_{\Omega_0^N}) \neq \widehat{\eta}_1(H^{\widehat{\eta}_1}_{\Omega_0^N})\right] &\leq P\left[\mathcal{E}(C_0N^3e^{-2\beta}) \leq T_\beta\right] + P\left[\mathcal{E}\left(\frac{2}{3}e^{-\beta}\right) > T_\beta\right] \\ &= 1 - \exp\left\{-C_0N^3e^{-2\beta}T_\beta\right\} + \exp\left\{-\frac{2}{3}e^{-\beta}T_\beta\right\} \\ &\leq C_0N^3e^{-2\beta}T_\beta + \exp\left\{-\frac{2}{3}e^{-\beta}T_\beta\right\} \\ &\leq \widetilde{C}N^3\beta e^{-\beta},\end{aligned}$$

by the definition of T_β. □

For α such that $N_\alpha = M$, and $k \neq 0$ define

$$g^N_\alpha(k) = \sum_{i=1}^{M-1} p^N_\alpha(i,k).$$

Recall that we have defined $r_\beta(k)$ as the jump rate from ω_0 to ω_k for the trace process $\{\eta_0(t) : t \geq 0\}$ on Ω_0^N. Next theorem expresses $r_\beta(k)$ in terms of $g^N_\alpha(k)$ with an error term $\psi(\beta)$, such that, as $\beta \uparrow \infty$, $e^{M\beta}\psi(\beta)$ vanishes, if we impose proper restrictions in the way that N grows with β.

Proposition 1.6.2. *Assume* (1.5.7). *There exist constants C_0 and β_0 such that for any $\beta > \beta_0$ and $k \in \Lambda_N$, $k \neq 0$,*

$$\left|r_\beta(k) - r(N_A, N_B, N_C, k)e^{-M\beta}\right| \leq \psi(\beta) \tag{1.6.4}$$

where

$$r(N_A, N_B, N_C, k) = \frac{d}{2}\mathbf{1}\{|k| = 1\} + \frac{2}{3}\sum_{\alpha : N_\alpha = M} g^N_\alpha(k) \tag{1.6.5}$$

and ψ is some function such that, for any $\beta > 0$,

$$\psi(\beta) \leq C_0\left(N^2 4^M + N^3 M\beta + N^6 4^M \beta e^{-\beta}\right)e^{-(M+1)\beta}. \tag{1.6.6}$$

Proof. Noting that $\{\eta_0(t) : t \geq 0\}$ is also the trace of the process $\{\eta_1(t) : t \geq 0\}$, by [3, Corollary 6.2]

$$\begin{aligned} r_\beta(k) &= R_1^\beta(\omega_0, \omega_k) + \sum_{\alpha:N_\alpha=M} \sum_{i=1}^{M-1} R_1^\beta(\omega_0, \xi^0_{\alpha,i}) \mathbf{P}^\beta_{\xi^0_{\alpha,i}} \left[H_{\Omega_0^N} = H_{\omega_k} \right] \\ &+ \sum_{\omega \in \mathcal{G}^N \setminus \bigcup_{\alpha:N_\alpha=M} \mathcal{G}^{N,0}_\alpha} R_1^\beta(\omega_0, \omega) \mathbf{P}^\beta_\omega \left[H_{\Omega_0^N} = H_{\omega_k} \right]. \end{aligned} \tag{1.6.7}$$

By Proposition 1.5.5 the first of the three terms above is equal to

$$\frac{d}{2} \mathbf{1}\{|k| = 1\} e^{-M\beta} + \mathcal{O}\left(N 4^M\right) e^{-(M+1)\beta}. \tag{1.6.8}$$

A simple analysis, such as the one made to obtain (1.7.1) below, indicates that $p^N_\alpha(i,k) \leq (3/5)^{\min\{i-1, M-i-1\}}$ for every $k \neq 0$, and then $g^N_\alpha(k) \leq C_0$, where C_0 is a constant independent of M. Using this observation, Proposition 1.5.5 and Lemma 1.6.1, we obtain that the second term in (1.6.7) is equal to

$$\frac{2}{3} \sum_{\alpha:N_\alpha=M} g^N_\alpha(k) e^{-M\beta} + \mathcal{O}\left(N4^M + N^3 M\beta + N^4 M 4^M \beta e^{-\beta}\right) e^{-(M+1)\beta}. \tag{1.6.9}$$

Now let's look at the third term in (1.6.7). For $\omega \in \mathcal{G}^N \setminus \bigcup_{\alpha:N_\alpha=M} \mathcal{G}^{N,0}_\alpha$, by Proposition 1.5.5, $R^\beta_1(\omega_0, \omega) \leq C_0 N 4^M e^{-(M+1)\beta}$. Now observe that for $\omega \in \mathcal{G}^{N,j}_\alpha$ with $|j-k| \geq 4$, $\alpha \in \{A, B, C\}$,

$$\mathbf{P}^\beta_\omega \left[H_{\Omega_0^N} = H_{\omega_k} \right] \leq C_0 \left((3/5)^N + N^3 \beta e^{-\beta} \right).$$

To see this we first approximate by the ideal process, as in Lemma 1.6.1, and then we make a simple analysis as in (1.7.1) below. Then, the third term in (1.6.7) is

$$\mathcal{O}\left(N^2 4^M + N^6 4^M \beta e^{-\beta}\right) e^{-(M+1)\beta}. \tag{1.6.10}$$

The result follows summing (1.6.8), (1.6.9) and (1.6.10). □

We obtain Theorem 1.2.5 as an immediate corollary of Proposition 1.6.2.

Proof of Theorem 1.2.5. The rates of the speeded up process $\{\eta_0(e^{M\beta} t) : t \geq 0\}$ are simply the rates for the process $\{\eta_0(t) : t \geq 0\}$ multiplied by $e^{M\beta}$. In the case where N_A, N_B and N_C are constants, we obtain, multiplying (1.6.4) by $e^{M\beta}$ and sending $\beta \uparrow \infty$, that the process $\{\eta_0(e^{M\beta} t) : t \geq 0\}$ converges to a Markov chain in Ω_0^N, which jumps from ω_i to ω_j with rate $r(N_A, N_B, N_C, j-i)$ given in (1.6.5). □

1.7 Understanding $g_\alpha^N(k)$

To understand the scaling limits of the system when $N \uparrow \infty$ with β, we need to estimate $g_\alpha^N(k)$. Consider the ideal random walk $\{\widehat{\eta}_1(t) : t \geq 0\}$ starting from $\xi_{\alpha,i}^0$, $1 \leq i \leq N_\alpha - 1$. For its jump chain, in each step, the probability of no absorption in Ω_0^N is less than or equal to $3/5$. To arrive at ω_k, $k \neq 0$, it is necessary to survive at least $(|k|-1)(M-2)$ steps without absorption in Ω_0^N. Therefore, for every $k \neq 0$ and $1 \leq i \leq M-1$,

$$p_\alpha^N(i,k) \leq \left(\frac{3}{5}\right)^{(M-2)(|k|-1)}. \tag{1.7.1}$$

This simple analysis indicates the fast decaying of $g_\alpha^N(k)$, both in M and in k, but it does not give information about $g_\alpha^N(1)$ or $g_\alpha^N(-1)$ which are not negligible. So, we need to go further into the calculations. The next lemma reduces the analysis of $g_\alpha^N(k)$ to the analysis of the terms $p_\alpha^N(1,k)$ and $p_\alpha^N(M-1,k)$.

Lemma 1.7.1. *Let α be such that $N_\alpha = M$. For every $k \in \Lambda_N$, $k \neq 0$, we have that*

$$g_\alpha^N(k) = \left(\frac{3}{2} + \frac{2}{3^{M-2}+1}\right)\left(p_\alpha^N(1,k) + p_\alpha^N(M-1,k)\right) \tag{1.7.2}$$

Proof. Let us fix N_A, N_B, N_C and $k \neq 0$. By the standard conditioning argument we have that, for $2 \leq i \leq M-2$,

$$p_\alpha^N(i,k) = \frac{3}{10}p_\alpha^N(i-1,k) + \frac{3}{10}p_\alpha^N(i+1,k). \tag{1.7.3}$$

This recurrence relation has characteristic equation $(3/10)\lambda^2 - \lambda + (3/10) = 0$, whose roots are $\lambda_1 = 3$ and $\lambda_2 = 1/3$. So that, we find the closed form

$$p_\alpha^N(i,k) = h_{N,k}^1 3^i + h_{N,k}^2 \left(\frac{1}{3}\right)^i, \quad i = 1, \ldots, M-1, \tag{1.7.4}$$

where $h_{N,k}^1$ and $h_{N,k}^2$ are constants independent of i, which may be computed in terms of $p_\alpha^N(1,k)$ and $p_\alpha^N(M-1,k)$ using the relation (1.7.4) for $i = 1$ and $i = M-1$. Now

$$g_\alpha^N(k) = \sum_{i=1}^{M-1} p_\alpha^N(i,k) = h_{N,k}^1 \sum_{i=1}^{M-1} 3^i + h_{N,k}^2 \sum_{i=1}^{M-1} \left(\frac{1}{3}\right)^i,$$

and we get (1.7.2) after elementary calculations. □

This lemma has an easy and useful corollary that would be sufficient to prove the particular case of Theorem 1.8.1 under the assumption (1.2.11).

Corollary 1.7.2. *There exists an universal constant C_0 such that for all N and $k \in \Lambda_N$, $k \neq 0$,*

$$\left| g_\alpha^N(k) - \frac{3}{4}\mathbf{1}\{|k| = 1\} \right| \leq C_0 \left(\frac{3}{5}\right)^M.$$

Proof. For $|k| > 1$, the result follows from the previous lemma and observation (1.7.1). Let us consider the case $k = 1$ (the case $k = -1$ is analogous). By the same argument that leads to (1.7.1) we get that $p_\alpha^N(M-1,1) \leq (3/5)^{M-2}$. So, using the previous lemma, we just need to care about $p_\alpha^N(1,1)$. If M is large, we expect that $p_\alpha^N(1,1)$ is near to $1/2$. A way of formalizing this without much effort involving computations is to couple the jump chain of $\{\widehat{\eta}_1(t) : t \geq 0\}$ with another process for which we can use symmetry. The idea is very simple but requires some notations. Let $(X_n)_{n\geq 0}$ be the discrete-time jump chain associated to the process $\{\widehat{\eta}_1(t) : t \geq 0\}$ starting from $\xi^0_{\alpha,1}$ (its jump probabilities are given in Figure 1.1). Define the hitting time H^X,

$$H^X = H^X_{\left\{\xi^{-1}_{(\alpha+1),1}, \xi^1_{(\alpha-1),1}, \omega_0, \omega_1\right\}},$$

as the first time the chain $(X_n)_{n\geq 0}$ visits any of the configurations $\xi^{-1}_{(\alpha+1),1}$, $\xi^1_{(\alpha-1),1}$, ω_0, ω_1. We can conclude that $p_\alpha^N(1,1) = 1/2 + \mathcal{O}((3/5)^M)$ if we show that both the event $H^X = H^X_{\omega_1}$ and the event $H^X = H^X_{\omega_0}$ have probability $1/2 + \mathcal{O}((3/5)^M)$.

To achieve this, consider an auxiliary discrete-time chain $(\widehat{X}_n)_{n\geq 0}$ defined on the infinite set $\mathbb{Z} \cup \{u_-, u_+\}$ starting from 0. To define the jump probabilities of this chain, consider $\widehat{S} : \mathbb{Z} \setminus \{0\} \to \{u_-, u_+\}$ defined as

$$\widehat{S}(i) = \begin{cases} u_- & \text{if } i < 0, \\ u_+ & \text{if } i > 0. \end{cases}$$

We define the chain $(\widehat{X}_n)_{n\geq 0}$ imposing that, from $i \in \mathbb{Z} \setminus \{0\}$, it jumps to $i \pm 1$ with probability $3/10$ and to $\widehat{S}(i)$ with probability $2/5$. From 0, it jumps to ± 1 with probability $3/14$ and to u_- and u_+ with probability $2/7$. We define u_- and u_+ as absorbing states. By symmetry, this chain is absorbed in u_-, with probability $1/2$, or in u_+, with probability $1/2$. There is an obvious correspondence between the states of the chain $(\widehat{X}_n)_{n\geq 0}$ near to 0 and the states of the chain $(X_n)_{n\geq 0}$ near to $\xi^0_{\alpha,1}$. We can couple these two chains in such a way that, with this correspondence, they walk together until the time H^X. Let $P^{X,\widehat{X}}$ denote such a coupling. As already done before, observe that $P^{X,\widehat{X}}\left[H^X \geq M-2\right] \leq (3/5)^{M-3}$. Therefore,

$$\begin{aligned} P^{X,\widehat{X}}\left[H^X = H^X_{\omega_1}\right] &= P^{X,Y}\left[H^X = H^X_{\omega_1}, H^X < M-2\right] + \mathcal{O}\left(\left(\frac{3}{5}\right)^M\right) \\ &= P^{X,\widehat{X}}\left[H^{\widehat{X}} = H^{\widehat{X}}_{u_+}, H^X < M-2\right] + \mathcal{O}\left(\left(\frac{3}{5}\right)^M\right) \\ &= \frac{1}{2} + \mathcal{O}\left(\left(\frac{3}{5}\right)^M\right), \end{aligned}$$

and the same holds changing ω_1 by ω_0 and u_+ by u_-. With this, we conclude that $p_\alpha^N(1,1) = 1/2 + \mathcal{O}\left((3/5)^M\right)$, and then the result follows from Lemma 1.7.1. □

Now, for $l, m \geq 3$ we will define a quantity $v(l,m)$ in terms of some absorbtion probabilities of a simple discrete-time Markov chain $(Y_n^{l,m})_{n\geq 0}$ that depends on l and m. We will see later that this quantity will represent the velocity of the ballistic process that appears in the statement of Theorem 1.2.7.

Let us define the chain $(Y_n^{l,m})_{n\geq 0}$. Its state space is the set $\mathbb{Z}\cup\{u_1, u_0, u_{-1}, u_{-2}\}$. To define its jump probabilities consider the function $S : \mathbb{Z}\setminus\{-(m-2), 0, l-2\} \to \{u_1, u_0, u_{-1}, u_{-2}\}$ defined as

$$S(i) = \begin{cases} u_{-2} & \text{if } i < -(m-2), \\ u_{-1} & \text{if } -(m-2) < i < 0, \\ u_0 & \text{if } 0 < i < l-2, \\ u_1 & \text{if } i > l-2. \end{cases}$$

We define the chain $(Y_n^{l,m})_{n\geq 0}$ imposing that, from $i \in \mathbb{Z}\setminus\{-(m-2), 0, l-2)\}$, it jumps to $i \pm 1$ with probability $3/10$ and to $S(i)$ with probability $2/5$. From $i \in \{-(m-2), 0, l-2)\}$ it jumps to $i \pm 1$ with probability $3/14$ and to $S(i \pm 1)$ with probability $2/7$. The states u_1, u_0, u_{-1} and u_{-2} are defined as absorbing states. Figure 1.7 illustrates the structure of this simple chain. Roughly speaking, after an identification of the states, $(Y_n^{l,m})_{n\geq 0}$ is the jump chain of the process $\{\widehat{\eta}_1(t) : t \geq 0\}$, illustrated in Figure 1.1, with $N_A = l$, $N_B = m$ and $N_C = \infty$.

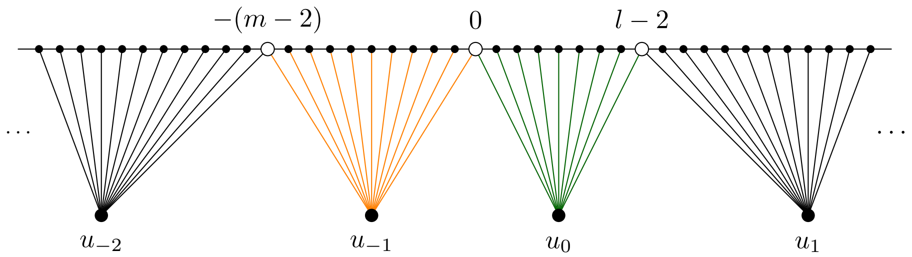

Figure 1.7: The graph structure of the chain $(Y_n^{l,m})_{n\geq 0}$.

For $0 \leq i \leq l-2$ and $k \in \{1, 0, -1, -2\}$ denote by $p^{l,m}(i, u_k)$ the probability for the chain $(Y_n^{l,m})_{n\geq 0}$ starting from i being absorbed in u_k. We define $v(l,m)$ as

$$v(l,m) := \frac{2}{3}\sum_{k=-2}^{1} k\left(\sum_{i=0}^{l-2} p^{l,m}(i, u_k)\right).$$

Repeating the proof of Lemma 1.7.1, with an obvious identification of the states, we get that

$$v(l,m) = \frac{2}{3}\left(\frac{3}{2} + \frac{2}{3^{l-2}+1}\right)\sum_{k\in\{-2,-1,1\}}\sum_{i\in\{0,l-2\}} kp^{l,m}(i, u_k). \tag{1.7.5}$$

Lemma 1.7.3. *There exists a constant C_0 such that for any $3 \le N_A < N_B < N_C$,*

$$\left| \frac{2}{3} \sum_{k \in \Lambda_N} k g_A^N(k) - v(N_A, N_B) \right| \le C_0 N_C^2 \left(\frac{3}{5} \right)^{N_C}$$

Proof. If $k \notin \{-2,-1,0,1\}$ we note that for $i = 1, N_A - 1$, starting from $\xi^0_{A,i}$, the chain $\{\widehat{\eta}_1(t) : t \ge 0\}$ must make at least N_C jumps to arrive at ω_k. So, using Lemma 1.7.1 we get that

$$g_A^N(k) \le C_0 (3/5)^{N_C}, \quad k \notin \{-2,-1,0,1\}. \tag{1.7.6}$$

For $k \in \{-2,-1,0,1\}$ we use the same coupling argument used in the last corollary, now coupling the jump chain of $\{\widehat{\eta}_1(t) : t \ge 0\}$ with the chain $(Y_n^{N_A,N_B})_{n \ge 0}$. If we do not survive at least N_C steps without absorption, we do not feel the difference of these two chains. So, in (1.7.2) we may change $p_A^N(i+1,k)$ by $p^{N_A,N_B}(i,u_k)$, $i = 0, N_A - 2$, causing errors of order $\mathcal{O}((3/5)^{N_C})$. □

The key to obtain the specific scenario in which the process will converge to a Brownian motion with drift is to understand the dependence of $v(N_A, N_B)$ on N_A and N_B. The next lemma is sufficient for this purpose.

Lemma 1.7.4. *Suppose that $3 \le N_A < N_B$, then*

$$v(N_A, N_B) = \left[-3 + \mathcal{O}\left(\left(\frac{1}{3} \right)^{N_A} \right) \right] \left(\frac{1}{3} \right)^{N_B} + \mathcal{O}\left(\left(\frac{1}{3} \right)^{2N_B} \right). \tag{1.7.7}$$

Proof. By (1.7.5), in order to explicitly compute $v(l,m)$ we just need to compute the six absorption probabilities

$$p^{l,m}(i, u_k), \quad i = 0, l-2, \quad k = 1, -1, -2. \tag{1.7.8}$$

Solving a recurrence as in (1.7.3), we can compute the distribution of the first visited state in the set $\{0, l-2, u_0\}$ if the chain $(Y_n^{l,m})_{n \ge 0}$ starts from 1. We find that, the process will first visit $l-2$, 0 or u_0 with probabilities p_l, q_l and r_l, respectively, where

$$p_l = \frac{3 - (1/3)}{3^{l-2} - (1/3)^{l-2}}, \quad q_l = \frac{3^{l-3} - (1/3)^{l-3}}{3^{l-2} - (1/3)^{l-2}}, \quad r_l = 1 - p_l - q_l. \tag{1.7.9}$$

This provides a simplification of the chain $(Y_n^{l,m})_{n \ge 0}$, which is best explained with Figure 1.8.

With this, we can easily compute the distribution of the first visited configuration in $\{-(m-2), u_{-1}, u_0, l-2\}$ if the process starts from 0. We obtain that the process will first visit $l-2$, u_0, $-(m-2)$, u_{-1} with, respectively, probabilities $p_{l,m}$, $q_{l,m}$, $p_{m,l}$ and $q_{m,l}$, where

$$p_{l,m} = \frac{\frac{3}{14} p_l}{1 - \frac{3}{14}(q_l + q_m)}, \quad q_{l,m} = \frac{\frac{2}{7} + \frac{3}{14} r_l}{1 - \frac{3}{14}(q_l + q_m)}. \tag{1.7.10}$$

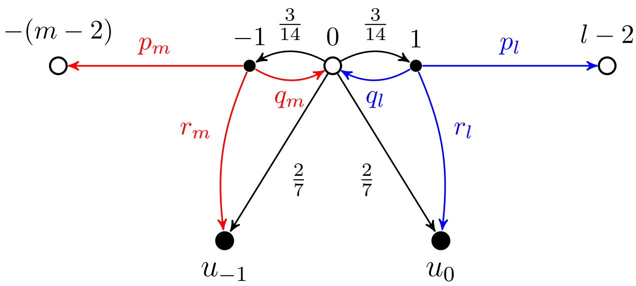

Figure 1.8: A first simplification in the dynamics of $(Y_n^{l,m})_{n\geq 0}$.

Now, if we define

$$p_{l,\infty} := \lim_{j\to\infty} p_{l,j}, \quad q_{l,\infty} := \lim_{j\to\infty} q_{l,j}, \quad q_{\infty,m} := \lim_{j\to\infty} q_{j,m},$$

this means that, in order to compute the probabilities in (1.7.8), we can consider the simple seven-state chain whose jump probabilities are given in Figure 1.9.

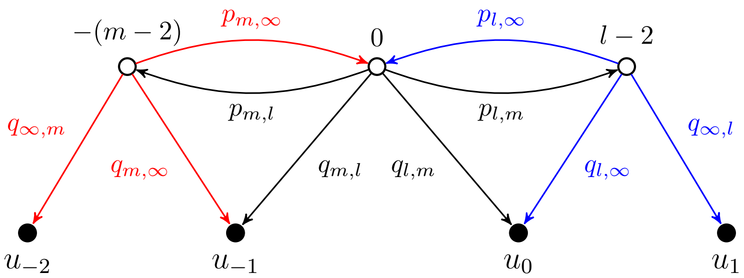

Figure 1.9: A further simplification in the dynamics of $(Y_n^{l,m})_{n\geq 0}$.

From this point, it is easy to find that

$$p^{l,m}(0,u_1) = \frac{p_{l,m}q_{\infty,l}}{1-(p_{l,m}p_{l,\infty}+p_{m,l}p_{m,\infty})},\ p^{l,m}(l-2,u_1) = q_{\infty,l} + p_{l,\infty}p^{l,m}(0,u_1),$$
$$p^{l,m}(0,u_{-1}) = \frac{q_{m,l}+p_{m,l}q_{m,\infty}}{1-(p_{l,m}p_{l,\infty}+p_{m,l}p_{m,\infty})},\ p^{l,m}(l-2,u_{-1}) = p_{l,\infty}p^{l,m}(0,u_{-1}),$$
$$p^{l,m}(0,u_{-2}) = \frac{p_{m,l}q_{\infty,m}}{1-(p_{l,m}p_{l,\infty}+p_{m,l}p_{m,\infty})},\ p^{l,m}(l-2,u_{-2}) = p_{l,\infty}p^{l,m}(0,u_{-2}).$$

To simplify the notations, in the next equations $\boldsymbol{x}$ and $\boldsymbol{y}$ will represent respectively $(1/3)^l$ and $(1/3)^m$. After many but elementary calculations we see from the last equations and the explicit expressions (1.7.9) and (1.7.10) that

$$\begin{aligned} p^{l,m}(0,u_1) &= \frac{3\boldsymbol{x}}{1-9\boldsymbol{x}^2} + \mathcal{O}(\boldsymbol{y}^2), \\ p^{l,m}(0,u_{-1}) &= \frac{1-27\boldsymbol{x}^2}{2-18\boldsymbol{x}^2} - (3+\mathcal{O}(\boldsymbol{x}))\boldsymbol{y} + \mathcal{O}(\boldsymbol{y}^2), \\ p^{l,m}(0,u_{-2}) &= (3+\mathcal{O}(\boldsymbol{x}))\boldsymbol{y} + \mathcal{O}(\boldsymbol{y}^2), \end{aligned}$$

and

$$\begin{aligned}
p^{l,m}(l-2,u_1) &= \frac{1-27\boldsymbol{x}^2}{2-18\boldsymbol{x}^2} + \mathcal{O}(\boldsymbol{y}^2) \\
p^{l,m}(l-2,u_{-1}) &= \frac{3\boldsymbol{x}}{1-9\boldsymbol{x}^2} + \mathcal{O}(\boldsymbol{x})\boldsymbol{y} + \mathcal{O}(\boldsymbol{y}^2), \\
p^{l,m}(l-2,u_{-2}) &= \mathcal{O}(\boldsymbol{x})\boldsymbol{y} + \mathcal{O}(\boldsymbol{y}^2),
\end{aligned}$$

From now, many cancellations take place and we see from (1.7.5) that $v(l,m) = [-3+\mathcal{O}(\boldsymbol{x})]\boldsymbol{y} + \mathcal{O}(\boldsymbol{y}^2)$, as desired. □

1.8 Scaling limits for the trace process on Ω_0^N when $N \uparrow \infty$

Recall the definition of the random walk $\{X(t) : t \geq 0\}$ presented just before Theorem 1.2.7.

Theorem 1.8.1. *Let θ_β be as in* (1.2.7)*. Assume that $\eta(0) = \omega_0$, $3 \leq N_A < N_B \leq N_C$ and that $N \uparrow \infty$ as $\beta \uparrow \infty$ in such a way that* (1.2.8) *holds and that*

$$\lim_{\beta\to\infty} (N_C^5 4^{N_A} + N_C^6 N_A \beta) e^{-\beta} = 0. \tag{1.8.1}$$

Then, as $\beta \uparrow \infty$, the process $\{X(t\theta_\beta)/N : t \geq 0\}$ converges in the uniform topology to a Brownian motion with drift $\{\mu t + \sigma B_t : t \geq 0\}$ on the circle $[-1,1]$. If $b = 0$ in (1.2.8)*, we may replace the assumption $N_A < N_B$ by $N_A \leq N_B$.*

In Theorem 1.8.1 the number of particles of type A can go to infinity or be constant. The parameters μ and σ can be explicitly computed. In the case where $N_A \uparrow \infty$ we have that $\mu = -3b/2$ and $\sigma = 1$. If N_A is constant, then there is a multiplicative correction $(1 + \mathcal{O}\left((1/3)^{N_A}\right)$ in these values. The restriction (1.8.1), which imposes that N can not increase too fast, is not optimal. It comes from our not very accurate estimate of $r_\beta(k)$ in Proposition 1.6.2. A more careful analysis would need to take into account a much larger combinatorial complexity.

In this section we will prove Theorems 1.2.7 and 1.8.1. The general strategy is the same for the two proofs, and so we start considering a general context.

For $\tilde{\theta}_\beta$, a function of β, define the process $\{Y^\beta(t) : t \geq 0\}$ by

$$Y^\beta(t) = \frac{X(\tilde{\theta}_\beta t)}{N}.$$

By [24, Theorem 8.7.1], in order to prove that, as $\beta \to \infty$, the Markov chain $\{Y^\beta(t) : t \geq 0\}$ converges to a diffusion $\{\mu t + \sigma B_t : t \geq 0\}$, it is enough to verify the convergence of the corresponding infinitesimal mean and covariance and a condition that rules out jumps in the limit. More precisely, we have to show that

$$\lim_{\beta\to\infty}\sum_{k\in\Lambda_N}\left(\frac{k}{N}\right)^2 r_\beta(k)\tilde{\theta}_\beta=\sigma^2,\quad \lim_{\beta\to\infty}\sum_{k\in\Lambda_N}\frac{k}{N}r_\beta(k)\tilde{\theta}_\beta=\mu, \tag{1.8.2}$$

and that, for every $\delta>0$

$$\lim_{\beta\to\infty}\sum_{|k|>N\delta} r_\beta(k)\tilde{\theta}_\beta=0. \tag{1.8.3}$$

By Proposition 1.6.2, if for $\psi(\beta)$ satisfying (1.6.6), we can prove that

$$\lim_{\beta\to\infty}N\tilde{\theta}_\beta\psi(\beta)=0, \tag{1.8.4}$$

then we may replace conditions (1.8.2) and (1.8.3) by the following:

$$\lim_{\beta\to\infty}\sum_{\alpha:N_\alpha=M}\left(1+\frac{2}{3}\sum_{k\in\Lambda_N}k^2g_\alpha^N(k)\right)e^{-M\beta}\tilde{\theta}_\beta N^{-2}=\sigma^2, \tag{1.8.5}$$

$$\lim_{\beta\to\infty}\frac{2}{3}\left(\sum_{\alpha:N_\alpha=M}\sum_{k\in\Lambda_N}kg_\alpha^N(k)\right)e^{-M\beta}\tilde{\theta}_\beta N^{-1}=\mu, \tag{1.8.6}$$

and, for every $\delta>0$

$$\lim_{\beta\to\infty}\sum_{\alpha:N_\alpha=M}\sum_{|k|>N\delta}g_\alpha^N(k)e^{-M\beta}\tilde{\theta}_\beta=0. \tag{1.8.7}$$

For the sake of clarity, from now on we look at each case separately. In fact, all the work has already been done.

Proof of Theorem 1.2.7. In this case $\tilde{\theta}_\beta=Ne^{N_A\beta}$. Since $N_A<N_B$ are constants, we get (1.8.4) from assumption (1.2.16). Just observing (1.7.6) we obtain (1.8.7) and (1.8.5) with $\sigma^2=0$. To conclude, observe that Lemma 1.7.3 gives (1.8.6) with $\mu=v(N_A,N_B)$. □

Proof of Theorem 1.8.1. In this case $\tilde{\theta}_\beta=\theta_\beta$. Consider first the case $b>0$. In this setting, since $N_A<N_B\le N_C$, (1.8.4) follows from assumption (1.8.1). As before, (1.8.7) follows from (1.7.6). For simplicity, let's suppose that we are in the case where $N_A\uparrow\infty$. By Lemma 1.7.3 the limit in (1.8.6) is equal to $\lim_{\beta\to\infty}(1/2)v(N_A,N_B)N$ and then, from Lemma 1.7.4 and assumption (1.2.8) we get (1.8.6) with $\mu=-3b/2$. To conclude, it remains to verify (1.8.5). By (1.7.6), the limit in (1.8.5) is equal to

$$\frac{1}{2}\left(1+\lim_{\beta\to\infty}\frac{2}{3}\sum_{k=-2}^{1}k^2g_A^N(k)\right). \tag{1.8.8}$$

Now, (1.8.5) with $\sigma^2 = 1$ follows easily from Corollary 1.7.2. If N_A is constant, we could, for example, analyze the limit (1.8.8) in the same way that we have estimated $\sum_{k\in\Lambda_N} kg_\alpha^N(k)$ in Lemmas 1.7.3 and 1.7.4, obtaining this way, after many (but elementary) calculations, that (1.8.5) holds with $\sigma^2 = 1 + \mathcal{O}((1/3)^{N_A})$. Now, noting that, by symmetry, (1.8.6) is equal to 0 if $N_A = N_B$ and recalling the definition of d, we see that the convergences still work for $N_A \leq N_B$ in the case $b = 0$. □

1.9 Proof of Lemma 1.2.1

1.9.1 Some estimates for the invariant measure

Recall the notations introduced in the beginning of Section 1.5. Let μ_β be the invariant measure of the ABC process $\{\eta(t) : t \geq 0\}$. In our context the invariance of the measure μ_β is characterized by the fact that, for every $\omega \in \Omega^N$,

$$e^{-\beta} \sum_{\xi\in B(\omega)} \mu_\beta(\xi) + \sum_{\xi\in R(\omega)} \mu_\beta(\xi) = |B(\omega)|\mu_\beta(\omega) + e^{-\beta}|R(\omega)|\mu_\beta(\omega). \tag{1.9.1}$$

Lemma 1.9.1. *For any $\beta > 0$, $k \in \Lambda_N$ and $1 \leq n \leq M$,*

$$\sum_{\omega\in\Delta_k^n} |B_k^*(\omega)|\mu_\beta(\omega) = e^{-\beta} \sum_{\xi\in\Delta_k^{n-1}} |R(\xi)|\mu_\beta(\xi). \tag{1.9.2}$$

Proof. Fix $k \in \Lambda_N$. We prove the result by induction in n. The case $n = 1$ is just the relation (1.9.1) for $\omega = \omega_k$. Now suppose that (1.9.2) holds for some $n \leq M-1$. Summing the relation (1.9.1) over all $\omega \in \Delta_k^n$ we obtain

$$\begin{aligned} e^{-\beta} \sum_{\omega\in\Delta_k^n} \sum_{\xi\in B(\omega)} \mu_\beta(\xi) &+ \sum_{\omega\in\Delta_k^n} \sum_{\xi\in R(\omega)} \mu_\beta(\xi) \\ &= \sum_{\omega\in\Delta_k^n} |B(\omega)|\mu_\beta(\omega) + e^{-\beta} \sum_{\omega\in\Delta_k^n} |R(\omega)|\mu_\beta(\omega) \end{aligned} \tag{1.9.3}$$

By (1.5.1), we note that in the first member on the left-hand side of (1.9.3), we are measuring configurations on Δ_k^{n-1}. Moreover, note that each configuration $\xi \in \Delta_k^{n-1}$ is counted repeatedly $|R(\xi)|$ times. This is due to the simple fact that there are exactly $|R(\xi)|$ configurations $\omega \in \Delta_k^n$ such that $\xi \in B(\omega)$. So, we may rewrite the first member on the left-hand side of (1.9.3) as $e^{-\beta} \sum_{\xi\in\Delta_k^{n-1}} |R(\xi)|\mu_\beta(\xi)$ and then, by the induction hypothesis it cancels with the first member on the right-hand side of the equality. Now note that in the second member of the left-hand side, we are measuring configurations in Δ_k^{n+1} and each configuration $\xi \in \Delta_k^{n+1}$ is counted repeatedly $|B_k^*(\xi)|$ times. Thus we get the relation (1.9.2) with n replaced by $n+1$, which concludes the proof. □

Corollary 1.9.2. *For any $\beta > 0$, $k \in \Lambda_N$ and $1 \le n \le M$*

$$\sum_{\omega \in \Delta_k^n} |B_k^*(\omega)| \mu_\beta(\omega) \le (4e^{-\beta})^n \mu_\beta(\omega_k),$$

and then, for β large enough,

$$\sum_{n=1}^{M} \sum_{\omega \in \Delta_k^n} |B_k^*(\omega)| \mu_\beta(\omega) \le 5e^{-\beta} \mu_\beta(\omega_k). \tag{1.9.4}$$

Proof. The proof consists in iterations of (1.9.2) using the inequality $|R(\xi)| \le 4|B_k^*(\xi)|$, which, by Lemma 1.5.1, holds for every $\xi \in V(\omega_k)$. □

For any set of configurations $\mathcal{H} \subseteq \Omega^N$, define inductively

$$B^0(\mathcal{H}) = \mathcal{H}, \quad B^n(\mathcal{H}) = \bigcup_{\omega \in B^{n-1}(\mathcal{H})} B(\omega), \ n = 1, 2, \dots, \tag{1.9.5}$$

and then define $B^\infty(\mathcal{H}) = \bigcup_{n=0}^\infty B^n(\mathcal{H})$. In the same way, just changing B by R in (1.9.5), define $R^n(\mathcal{H})$, $n \ge 1$. When $\mathcal{H} = \{\omega_k\}$ we write simply R_k^n instead of $R^n(\{\omega_k\})$. We omit the index n when $n = 1$.

Lemma 1.9.3. *For any $\beta > 0$, $k \in \Lambda_N$ and $n \ge 1$,*

$$\begin{aligned} \sum_{\omega \in R_k^{M+n}} |B_k^*(\omega)| \mu_\beta(\omega) + e^{-\beta} \sum_{i=0}^{n-1} \sum_{\omega \in R_k^{M+i}} \sum_{\zeta \in D_k^*(\omega)} \mu_\beta(\zeta) \\ = e^{-\beta} \sum_{\xi \in R_k^{M+n-1}} |R(\xi)| \mu_\beta(\xi) + \sum_{i=0}^{n-1} \sum_{\xi \in R_k^{M+i}} |D_k^*(\xi)| \mu_\beta(\xi) \end{aligned} \tag{1.9.6}$$

Proof. Fix $k \in \Lambda_N$. The proof by induction is very similar to the proof of Lemma 1.9.1. To pass from the case n to the case $n+1$, sum the relation (1.9.1) over all $\omega \in R_k^{M+n}$ decomposing $B(\omega) = B_k^*(\omega) \cup D_k^*(\omega)$. The inductive argument is completed observing that

$$\sum_{\omega \in R_k^{M+n}} \sum_{\xi \in B_k^*(\omega)} \mu_\beta(\xi) = \sum_{\xi \in R_k^{M+n-1}} |R(\xi)| \mu_\beta(\xi),$$

and

$$\sum_{\omega \in R_k^{M+n}} \sum_{\xi \in R(\omega)} \mu_\beta(\xi) = \sum_{\xi \in R_k^{M+n+1}} |B_k^*(\xi)| \mu_\beta(\xi).$$

In the same way, we obtain the base case $n = 1$ from the case $n = M$ of Lemma 1.9.1. □

Remind that we have defined $M^* = \max\{N_A, N_B, N_C\}$.

Corollary 1.9.4. *There exists a constant C_0 such that, for any $\beta > 0$,*

$$\mu_\beta\left(\bigcup_{k\in\Lambda_N}\bigcup_{n=M}^{M^*} R_k^n\right) \leq C_0 4^{M^*} e^{-M\beta}\mu_\beta(\Omega_0^N), \quad (1.9.7)$$

$$\mu_\beta\left(\mathcal{G}^N\right) \leq C_0 4^{M^*} e^{-(M-1)\beta}\mu_\beta(\Omega_0^N), \quad (1.9.8)$$

$$\mu_\beta\left(R(\mathcal{G}^N)\right) \leq C_0 4^{M^*} e^{-M\beta}\mu_\beta(\Omega_0^N). \quad (1.9.9)$$

Proof. Fix $k \in \Lambda_N$. Let $Z_k(0) = \sum_{\omega\in\Delta_k^M} |B_k^*(\omega)|\mu_\beta(\omega)$ and, for $n \geq 1$, let $Z_k(n)$ be the expression in (1.9.6). Obviously, for any $\omega \in V(\omega_k)\setminus\{\omega_k\}$ we have $|B_k^*(\omega)| \geq 1$. Let's label the particles of the system in such a way that for the configuration ω_k, the labels $A_1, A_2, \dots, A_{N_A}, B_1, B_2, \dots$ are placed clockwise and the particle A_1 is the particle of type A that is adjacent to a particle of type C, which is C_{N_C}. With these labels we note that, when they exist, the blue edges of a configuration $\omega \in V(\omega_k)$ of the type whose transposition leads to configurations in $D_k^*(\omega)$ connect the adjacent particles $(\alpha-1)_{N_{(\alpha-1)}}$ and $(\alpha+1)_1$, for some $\alpha \in \{A, B, C\}$, see Figure 1.2. So, for configurations in $V(\omega_k)$ there are at most three of such blue edges, that is $|D_k^*(\omega)| \leq 3$. Moreover, from ω_k to achieve a configuration $\omega \in V(\omega_k)$ with $|D_k^*(\omega)| = 3$, at least $N_A + N_B + N_C - 3 > M^*$ jumps are necessary. So, for configurations $\omega \in \bigcup_{n=M}^{M^*} R_k^n$, we have $|D_k^*(\omega)| \leq 2$. These inequalities and the one of Lemma 1.5.1 applied to equality (1.9.6) allow us to conclude that, for $1 \leq n \leq M^* - M + 1$

$$Z_k(n) \leq (4e^{-\beta})Z_k(n-1) + 2\sum_{i=0}^{n-1} Z_k(i).$$

Thus, just using that $4e^{-\beta} < 1$ and Corollary 1.9.2, we get

$$Z_k(n) \leq 4^n Z_k(0) \leq 4^n 4^M e^{-\beta}\mu_\beta(\omega_k). \quad (1.9.10)$$

Now note that

$$\mathcal{G}^N \subseteq \bigcup_{k\in\Lambda_N}\ \bigcup_{m\in\{N_A,N_B,N_C\}}\ \bigcup_{\omega\in R_k^m} D_k^*(\omega).$$

So, by the definition of $Z_k(n)$ and (1.9.10),

$$\mu_\beta\left(\bigcup_{k\in\Lambda_N}\bigcup_{n=M}^{M^*} R_k^n\right) + e^{-\beta}\mu_\beta(\mathcal{G}^N) \leq \sum_{k\in\Lambda_N}\sum_{n=0}^{M^*-M+1} Z_k(n) \leq C_0 4^{M*} e^{-M\beta}\mu_\beta(\Omega_0^N),$$

which proves (1.9.7) and (1.9.8). To obtain the inequality (1.9.9), just note that for each $\omega \in \mathcal{G}^N$, the invariance of μ_β says that $\sum_{v\in R(\omega)}\mu_\beta(v) = 6e^{-\beta}\mu_\beta(\omega)$, and so $\mu_\beta(R(\mathcal{G}^N)) \leq 6e^{-\beta}\mu_\beta(\mathcal{G}^N)$. □

1.9.2 The set that the process never leaves

The proof of Lemma 1.2.1 consists in finding a set of configurations Ξ^N that the process never leaves in the time scale $e^{M\beta}$. The set Ξ^N needs to be sufficiently small so that $\mu_\beta(\Xi^N \setminus \Omega_0^N)/\mu_\beta(\Omega_0^N)$ vanishes as $\beta \uparrow \infty$, which will allow us to conclude that, in fact, the process stays almost always in Ω_0^N. The analysis of the excursions between two consecutive visits to the set Ω_0^N, which we have made in Section 1.5, suggests a natural candidate. We define Ξ^N as

$$\Xi^N = B^\infty \left(\bigcup_{k\in\Lambda_N} \bigcup_{n=0}^{M} R_k^n \right) \cup B^\infty \left(R(\mathcal{G}^N) \right). \tag{1.9.11}$$

This choice is optimal in the sense that, starting from Ω_0^N, any configuration in Ξ^N can, in fact, be visited after a time of order $e^{M\beta}$. It is interesting to note that the configurations in Ξ^N that are not in $\bigcup_{k\in\Lambda_N} \bigcup_{n=0}^{M} \Delta_k^n$ are very similar to the configurations in Ω_0^N, differing by at most two particles that are detached from their corresponding blocks. This observation, which will be crucial for Section 1.10, justifies the inclusion $\Xi^N \subseteq \Gamma^N$ stated in Section 1.2.2.

Let $\partial\Xi^N$ denote the boundary of Ξ^N, that is

$$\partial\Xi^N = \left\{ \omega \in \Xi^N : \text{there exists } \xi \in \Omega^N \setminus \Xi^N \text{ and } i \in \Lambda_N \text{ such that } \xi = \sigma^{i,i+1}\omega \right\}.$$

Note that Ξ^N was defined in such a way that

$$B(\xi) \subseteq \Xi^N, \text{ if } \xi \in \partial\Xi^N. \tag{1.9.12}$$

Lemma 1.9.5. *There exists a constant C_0 such that, for any $\beta > 0$,*

$$\mu_\beta(\Xi^N \setminus \Omega_0^N) \le C_0 4^{M^*} e^{-\beta} \mu_\beta(\Omega_0^N) \tag{1.9.13}$$

and

$$\mu_\beta(\partial\Xi^N) \le C_0 4^{M^*} e^{-M\beta} \mu_\beta(\Omega_0^N). \tag{1.9.14}$$

Proof. Note that

$$\Xi^N \setminus \Omega_0^N \subseteq \left(\bigcup_{k\in\Lambda_N} \bigcup_{n=1}^{M^*} R_k^n \right) \cup \mathcal{G}^N \cup R(\mathcal{G}^N)$$

and

$$\partial\Xi^N \subseteq \left(\bigcup_{k\in\Lambda_N} \bigcup_{n=M}^{M^*} R_k^n \right) \cup R(\mathcal{G}^N).$$

Now use Corollaries 1.9.2 and 1.9.4. ☐

Proof of Lemma 1.2.1. We follow the strategy presented in [31]. Fix $k \in \Lambda_N$ and $t \geq 0$. We first claim that

$$\lim_{\beta\to\infty} \mathbf{E}^{\beta}_{\omega_k}\left[\int_0^t \mathbf{1}\{\eta(sN^2e^{M\beta}) \notin \Xi^N\}ds\right] = 0. \tag{1.9.15}$$

For each $\omega \in \partial\Xi^N$, denote by $J(\omega, t)$ the number of jumps from ω to configurations in $\Omega^N \setminus \Xi^N$ in the time interval $[0, t]$ and let $R^\beta(\omega, \Omega^N \setminus \Xi^N)$ be the total jump rate from ω to $\Omega^N \setminus \Xi^N$. Note that the process $\{(\eta(t), J(\omega, t)) : t \geq 0\}$ is a Markov chain. If $\tilde{L}_\beta$ stands for the generator of this chain and $f(\xi, n) = n$, it is easy to see that $\tilde{L}_\beta f(\xi, n) = \mathbf{1}\{\xi = \omega\}R^\beta(\omega, \Omega_0^N \setminus \Xi^N)$, so that

$$\{J(\omega, t) - \int_0^t R^\beta(\omega, \Omega_0^N \setminus \Xi^N)\mathbf{1}\{\eta(s) = \omega\}ds : \ t \geq 0\}$$

is a martingale, and thus

$$\mathbf{E}^{\beta}_{\omega_k}\left[J(\omega, t)\right] = \mathbf{E}^{\beta}_{\omega_k}\left[\int_0^t R^\beta(\omega, \Omega_0^N \setminus \Xi^N)\mathbf{1}\{\eta(s) = \omega\}ds\right].$$

Therefore, if we define $J(t) = \sum_{\omega\in\partial\Xi^N} J(\omega, t)$, by observation (1.9.12) we get that

$$\mathbf{P}^{\beta}_{\omega_k}\left[J(t) \geq 1\right] \leq \mathbf{E}^{\beta}_{\omega_k}\left[J(t)\right] \leq C_0Ne^{-\beta}\mathbf{E}^{\beta}_{\omega_k}\left[\int_0^t \mathbf{1}\{\eta(s) \in \partial\Xi^N\}ds\right].$$

By symmetry,

$$\begin{aligned}\mathbf{E}^{\beta}_{\omega_k}\left[\int_0^t \mathbf{1}\{\eta(s) \in \partial\Xi^N\}ds\right] &= \frac{1}{|\Omega_0^N|}\sum_{j\in\Lambda_N}\mathbf{E}^{\beta}_{\omega_j}\left[\int_0^t \mathbf{1}\{\eta(s) \in \partial\Xi^N\}ds\right] \\ &= \frac{1}{|\Omega_0^N|\mu_\beta(\omega_0)}\sum_{j\in\Lambda_N}\mu_\beta(\omega_j)\mathbf{E}^{\beta}_{\omega_j}\left[\int_0^t \mathbf{1}\{\eta(s) \in \partial\Xi^N\}ds\right].\end{aligned} \tag{1.9.16}$$

The sum is bounded above by

$$\mathbf{E}^{\beta}_{\mu_\beta}\left[\int_0^t \mathbf{1}\{\eta(s) \in \partial\Xi^N\}ds\right] = t\mu_\beta(\partial\Xi^N)$$

and the denominator is equal to $\mu_\beta(\Omega_0^N)$, and so

$$\mathbf{P}^{\beta}_{\omega_k}\left[J(tN^2e^{M\beta}) \geq 1\right] \leq \frac{C_0tN^3e^{-\beta}e^{M\beta}\mu_\beta(\partial\Xi^N)}{\mu_\beta(\Omega_0^N)}.$$

By (1.9.14) the above expression is less than or equal to $C_0tN^34^{M^*}e^{-\beta}$, which vanishes as $\beta \uparrow \infty$, in view of assumption (1.2.2). Therefore, we have proved (1.2.5), that is, for any $t \geq 0$, starting from ω_k, with probability converging to 1, the process $\{\eta(s) : s \geq 0\}$ does not leave the set Ξ^N in the time interval $[0, tN^2e^{M\beta}]$, which is a result stronger than (1.9.15). To conclude the proof of the lemma it remains to show that

$$\lim_{\beta\to\infty} \mathbf{E}^{\beta}_{\omega_k}\left[\int_0^t \mathbf{1}\{\eta(sN^2e^{M\beta}) \in \Xi^N \setminus \Omega_0^N\}ds\right] = 0.$$

By repeating the arguments used in (1.9.16) we obtain that the previous expectation is bounded by $t\mu_\beta(\Xi^N \setminus \Omega_0^N)/\mu_\beta(\Omega_0^N)$. By (1.9.13) this is bounded by $C_0 t 4^{M^*} e^{-\beta}$, which, in view of assumption (1.2.2), vanishes as $\beta \uparrow \infty$. □

About Remark 1.2.4. Now we prove that, for the equal densities case $N_A = N_B = N_C$, (1.2.13) holds without assumptions controlling the growth of N. In fact, this can be derived from the estimates of the partition function Z_β presented in [26, 27]. However, for completeness we present a proof here. Subtracting a function of M in the Hamiltonian (1.2.1) (in fact, this function is M^2 but this not relevant) and incorporating this correction in the partition function Z_β, we may suppose that the ground states ω_k, $k \in \Lambda_N$, have energy zero. For each n, the number of configurations with energy n is bounded by 3^{3M}, since this is a bound for the total number of configurations. So,

$$\mu_\beta(\{\omega : \mathbb{H}(\omega) > M/2\}) \leq \frac{\sum_{n>M/2} 3^{3M} e^{-n\beta}}{Z_\beta} \leq C_0\left(27e^{-\beta/2}\right)^M,$$

and this goes to zero when $\beta \uparrow \infty$ (for this term is even better if M grows fast). For configurations with energy at most $M/2$ (which are configurations at distance at most $M/2$ from some ground state) we can use the estimate (1.9.4). So, in the limit $\beta \uparrow \infty$, in the equal densities case, the invariant measure is concentrated in Ω_0^N, no matter how fast $N \uparrow \infty$. □

1.10 Convergence of the center of mass

In this section we assume the hypothesis of Theorem 1.2.2, under which we will show that, when $\beta \uparrow \infty$, the process $\{\mathcal{C}(\eta(tN^2e^{M\beta}) : t \geq 0)\}$ is close to the process $\{X(tN^2e^{M\beta})/N + r_A/2 : t \geq 0\}$ in the Skohorod space $D([0,\infty),[-1,1])$.

In the previous section we showed that under (1.2.2) we have (1.2.5), where Ξ^N is the set defined in (1.9.11). Later it will be useful to note that Ξ^N can also be expressed as the union $\Xi^N = \bigcup_{k\in\Lambda_N} \Xi^N_k$ where

$$\Xi^N_k = \bigcup_{n=0}^{M} \Delta^n_k \;\cup \bigcup_{\alpha\in\{A,B,C\}} B^\infty\left(R(\mathcal{G}^{N,k}_\alpha)\right).$$

In order to compare the process $\{\mathcal{C}(\eta(tN^2e^{M\beta}) : t \geq 0)\}$ with the trace process $\{X(tN^2e^{M\beta})/N + r_A/2 : t \geq 0\}$ we will use the process, derived from $\{\eta(t) : t \geq 0\}$, that records the last visit to the set Ω_0^N. Define

$$\hat{X}(t) := \begin{cases} \mathbf{X}(\eta(t)) & \text{if } \eta(t) \in \Omega_0^N, \\ \mathbf{X}(\eta(\sigma(t)^-)) & \text{if } \eta(t) \notin \Omega_0^N. \end{cases}$$

where $\sigma(t) = \sup\{s \le t : \eta(s) \in \Omega_0^N\}$. As we have done for $\{X(t) : t \ge 0\}$, we are omitting the dependence on β. The last visit process $\{\hat{X}(t) : t \ge 0\}$ has the advantage with respect to the trace process that it does not translate in time the original trajectory.

With the same proof of [3, Proposition 4.4], with obvious small modifications for our case, under (1.2.3) we have that

$$\lim_{\beta\to\infty} \mathbf{E}^\beta_{\omega_0}\left[\rho(X^*, \hat{X}^*)\right] = 0, \tag{1.10.1}$$

where X^* and $\hat{X}^*$ denote the speeded up processes $\{X(tN^2e^{M\beta})/N : t \ge 0\}$ and $\{\hat{X}(tN^2e^{M\beta})/N : t \ge 0\}$, respectively, and ρ is a distance that generates the Skohorod topology in $D([0,\infty), [-1,1])$.

Now we prove that the last visit process is close to the center of mass in the uniform metric.

Proposition 1.10.1. *Assume the hypothesis of Theorem 1.2.2. For any $\varepsilon > 0$ and $t > 0$,*

$$\lim_{\beta\to\infty} \mathbf{P}^\beta_{\omega_0}\left[\sup_{0\le s\le tN^2e^{M\beta}} |\hat{X}(s)/N + r_A/2 - \mathcal{C}(\eta(s))| > \varepsilon\right] = 0.$$

Proof. Let $\hat{N}(t)$ be the number of jumps of the process $\{\hat{X}(s) : s \ge 0\}$ during the time interval $[0, tN^2e^{M\beta}]$. We claim that there exists a constant L, depending on t, such that

$$\lim_{\beta\to\infty} \mathbf{P}^\beta_{\omega_0}\left[\frac{N^2}{L} < \hat{N}(t) < LN^2\right] = 1. \tag{1.10.2}$$

In fact, let $N(t)$ be the number of jumps of $\{X(s) : s \ge 0\}$ during the time interval $[0, tN^2e^{M\beta}]$. Observing that

$$N(t) = \hat{N}\left(t + \int_0^t \mathbf{1}\{\eta(sN^2e^{M\beta}) \notin \Omega_0^N\}ds\right),$$

the claim will be proved if we prove (1.10.2) for $\hat{N}(t)$ changed by $N(t)$. Now note that

$$\mathbf{P}^\beta_{\omega_0}\left[N(t) \ge LN^2\right] = P\left[T_1^\beta + T_2^\beta + \ldots + T^\beta_{LN^2} < tN^2e^{M\beta}\right], \tag{1.10.3}$$

where, T_i^β, $i = 1, 2, \ldots$ are independent mean $1/\lambda_\beta$ exponential random variables, with $\lambda_\beta = \sum_{k\in\Lambda_N} r_\beta(k)$. By Proposition 1.6.2, because of (1.2.9), there exist constants $1 < c_0 < C_0 < \infty$ such that $e^{M\beta}\lambda_\beta \in (c_0, C_0)$, for all $\beta > 0$. Hence, the expression in (1.10.3) goes to zero as $\beta \uparrow \infty$, if $t/L < 1/C_0$. In the same way, we show that $\lim_{\beta\uparrow\infty} \mathbf{P}^{\beta}_{\omega_0}\left[N(t) \leq N^2\right] = 0$, and the claim is proved.

Let $\tau = H_{\Omega_0^N \setminus \{\omega_0\}}$. Using (1.2.5), (1.10.2), the strong Markov property and translation invariance we see that the proposition will be proved if we prove that

$$\lim_{\beta\to\infty} N^2 \mathbf{P}^{\beta}_{\omega_0}\left[\sup_{0\leq s\leq\tau} |\mathcal{C}(\eta(s)) - \mathcal{C}(\omega_0)| > \varepsilon,\ \eta([0,\tau]) \subseteq \Xi^N\right] = 0. \tag{1.10.4}$$

Observe that if $\omega \in \Xi^N_k$ then $|\mathcal{C}(\omega) - \mathcal{C}(\omega_k)| < 1/N_A < \varepsilon/2$, for β large enough. So, if ν denotes the hitting time of $\bigcup_{|k|>N\varepsilon/2} \Xi^N_k$, (1.10.4) will be proved if we prove that

$$\lim_{\beta\to\infty} N^2 \mathbf{P}^{\beta}_{\omega_0}\left[\nu \leq \tau,\ \eta([0,\tau]) \subseteq \Xi^N\right] = 0. \tag{1.10.5}$$

For $k \in \Lambda_N$, let $\mathcal{B}_k = \{\omega \in V(\omega_k) \cap \Xi^N :\ D^*_k(\omega) = \emptyset\}$. Note that

$$\bigcup_{n=0}^{M} \Delta^n_k \setminus \bigcup_{\alpha\in\{A,B,C\}} \mathcal{F}^{N,k}_{\alpha} \subseteq \mathcal{B}_k \subseteq \Xi^N_k$$

and the first inclusion is an equality in the special case of equal densities. The set $\mathcal{B}_k$ is formed by the configurations in Ξ^N from which the process is attracted to ω_k. In the same way we proved Lemma 1.5.6, we see that

$$\mathbf{P}^{\beta}_{\omega}\left[H_{\mathcal{B}^c_k} < H_{\omega_k}\right] \leq C_0 N e^{-\beta}, \quad \text{if } \omega \in \mathcal{B}_k. \tag{1.10.6}$$

Let $\tilde{\nu}$ denote the hitting time of $\bigcup_{0<|k|<N\varepsilon/2} \mathcal{B}_k$. Using the strong Markov property and (1.10.6), we see that $\mathbf{P}^{\beta}_{\omega_0}[\tilde{\nu} \leq \nu \leq \tau] \leq C_0 N e^{-\beta}$ and then, decomposing the event appearing in (1.10.5) in the partition $\{\tilde{\nu} \leq \nu\} \cup \{\nu < \tilde{\nu}\}$, we see that the proof will be completed once we show that

$$\lim_{\beta\to\infty} N^2 \mathbf{P}^{\beta}_{\omega_0}\left[\nu < \tilde{\nu},\ \eta([0,\nu]) \subseteq \Xi^N\right] = 0. \tag{1.10.7}$$

Observing that, for each $k \in \Lambda_N$

$$\Xi^N_k \setminus \bigcup_{j=k-1}^{k+1} \mathcal{B}_j = \bigcup_{\alpha\in\{A,B,C\}} \left(\mathcal{G}^{N,k}_{\alpha} \cup R(\mathcal{G}^{N,k}_{\alpha}) \cup \{\xi^{k+1}_{\alpha,2}, \xi^{k-1}_{N_\alpha-2}\}\right) \cup \bigcup_{\alpha:N_\alpha=M} \{\zeta^k_{\alpha,0}, \zeta^k_{\alpha,N_\alpha}\},$$

we note that the only possible paths from ω_0 to $\bigcup_{|k|>N\varepsilon/2} \Xi^N_k$ contained in Ξ^N that avoid the set $\bigcup_{0<|k|<N\varepsilon/2} \mathcal{B}_k$ are those passing through the intermediate metastates in $\mathcal{G}^N$. Now we will use that, starting from $\mathcal{G}^N$ the trace of $\{\eta(t) : t \geq 0\}$ in Ω^N_1 is well approximated by the ideal process $\{\widehat{\eta}_1(t) : t \geq 0\}$ whose jump probabilities are given in Figure 1.1. A small modification of Lemma 1.6.1 is needed to justify this approximation. To arrive in $\bigcup_{|k|>N\varepsilon/2} \Xi^N_k$ we have to pass first at some configuration in $\bigcup_{|k|=\lfloor N\varepsilon/4\rfloor} \Xi^N_k$. From this point we make the same coupling as in Lemma 1.6.1.

Observe now that from $\bigcup_{|k|=\lfloor N\varepsilon/4\rfloor} \Xi_k^N$ the ideal process must make at least $\delta N^2\varepsilon$ jumps without absorption in Ω_0^N, for some constant δ. This gives the bound

$$\mathbf{P}^\beta_{\omega_0}\left[\nu < \tilde{\nu},\ \eta([0,\nu]) \subseteq \Xi^N\right] \leq \left(\frac{3}{5}\right)^{\delta N^2 \varepsilon} + C_0 N^3 \beta e^{-\beta}.$$

So, (1.10.7) follows by (1.2.9) which imposes that N increases slowly with β. This completes the proof of the proposition. □

Now, Theorem 1.2.2 follows from (1.10.1), Proposition 1.10.1 and Theorem 1.8.1.

1.11 Appendix

Lemma 1.11.1. *For any integers M and $1 \leq i \leq M-1$,*

$$\sum_{j=1}^{i} \binom{M-j-1}{i-j} \left(\frac{1}{2}\right)^{M-j} + \sum_{r=1}^{M-i} \binom{M-r-1}{M-i-r} \left(\frac{1}{2}\right)^{M-r} = 1 \tag{1.11.1}$$

Proof. Fix M. For any $i \in \{1, \dots, M-1\}$ define

$$\phi(i) = \sum_{j=1}^{i} \binom{M-j-1}{i-j} 2^{j-1}.$$

Multiplying (1.11.1) by 2^{M-1}, the equality to be proved becomes

$$\phi(i) + \phi(M-i) = 2^{M-1}.$$

We claim that, for any $1 \leq i \leq M-1$, $\phi(i)$ counts the number of subsets of $\{1, \dots, M-1\}$ with at most $i-1$ elements, which implies the above equality. The proof of this claim relies on a suitable way of classifying the elements of

$$\binom{[M-1]}{\leq i-1} := \{E \subseteq \{1, \dots, M-1\} : |E| \leq i-1\}.$$

We first observe that for any $E \in \binom{[M-1]}{\leq i-1}$ there exists $1 \leq k_0 \leq i$ such that

$$|E \cap \{k_0, \dots, M-1\}| = i - k_0.$$

To see this, note that if we define h on $\{1, \dots, i\}$ as $h(k) = i-k-|E\cap\{k, \dots, M-1\}|$, then $h(k+1) \in \{h(k), h(k)-1\}$, $h(1) \geq 0$, $h(i) \leq 0$. So, there must exist some $k_0 \in \{1, \dots, i\}$ such that $h(k_0) = 0$. Therefore, we may decompose

$$\binom{[M-1]}{\leq i-1} = \bigcup_{j=1}^{i} \mathcal{D}_j^i \tag{1.11.2}$$

into a disjoint union, where

$$\mathcal{D}_j^i := \left\{ E \in \binom{[M-1]}{\leq i-1} : j = \max\{1 \leq k \leq i : |E \cap \{k, \dots, M-1\}| = i-k\} \right\}.$$

Now note that if $E \in \mathcal{D}_j^i$ then $j \notin E$. Another simple argument, using again the function h defined above, shows that, in fact,

$$\mathcal{D}_j^i = \{E \subseteq \{1, \dots, M-1\} : j \notin E,\ |E \cap \{j+1, \dots, M-1\}| = i-j\}\},$$

and so, $|\mathcal{D}_j^i| = \binom{M-j-1}{i-j} 2^{j-1}$. As the union in (1.11.2) is disjoint, summing in j, from 1 to i, we get that $\phi(i)$ is the cardinality of $\binom{[M-1]}{\leq i-1}$, as claimed. □

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CHAPTER 2

Metastability of reversible random walks in potential fields

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ABSTRACT. Let Ξ be an open and bounded subset of $\mathbb{R}^d$ and let $F : \Xi \to \mathbb{R}$ be a twice continuously differential function. Denote by Ξ_N the discretization of Ξ, $\Xi_N = \Xi \cap (N^{-1}\mathbb{Z}^d)$, and denote by $\{X_N(t) : t \geq 0\}$ the continuous-time, nearest-neighbor, random walk on Ξ_N which jumps from $\boldsymbol{x}$ to $\boldsymbol{y}$ at rate $e^{-(1/2)N[F(\boldsymbol{y})-F(\boldsymbol{x})]}$. We examine in this article the metastable behavior of $\{X_N(t) : t \geq 0\}$ among the wells of the potential F.

2.1 Introduction

We introduced recently in [3, 6] an approach to prove the metastable behavior of Markov chains which has been successfully applied in several different contexts. We refer to [7, 33] for a description of the method and for examples of Markov chains whose metastable behavior has been established with this approach.

We examine in this article the metastable behavior of reversible random walks in force fields. This is an old problem whose origin can be traced back at least to Kramers [32]. It has been adressed by Freidlin and Wentsell [28] and by Galves, Olivieri and Vares [29] in the context of small random perturbations of dynamical systems, and, more recently, by Bovier, Eckhoff, Gayrard and Klein in a series of papers [15, 16, 17, 18] through the potential theoretic approach. This problem has raised interest and has found applications in many areas, as computer sciences [20] and chemical physics [38].

The first main result of this article, Theorem 2.2.4, states that starting from a neighborhood of a local minimum of the force field, in an appropriate time-scale, the evolution of the random walk can be described by a reversible Markov chain in a finite graph, in which the vertices represent the wells of the force field and the edges the saddle points.

More precisely, denote by $X_N(t)$ a reversible random walk evolving in a discretization of a bounded domain $\Xi \subset \mathbb{R}^d$ according to a force field $F : \Xi \to \mathbb{R}$. A precise definition of the dynamics is given below in (2.2.1). Let $\boldsymbol{x}_1, \dots, \boldsymbol{x}_L$ be the local minima of the field F, and let $Y_N(t)$ be the process which records the minima visited: $Y_N(t)$ is equal to j if the chain $X_N(t)$ belongs to a neighborhood of $\boldsymbol{x}_j$, $1 \le j \le L$, and 0 otherwise. Clearly, $Y_N(t)$ is not Markovian. Theorem 2.2.4 asserts that starting from a neighborhood of a local minimum $\boldsymbol{x}_j$, there exists a time scale β_N, which depends on j, in which $Y_N(t\beta_N)$ converges in some topology to a Markovian dynamics whose state space is a subset of $\{1, \dots, L\}$. This asymptotic dynamics may have absorbing points, and its jump rates depend solely on the behavior of the potential in the neighborhoods of the local minima and in the neighborhoods of the saddle points. Theorem 2.2.4 is similar in spirit to the one of Noé, Wu, Prinz and Plattner [38], who proved that projected metastable Markovian dynamics can be well approximated by hidden Markovian dynamics.

The second main result, Theorem 2.2.7, adresses the problem of the exit points from a domain. Consider a local minimum $\boldsymbol{x}_j$ of the force field and denote by $\{\boldsymbol{z}_1, \dots, \boldsymbol{z}_K\}$ the lowest saddle points of F which separate $\boldsymbol{x}_j$ from the other local minima. Theorem 2.2.7 provides the asymptotic probabilities that the chain $X_N(t)$ will traverse a mesoscopic neighborhood of a saddle point $\boldsymbol{z}_i$ before hitting another local minima of the force field.

We explained already in [7] the main differences between our approach and the potential theoretic one [15, 16], and between our approach and the pathwise one due to Cassandro, Galves, Olivieri and Vares [21]. We will not repeat this exposition here. Our approach does not aim to characterize the typical paths in a transition between two metastable states, in contrast with the transition path theory [25]. Nevertheless, in the case where the number of wells is small, as in the examples presented in [36], Theorems 2.2.4 and 2.2.7 describe the distribution of the transition paths, at least at the scale of the metastable sets, by indicating the sequence of metastable sets visited in a transition between two metastable sets.

In the case of complex networks, the Lennard–Jones clusters analyzed in [20] for instance, to give a rough view of the transition paths from two metastable states, we may proceed in two ways. One possibility is to reduce the number of nodes by considering the trace of the original chain on a subset of the state space (cf. [3, Section 6.1] for the definition of trace processes). Avena and Gaudillière [1] proposed a natural algorithm to reduce the number of vertices of a chain. The algorithm produces a subset V with the property that the mean hitting time of V does not depend on the starting point. In this sense the vertices of V are "uniformly" distributed among the set of nodes. The algorithm can also be callibrated to provide a large or small set of nodes V.

Another possibility is to identify certain nodes, losing the Markov property, and to apply Theorem 2.2.4 below to approximate this new dynamics by a Markovian dynamics. To describe the transition paths at this level of accuracy, one can compute for these reduced dynamics the equilibrium potential between two metastable sets (the committor in the terminology of [20]), and the optimal flow for Thomson's principle (the probability current of reactive trajectories).

In both cases, the selection of the set of nodes or the selection of nodes to be merged have to be carried out judiciously, to reduce as much as possible the number of nodes without losing the essential features of the original chain. From a computational point of view, the jump rates of trace process are easily calculated, while the jump rates of projected processes are more difficult to derive. In the first case, it suffices to apply recursively the first displayed equation below the proof of Corollary 6.2 in [3], while in the second case, one has to calculate the capacities between the metastable sets.

2.2 Notation and Results

Let Ξ be an open and bounded subset of $\mathbb{R}^d$, and denote by $\partial\,\Xi$ its boundary, which is assumed to be a smooth manifold. Fix a twice continuously differentiable function $F : \Xi \cup \partial\,\Xi \to \mathbb{R}$, with a finite number of critical points, satisfying the following assumptions:

(H1) The second partial derivatives of F are Lipschitz continuous. Denote by C_1 the Lipschitz constant;

(H2) All the eigenvalues of the Hessian of F at the critical points which are local minima are *strictly* positive.

(H3) The Hessian of F at the critical points which are not local minima or local maxima has one strictly negative eigenvalue, all the other ones being strictly positive.

(H4) For every $\boldsymbol{x} \in \partial\,\Xi$, $(\nabla F)(\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) < 0$, where $\boldsymbol{n}(\boldsymbol{x})$ represents the exterior normal to the boundary of Ξ, and $\boldsymbol{x} \cdot \boldsymbol{y}$ the scalar product of $\boldsymbol{x}\ \boldsymbol{y} \in \mathbb{R}^d$.

Denote by Ξ_N the discretization of Ξ: $\Xi_N = \Xi \cap (N^{-1}\mathbb{Z}^d)$, $N \geq 1$, where $N^{-1}\mathbb{Z}^d = \{\boldsymbol{k}/N : \boldsymbol{k} \in \mathbb{Z}^d\}$. The elements of Ξ_N are represented by the symbols

$\boldsymbol{x} = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_d)$, $\boldsymbol{y}$ and $\boldsymbol{z}$. Let μ_N be the probability measure on Ξ_N defined by

$$\mu_N(\boldsymbol{x}) \;=\; \frac{1}{Z_N} e^{-NF(\boldsymbol{x})} \;, \quad \boldsymbol{x} \in \Xi_N \;,$$

where Z_N is the partition function $Z_N = \sum_{\boldsymbol{x}\in\Xi_N} \exp\{-NF(\boldsymbol{x})\}$. Let $\{X_N(t) : t \geq 0\}$ be the continuous-time Markov chain on Ξ_N whose generator L_N is given by

$$(L_N f)(\boldsymbol{x}) \;=\; \sum_{\substack{\boldsymbol{y}\in\Xi_N \\ \|\boldsymbol{y}-\boldsymbol{x}\|=1/N}} e^{-(1/2)N[F(\boldsymbol{y})-F(\boldsymbol{x})]} \, [f(\boldsymbol{y}) - f(\boldsymbol{x})] \;, \tag{2.2.1}$$

where $\|\cdot\|$ represents the Euclidean norm of $\mathbb{R}^d$. The rates were chosen for the measure μ_N to be reversible for the dynamics. Denote by $R_N(\boldsymbol{x}, \boldsymbol{y})$, $\lambda_N(\boldsymbol{x})$, $\boldsymbol{x}$, $\boldsymbol{y} \in \Xi_N$, the jump rates, holding rates of the chain $X_N(t)$, respectively:

$$R_N(\boldsymbol{x}, \boldsymbol{y}) \;=\; \begin{cases} e^{-(1/2)N[F(\boldsymbol{y})-F(\boldsymbol{x})]} & \|\boldsymbol{y}-\boldsymbol{x}\| = 1/N \;,\; \boldsymbol{x} \;,\; \boldsymbol{y} \in \Xi_N \;, \\ 0 & \text{otherwise} \;. \end{cases}$$

$$\lambda_N(\boldsymbol{x}) \;=\; \sum_{\substack{\boldsymbol{y}\in\Xi_N \\ \|\boldsymbol{y}-\boldsymbol{x}\|=1/N}} R_N(\boldsymbol{x}, \boldsymbol{y}) \;.$$

Denote by $D(\mathbb{R}_+, \Xi_N)$ the space of right-continuous trajectories $f : \mathbb{R}_+ \to \Xi_N$ with left-limits, endowed with the Skorohod topology. Let $\mathbf{P}_{\boldsymbol{x}} = \mathbf{P}^N_{\boldsymbol{x}}$, $\boldsymbol{x} \in \Xi_N$, be the measure on $D(\mathbb{R}_+, \Xi_N)$ induced by the chain $X_N(t)$ starting from $\boldsymbol{x}$. Expectation with respect to $\mathbf{P}_{\boldsymbol{x}}$ is denoted by $\mathbf{E}_{\boldsymbol{x}}$.

For a subset A of Ξ_N, denote by H_A (resp. H_A^+) the hitting time of (resp. return time to) the set A:

$$\begin{aligned} H_A \;&:=\; \inf\{t > 0 : X_N(t) \in A\} \;, \\ H_A^+ \;&:=\; \inf\{t > 0 : X_N(t) \in A \,,\; X_N(s) \neq X_N(0) \;\text{ for some } 0 < s < t\} \,. \end{aligned}$$

The capacity between two disjoint sets A, B of Ξ_N, denoted by $\text{cap}_N(A, B)$, is given by

$$\text{cap}_N(A, B) \;=\; \sum_{\boldsymbol{x}\in A} \mu_N(\boldsymbol{x}) \, \lambda_N(\boldsymbol{x}) \, \mathbf{P}_{\boldsymbol{x}}\big[H_B < H_A^+\big] \;.$$

A. The wells and their capacities. Denote by $\mathfrak{M}$ the set of local minima and by $\mathfrak{S}$ the set of saddle points of F in Ξ. Let $\mathfrak{S}_1$ be the set of the lowest saddle points:

$$\mathfrak{S}_1 \;=\; \Big\{\boldsymbol{z} \in \mathfrak{S} : F(\boldsymbol{z}) = \min\{F(\boldsymbol{y}) : \boldsymbol{y} \in \mathfrak{S}\}\Big\} \;.$$

We represent by $\boldsymbol{z}^{1,1}, \dots, \boldsymbol{z}^{1,n_1}$ the elements of $\mathfrak{S}_1$, $\mathfrak{S}_1 = \{\boldsymbol{z}^{1,1}, \dots, \boldsymbol{z}^{1,n_1}\}$. Starting from $\mathfrak{S}_1$, we define inductively a finite sequence of disjoint subsets of $\mathfrak{S}$. Assume that $\mathfrak{S}_1, \dots, \mathfrak{S}_i$ have been defined, let $\mathfrak{S}_i^+ = \mathfrak{S}_1 \cup \dots \cup \mathfrak{S}_i$, and let

$$\mathfrak{S}_{i+1} \;=\; \Big\{\boldsymbol{z} \in \mathfrak{S} : F(\boldsymbol{z}) = \min\{F(\boldsymbol{y}) : \boldsymbol{y} \in \mathfrak{S} \setminus \mathfrak{S}_i^+\}\Big\} \;.$$

We denote by $\boldsymbol{z}^{i,j}$, $1 \le j \le n_i$ the elements of $\mathfrak{S}_i$. We obtain in this way a partition $\{\mathfrak{S}_i : 1 \le i \le i_0\}$ of $\mathfrak{S}$.

We will refer to the index i as the level of a saddle point. Denote by H_i the height of the saddle points in $\mathfrak{S}_i$:

$$H_i \;=\; F(\boldsymbol{z}^{i,1})\,, \quad 1 \le i \le i_0\,,$$

so that $H_1 < H_2 < \cdots < H_{i_0}$.

For each $1 \le i \le i_0$, let $\widehat{\Omega}^i$ be the subset of Ξ defined by

$$\widehat{\Omega}^i \;=\; \big\{\boldsymbol{x} \in \Xi : F(\boldsymbol{x}) \le F(\boldsymbol{z}^{i,1})\big\}\,.$$

By definition, $\widehat{\Omega}^i \subset \widehat{\Omega}^{i+1}$. The set $\widehat{\Omega}^i$ can be written as a disjoint union of connected components: $\widehat{\Omega}^i = \cup_{1\le j\le \varkappa_i} \widehat{\Omega}^i_j$, where $\widehat{\Omega}^i_j \cap \widehat{\Omega}^i_k = \varnothing$, $j \ne k$, and where each set $\widehat{\Omega}^i_j$ is connected. Some connected component may not contain any saddle point in $\mathfrak{S}_i$, and some may contain more than one saddle point. Denote by Ω^i_j, $1 \le j \le \ell_i$, the connected components $\widehat{\Omega}^i_{j'}$ which contain a point in $\mathfrak{S}_i$, and let $\Omega^i = \cup_{1\le j\le \ell_i} \Omega^i_j$. Clearly, the number of components Ω^i_j is smaller than the number of elements of $\mathfrak{S}_i$, $\ell_i \le n_i$.

Each component Ω^i_j is a union of wells, $\Omega^i_j = W^i_{j,1} \cup \cdots \cup W^i_{j,\ell^i_j}$. The sets $W^i_{j,a}$ are defined as follows. Let $\mathring{\Omega}^i_j$ be the interior of Ω^i_j. Each set $W^i_{j,a}$ is the closure of a connected component of $\mathring{\Omega}^i_j$. The intersection of two wells is a subset of the set of saddle points: $W^i_{j,a} \cap W^i_{j,b} \subset \mathfrak{S}_i$. Figure 2.1 illustrates the wells of two connected components of some level. The sets W^ϵ_a are introduced just before (2.2.2).

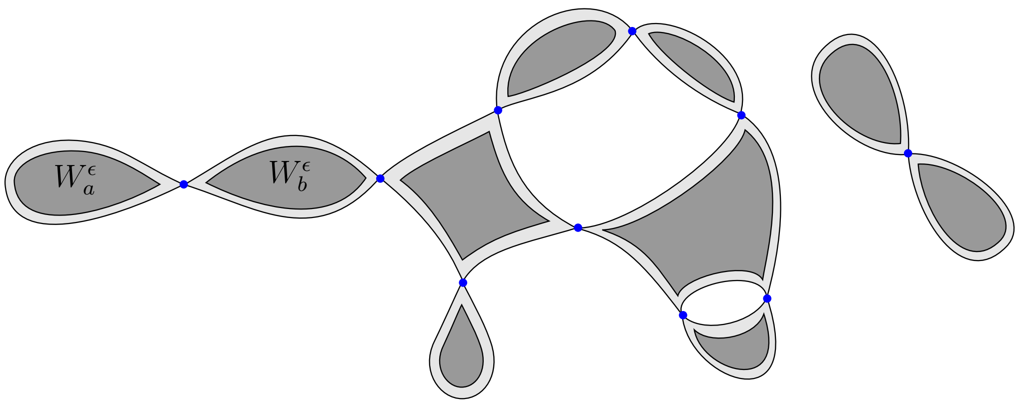

Figure 2.1: Some wells which form two connected components Ω^i_1 and Ω^i_2.

Fix $1 \le i \le i_0$ and $1 \le j \le \ell_i$ and a connected component $\Omega = \Omega^i_j$. To avoid heavy notation, unless when strictly required, we omit from now on the dependence of the sets $\mathfrak{S}_i$, $W^i_{j,a}$ and the numbers ℓ^i_j on the indices i and j which are fixed.

Let $S = \{1, \dots, \ell\}$ denote the set of the indices of the wells forming the connected component Ω. For $a \ne b \in S$, denote by $\mathfrak{S}_{a,b}$ the set of saddle points separating W_a

from W_b,

$$\mathfrak{S}_{a,b} \;=\; \big\{ \boldsymbol{z} \in \mathfrak{S} : \boldsymbol{z} \in W_a \cap W_b \big\}\;,$$

and denote by $\mathfrak{S}(A)$, $A \subset S$, the set of saddle points separating $\cup_{a\in A} W_a$ from $\cup_{a\in A^c} W_a$:

$$\mathfrak{S}(A) \;=\; \bigcup_{a\in A\,,\, b\in A^c} \mathfrak{S}_{a,b}\;.$$

For a saddle point $\boldsymbol{z} \in \mathfrak{S}$, denote by $-\mu(\boldsymbol{z})$ the unique negative eigenvalue of the Hessian of F at $\boldsymbol{z}$.

Recall that $F(\boldsymbol{z}) = H_i$, $\boldsymbol{z} \in \mathfrak{S} = \mathfrak{S}_i$. For $0 < \epsilon < H_i - H_{i-1}$, $1 \le a \le \ell$, let $W_a^\epsilon = \{\boldsymbol{x} \in W_a : F(\boldsymbol{x}) < H_i - \epsilon\}$, and let

$$\mathcal{E}_N^a \;=\; W_a^\epsilon \cap \Xi_N\;,\;\; 1 \le a \le \ell\,, \quad \mathcal{E}_N(A) = \bigcup_{a\in A} \mathcal{E}_N^a\;,\;\; A \subset S\;. \tag{2.2.2}$$

Each well $W_{j,a}^1$ contains exactly one local minimum of F, while the wells $W_{j,a}^i$, $1 < i \le i_0$, may contain more than one local minimum. Denote by $\{\boldsymbol{m}_{a,1}, \dots, \boldsymbol{m}_{a,q}\}$, $q = q_a$, the deepest local minima of F which belong to $W_{j,a}^i$:

$$\{\boldsymbol{m}_{a,1}, \dots, \boldsymbol{m}_{a,q}\} \;=\; \Big\{ \boldsymbol{y} \in W_a \cap \mathfrak{M} : F(\boldsymbol{y}) = \min\{F(\boldsymbol{y}') : \boldsymbol{y}' \in W_a \cap \mathfrak{M}\} \Big\}\;.$$

Let $h_a = F(\boldsymbol{m}_{a,1})$ and let

$$\boldsymbol{\mu}(a) \;=\; \sum_{k=1}^{q_a} \frac{1}{\sqrt{\det \mathrm{Hess}\, F(\boldsymbol{m}_{a,k})}}\;,\;\; a \in S\;,$$

where $\mathrm{Hess}\, F(\boldsymbol{x})$ represents the Hessian of F calculated at $\boldsymbol{x}$, and $\det \mathrm{Hess}\, F(\boldsymbol{x})$ its determinant. A calculation, presented in (2.6.5), shows that for each $a \in S$,

$$\mu_N(\mathcal{E}_N^a) \;=\; [1 + o_N(1)]\, \frac{(2\pi N)^{d/2}}{Z_N}\, e^{-N h_a}\, \boldsymbol{\mu}(a)\;. \tag{2.2.3}$$

The next result and Theorem 2.2.2 below are discrete versions of a result of Bovier, Eckhoff, Gayrard and Klein [17]. The proofs are based on the proof of Theorem 3.1 in [17] and on [10, 11].

Theorem 2.2.1. *For every proper subset A of S,*

$$\lim_{N\to\infty} \frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{N H_i}\, \mathrm{cap}_N(\mathcal{E}_N(A), \mathcal{E}_N(A^c)) \;=\; \sum_{\boldsymbol{z}\in\mathfrak{S}(A)} \frac{\mu(\boldsymbol{z})}{\sqrt{-\det \mathrm{Hess}\, F(\boldsymbol{z})}}\;.$$

This result together with two other estimates permit to prove the metastable behavior of the Markov chain $X_N(t)$ among the shallowest valleys $\mathcal{E}_N^a$. To examine the metastable behavior of the chain $X_N(t)$ on deeper wells we need to extend

Theorem 2.2.1 to disjoint sets A, B which do not form a partition of S, $A \cup B \neq S$. The statement of this extension and its proof requires the introduction of a graph.

B. A Graph associated to the chain. Let $\mathbb{G} = (S, E)$ be the weighted graph whose vertices are $S = \{1, \dots, \ell\}$, the indices of the sets W_a. Place an edge between a and $b \in S$ if and only if there exists a saddle point $\boldsymbol{z}$ belonging to $W_a \cap W_b$, i.e., if $\mathfrak{S}_{a,b} \neq \varnothing$. The weight of the edge between a and b, denoted by $\boldsymbol{c}(a, b)$, is set to be

$$\boldsymbol{c}(a,b) \;=\; \sum_{\boldsymbol{z}\in\mathfrak{S}_{a,b}} \frac{\mu(\boldsymbol{z})}{\sqrt{-\det \operatorname{Hess} F(\boldsymbol{z})}}\;. \tag{2.2.4}$$

Note that $\boldsymbol{c}(a, b)$ vanishes if there is no saddle point $\boldsymbol{z}$ belonging to $W_a \cap W_b$ and that the weights are independent of N. Figure 2.2 present the weighted graph associated to one of the connected component of Figure 2.1.

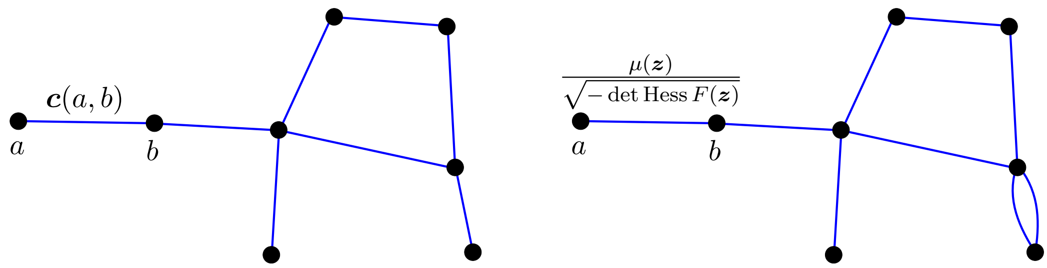

Figure 2.2: The simple weighted graph and the graph with multiple edges associated to one of the connected components of Figure 2.1.

The graph $\mathbb{G}$ has to be interpreted as an electrical network, where the weights $\boldsymbol{c}(a, b)$ represent the conductances. It would be more natural to start with a graph with multiple edges, each edge corresponding to a saddle point $\boldsymbol{z}$. However, adding the parallel conductances one can reduce the graph with multiple edges to the above graph.

Let

$$c_N(a,b) \;=\; \frac{(2\pi N)^{d/2}}{Z_N}\,\frac{e^{-NH_i}}{2\pi N}\,\boldsymbol{c}(a,b)\;,\quad a\;,\; b\in S\;.$$

It follows from Theorem 2.2.1 and from a calculation that

$$c_N(a,b) \;=\; [1+o_N(1)]\,\frac{1}{2}\Big\{\operatorname{cap}_N(\mathcal{E}^a_N,\breve{\mathcal{E}}^a_N) \;+\; \operatorname{cap}_N(\mathcal{E}^b_N,\breve{\mathcal{E}}^b_N) \;-\; \operatorname{cap}_N\big(\mathcal{E}^a_N\cup\mathcal{E}^b_N,\cup_{c\neq a,b}\mathcal{E}^c_N\big)\Big\}\;, \tag{2.2.5}$$

where, $\breve{\mathcal{E}}^a_N = \cup_{c\neq a}\mathcal{E}^c_N$. This explains the definition of $c_N(a, b)$. Moreover, by [3, Lemma 6.8], $c_N(a, b)$ is equal to $\mu_N(\mathcal{E}^a_N) r_N(\mathcal{E}^a_N, \mathcal{E}^b_N)$, where $r_N = r^1_N$ represents the average rates introduced below in (2.6.1).

For two disjoint subsets A, B of S, denote by $\mathrm{cap}_{\mathbb{G}}(A,B)$ the *conductance* between A and B. To define the conductance, denote by $\{Y_k : k \ge 0\}$ the discrete-time random walk on S which jumps from a to b with probability

$$p(a,b) \;=\; \frac{\boldsymbol{c}(a,b)}{\sum_{b'\in S}\boldsymbol{c}(a,b')} \,. \tag{2.2.6}$$

Denote by $\mathbb{P}^Y_a$, $a\in S$, the distribution of the chain Y_k starting from a and by $V_{A,B}$, A, $B\subset S$, $A\cap B=\varnothing$, the equilibrium potential between A and B:

$$V_{A,B}(b) \;=\; \mathbb{P}^Y_b\big[H_A < H_B\big]\;,\quad b\in S\;,$$

where H_C, $C\subset S$, represents the hitting time of C: $H_C=\min\{k\ge 0 : Y_k\in C\}$. The conductance between A and B is defined as

$$\mathrm{cap}_{\mathbb{G}}(A,B) \;=\; \frac{1}{2}\sum_{a,b\in S}\boldsymbol{c}(a,b)\big[V_{A,B}(b)-V_{A,B}(a)\big]^2\,.$$

By [30, Proposition 3.1.2] the conductance between A and B coincides with the capacity between A and B. The next result establishes that the capacities for the chain $X_N(t)$ can be computed from the conductances on the finite graph $\mathbb{G}$.

Theorem 2.2.2. *For every disjoint subsets A, B of S,*

$$\mathrm{cap}_N(\mathcal{E}_N(A),\mathcal{E}_N(B)) \;=\; [1+o_N(1)]\,\frac{(2\pi N)^{d/2}}{Z_N}\,\frac{e^{-NH_i}}{2\pi N}\,\mathrm{cap}_{\mathbb{G}}(A,B)\;.$$

Remark 2.2.3. *It follows from the proofs of Theorems 2.2.1 and 2.2.2 that both statements remain in force if we replace the sets $\mathcal{E}^a_N$ by singletons $\{\boldsymbol{x}^a_N\}$, where $\boldsymbol{x}^a_N\in\mathcal{E}^a_N$. In this case the sets $\mathcal{E}_N(A)$ become $\{\boldsymbol{x}^a_N : a\in A\}$.*

C. Metastability. The Markov chain $X_N(t)$ exhibits a metastable behavior among the wells of each connected component Ω^i_j. The description of this behavior requires some further notation.

Recall that $h_a = F(\boldsymbol{m}_{a,1})$ represents the value of F at a deepest minima of the well W_a. Let $\hat\theta_a = H_i - h_a > 0$, $a\in S$, be the depth of the well W_a. The depths $\hat\theta_a$ provide the time-scale at which a metastable behavior is observed. Let $\theta_1<\theta_2<\cdots<\theta_n$, $n\le\ell$, be the increasing enumeration of the sequence $\hat\theta_a$, $1\le a\le\ell$:

$$\{\hat\theta_1,\dots,\hat\theta_\ell\} \;=\; \{\theta_1,\dots,\theta_n\}\;.$$

Of course, n and θ_m depend on the component Ω^i_j. If we need to stress this dependence, we will denote n, θ_m by $n_{i,j}$, $\theta^{i,j}_m$, respectively.

The chain exhibits a metastable behavior on n different time scales in the set Ω. Let $T_m=\{a\in S : \hat\theta_a=\theta_m\}$, $1\le m\le n$, so that $T_1,\dots,T_n$ forms a partition of S, and let

$$S_m \;=\; T_m\cup\cdots\cup T_n\;,\quad 1\le m\le n\;.$$

Define the projection $\Psi_N^m : \Xi_N \to S_m \cup \{N\}$, $1 \le m \le n$, as

$$\Psi_N^m(\boldsymbol{x}) \;=\; \sum_{a\in S_m} a\, \mathbf{1}\{\boldsymbol{x} \in \mathcal{E}_N^a\} \;+\; N\, \mathbf{1}\Big\{\boldsymbol{x} \notin \bigcup_{a\in S_m} \mathcal{E}_N^a\Big\}\,. \tag{2.2.7}$$

Denote by $\boldsymbol{X}_N^m(t)$ the projection of the Markov chain $X_N(t)$ by Ψ_N^m:

$$\boldsymbol{X}_N^m(t) \;=\; \Psi_N^m(X_N(t))\,.$$

Fix $1 \le m \le n$. We introduce some notation to define the asymptotic dynamics of the process $\boldsymbol{X}_N^m(t)$. The time scale in which the process $\boldsymbol{X}_N^m$ evolves, denoted by $\beta_m = \beta_m(N)$, is given by

$$\beta_m \;=\; 2\pi N\, e^{\theta_m N}\,.$$

For a, b in S_m, let

$$\boldsymbol{c}_m(a,b) \;=\; \frac{1}{2}\Big\{\mathrm{cap}_{\mathbb{G}}(\{a\}, S_m\backslash\{a\}) + \mathrm{cap}_{\mathbb{G}}(\{b\}, S_m\backslash\{b\}) - \mathrm{cap}_{\mathbb{G}}(\{a,b\}, S_m\backslash\{a,b\})\Big\}\,. \tag{2.2.8}$$

Note that $\boldsymbol{c}_m(a,b)$ represents the conductance between a and b for the electrical circuit obtained from $\mathbb{G}$ by removing the vertices in S_m^c. In particular, $\boldsymbol{c}_1(a,b) = \boldsymbol{c}(a,b)$ for a, $b \in S_m$. Let

$$\boldsymbol{r}_m(a,b) \;=\; \begin{cases} \boldsymbol{c}_m(a,b)/\boldsymbol{\mu}(a) & a \in T_m\,,\ b \in S_m\,, \\ 0 & a \in S_{m+1}\,,\ b \in S_m\,. \end{cases} \tag{2.2.9}$$

Recall from [33] the definition of the soft topology.

Theorem 2.2.4. *Fix $1 \le i \le i_0$, $1 \le j \le \ell_i$, $1 \le m \le n_{i,j}$, $a \in S_m$ and a sequence of configurations $\boldsymbol{x}_N$ in $\mathcal{E}_N^a$. Under $\mathbf{P}_{\boldsymbol{x}_N}$, the time re-scaled projection $\mathbb{X}_N^m(t) = \boldsymbol{X}_N^m(t\beta_m)$ converges in the soft topology to a S_m-valued continuous-time Markov chain $\mathbb{X}^m(t)$ whose jump rates are given by* (2.2.9)*. In particular, the points in S_{m+1} are absorbing for the chain $\mathbb{X}^m(t)$.*

Remark 2.2.5. *Theorem 2.2.4 states that the weighted graph $\mathbb{G}$, the measure $\boldsymbol{\mu}$ and the sequence $\beta_m(N)$ describe the evolution of the chain $X_N(t)$ in the connected component Ω. The weighted graph with multiple edges would describe more accurately the chain $X_N(t)$, providing the probability that the chain leaves a well W_a through a mesoscopic neighborhood of a saddle point $\boldsymbol{z} \in \mathfrak{S}$. This statement is made precise in Theorem 2.2.7 below.*

Remark 2.2.6. *Nothing prevent two time-scales at different levels to be equal, or two time scales in different connected components of the same level to be equal. It is possible that $\theta_m^{i,j} = \theta_{m'}^{i',j'}$ for some $i \neq i'$ or that $\theta_m^{i,j} = \theta_{m'}^{i,j'}$ for some $j \neq j'$.*

D. Exit points from a well. Fix $1 \le i \le i_0$, $1 \le j \le \ell_i$, and recall that we denote by $W_a = W^i_{j,a}$, $a \in S = \{1, \dots, \ell^i_j\}$, the wells which form the connected component Ω^i_j. The last result of this article states that the chain $X_N(t)$ leaves the set W_a through a neighborhood of a saddle point $\boldsymbol{z}$ in the boundary of W_a with probability $\omega(\boldsymbol{z})/\sum_{\boldsymbol{z}'} \omega(\boldsymbol{z}')$, where the summation is carried over all saddle points in the boundary of W_a and where

$$\omega(\boldsymbol{z}) \;=\; \frac{\mu(\boldsymbol{z})}{\sqrt{-\det \operatorname{Hess} F(\boldsymbol{z})}} \,\cdot \tag{2.2.10}$$

Let δ_N be a sequence such that $\delta_N \ll N^{-3/4}$, $N^{d+1} \exp\{-N\delta_N\} \to 0$. Denote by $\Omega_N = \Omega^i_{j,N}$ the connected component of the set $\{\boldsymbol{x} \in \Xi : F(\boldsymbol{x}) \le H_i + \delta_N\}$ which contains Ω^i_j. Since $\delta_N \downarrow 0$, for N large enough, $\Omega^i_{j,N} \cap \Omega^i_{j',N} = \varnothing$ for all $j' \ne j$. In particular, for N large enough there is a one-to-one correspondance between Ω^i_j and $\Omega^i_{j,N}$.

Fix $a \in S$ and let $\mathfrak{S}_a$ be the set of saddle points in the boundary of W_a, $\mathfrak{S}_a = \cup_{b \in S, b \ne a} \mathfrak{S}_{a,b}$. Denote by $\partial\Omega_N$ the boundary of Ω_N and by $B_\epsilon(\boldsymbol{x})$ the open ball of radius $\epsilon > 0$ around $\boldsymbol{x} \in \Xi$. We modify the set $\partial\Omega_N$ around each saddle point $\boldsymbol{z} \in \mathfrak{S}_a$ to obtain a closed manifold $D_a \subset \Omega_N$.

Fix a saddle point $\boldsymbol{z} \in \mathfrak{S}_a$ and recall condition (H3) on F. Denote by $-\mu < 0 < \lambda_2 \le \cdots \le \lambda_d$ the eigenvalues of Hess $F(\boldsymbol{z})$, and by $\boldsymbol{v}$, $\boldsymbol{w}^i$, $2 \le i \le d$, an associated orthonormal basis of eigenvectors. Let $\mathbb{H} = \mathbb{H}_{\boldsymbol{z}}$ be the $(d-1)$-dimensional hyperplane generated by the vectors $\boldsymbol{w}^i$, $2 \le i \le d$. By a Taylor expansion, there exists $\epsilon > 0$ such that

$$F(\boldsymbol{x}) \;\ge\; H_i \;+\; \frac{\lambda_2}{4}\, \|\boldsymbol{x} - \boldsymbol{z}\|^2 \tag{2.2.11}$$

for $\boldsymbol{x} \in \boldsymbol{z} + \mathbb{H} = \{\boldsymbol{z} + \boldsymbol{y} : \boldsymbol{y} \in \mathbb{H}\}$ such that $\|\boldsymbol{x} - \boldsymbol{z}\| \le \epsilon$. Let

$$D_{\boldsymbol{z}} \;=\; \big\{\boldsymbol{y} \in (\boldsymbol{z} + \mathbb{H}) \cap B_\epsilon(\boldsymbol{z}) : F(\boldsymbol{y}) \le H_i + \delta_N\big\}\,. \tag{2.2.12}$$

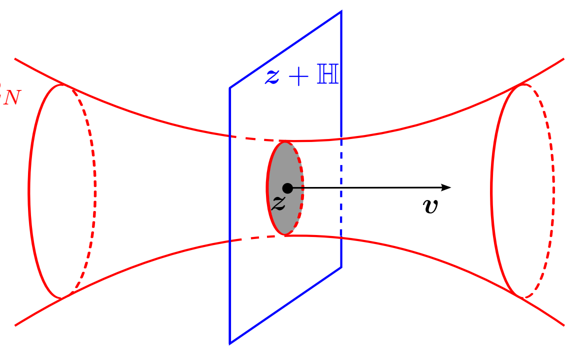

Figure 2.3: In gray the set $D_{\boldsymbol{z}}$.

We intersected the set $\boldsymbol{z} + \mathbb{H}$ with the set $B_\epsilon(\boldsymbol{z})$ to avoid including in $D_{\boldsymbol{z}}$ points which are far from $\boldsymbol{z}$.

The set $D_a = D_a^N$ is defined as follows. For each $\boldsymbol{z} \in \mathfrak{S}_a$, remove from $\partial\Omega_N$ the set $(\boldsymbol{z} + \mathbb{H}) \cap \partial\Omega_N \cap B_\epsilon(\boldsymbol{z})$. As before, the set $B_\epsilon(\boldsymbol{z})$ has been introduced to avoid removing from $\partial\Omega_N$ points which are far from $\boldsymbol{z}$. Denote by Ω_N^1 the set obtained after this operation, which is a finite union of connected sets. Remove from Ω_N^1 all connected component which contain a point close to some saddle point which does not belong to $\mathfrak{S}_a$. Denote this new set by Ω_N^2. D_a is the union of Ω_N^2 with all set $D_{\boldsymbol{z}}$, $\boldsymbol{z} \in \mathfrak{S}_a$:

$$D_a \;=\; \bigcup_{\boldsymbol{z}\in\mathfrak{S}_a} D_{\boldsymbol{z}} \;\cup\; \Omega_N^2\;.$$

Denote by $\mathcal{D}_a$, $\mathcal{D}_{\boldsymbol{z}} \subset \Xi_N$ the discretizations of the sets D_a and $D_{\boldsymbol{z}}$, that is $\mathcal{D}_a = \{\boldsymbol{x} \in \Xi_N : d(\boldsymbol{x}, D_a) \le 1/N\}$, where d stands for the Euclidean distance, $d(\boldsymbol{x}, A) = \inf_{\boldsymbol{y}\in A} \|\boldsymbol{x} - \boldsymbol{y}\|$.

Theorem 2.2.7. *Fix $1 \le i \le i_0$, $1 \le j \le \ell_i$, and $a \in S = \{1, \dots \ell_j^i\}$. Let . For all $\boldsymbol{z} \in \mathfrak{S}_a$, and all sequences $\{\boldsymbol{x}_N : N \ge 1\}$, $\boldsymbol{x}_N \in \mathcal{E}_N^a$,*

$$\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N}\Big[H_{\mathcal{D}_a} = H_{\mathcal{D}_{\boldsymbol{z}}}\Big] \;=\; \frac{\omega(\boldsymbol{z})}{\sum_{\boldsymbol{z}'\in\mathfrak{S}_a}\omega(\boldsymbol{z}')}\;\cdot$$

The proof of Lemma 2.7.1 yields the last result.

Proposition 2.2.8. *Let $D \subset \Xi$ be a domain with a smooth boundary, and let $m =: \inf_{\boldsymbol{y}\in\partial D} F(\boldsymbol{y})$. Fix a sequence $\{\epsilon_N : N \ge 1\}$ of positive numbers such that $\lim_N N^{d+1} \exp\{-N\epsilon_N\} = 0$, and let $D_N = \Xi_N \cap D$, $B_N = \{\boldsymbol{x} \in \partial D_N : F(\boldsymbol{x}) \le m + 2\epsilon_N\}$. Fix a point $\boldsymbol{x} \in D$ such that $F(\boldsymbol{x}) < m$ and for which there exists a continuous path $\boldsymbol{x}(t)$, $0 \le t \le 1$, from B_N to $\boldsymbol{x}$ such that $F(\boldsymbol{x}(t)) \le m + \epsilon_N$ for all $0 \le t \le 1$. Then,*

$$\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N}\big[H_{\partial D_N} = H_{B_N}\big] \;=\; 1\;,$$

where $\boldsymbol{x}_N \in D_N$, $\|\boldsymbol{x}_N - \boldsymbol{x}\| \le 1/N$.

We conclude this section with some comments. Bianchi, Bovier and Ioffe [10, 11] examined the metastable behavior of the Curie-Weiss model with random external fields. In this case the potential F becomes a sequence of potentials F_N which converges to some function F_∞. The authors assumed that the parameter of the model, the distribution of the external field, were chosen to guarantee that all wells do not have saddle points at the same height. In this case, the metastable behavior of the chain consists in staying for an exponential time in some well and then to jump to a deeper well in which the chain remains trapped for ever.

To observe a metastable behavior similar to the one described in Theorem 2.2.4, one has to tune the distribution of the external field in a way that the wells associated to F_∞ have more than one saddle point at the same height. In this case, however, the metastable behavior might depend on the subsequence of N.

To illustrate this possibility, consider the following one-dimensional example. Let F_N be a sequence of potentials which converge uniformly to a potential F_∞. Fix two local maxima of F_∞, supposed to be at the same height, $F_\infty(\boldsymbol{z}) = F_\infty(\boldsymbol{z}')$, and assume that the interval $(\boldsymbol{z}, \boldsymbol{z}')$ is a well, $F_\infty(\boldsymbol{x}) < F_\infty(\boldsymbol{z})$ for $\boldsymbol{z} < \boldsymbol{x} < \boldsymbol{z}'$. Suppose also that F_N has two local maxima $\boldsymbol{z}_N$, $\boldsymbol{z}'_N$ such that $\boldsymbol{z}_N \to \boldsymbol{z}$, $\boldsymbol{z}'_N \to \boldsymbol{z}'$, that $(\boldsymbol{z}_N, \boldsymbol{z}'_N)$ is a well for F_N, and that there exists subsequences N' and N'' such that

$$N'\big[F_{N'}(\boldsymbol{z}'_{N'}) - F_{N'}(\boldsymbol{z}_{N'})\big] \;\le\; -\epsilon\;, \quad N''\big[F_{N''}(\boldsymbol{z}'_{N''}) - F_{N''}(\boldsymbol{z}_{N''})\big] \;\ge\; \epsilon$$

for some $\epsilon > 0$. In this case, in view of the results presented in this section, starting from a local minima in $(\boldsymbol{z}_N, \boldsymbol{z}'_N)$, along the subsequence N', almost surely the chain will escape from $(\boldsymbol{z}_N, \boldsymbol{z}'_N)$ through a neighborhood of $\boldsymbol{z}'_N$, while along the subsequence N'' almost surely it will escape from $(\boldsymbol{z}_N, \boldsymbol{z}'_N)$ through a neighborhood of $\boldsymbol{z}_N$.

This is what happens for the Curie-Weiss model with an external field, random or not, if there exist saddle points at the same height. For the metastable behavior not to depend on particular subsequences, one needs to impose some strong conditions on the asymptotic behavior of the sequence F_N.

The article is divided as follows. In Section 2.3 we prove the upper bound for the capacities appearing in the statement of Theorem 2.2.1 and in Section 2.4 the lower bound. In Section 2.5 we prove Theorem 2.2.2, in Section 2.6, Theorem 2.2.4, and in Section 2.7, Theorem 2.2.7.

2.3 Upper bound for the capacities

We prove in this section the upper bound of Theorem 2.2.1. The proof is based on ideas of [17, 10, 11] and on the Dirichlet principle [30, Proposition 3.1.3] which expresses the capacity between two sets as an infimum of the Dirichlet form: for two disjoint subsets A, B of Ξ_N,

$$\mathrm{cap}_N(A,B) \;=\; \inf_f D_N(f)\;,$$

where the infimum is carried over all functions $f : \Xi_N \to \mathbb{R}$ such that $f(\boldsymbol{x}) = 1$, $\boldsymbol{x} \in A$, $f(\boldsymbol{y}) = 0$, $\boldsymbol{y} \in B$, and where $D_N(f)$ stands for the Dirichlet form of f,

$$D_N(f) \;=\; \sum_{\boldsymbol{x}\in\Xi_N} f(\boldsymbol{x})\,(-L_N f)(\boldsymbol{x})\,\mu_N(\boldsymbol{x}) \;=\; \frac{1}{2}\sum_{\boldsymbol{x},\boldsymbol{y}\in\Xi_N} \mu_N(\boldsymbol{x}) R_N(\boldsymbol{x},\boldsymbol{y})[f(\boldsymbol{y}) - f(\boldsymbol{x})]^2\;.$$

Proposition 2.3.1. *For every proper subset A of $\{1,\dots,\ell\}$,*

$$\limsup_{N\to\infty} \frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NF(\boldsymbol{z})}\, \mathrm{cap}_N(\mathcal{E}_N(A), \mathcal{E}_N(A^c)) \;\le\; \sum_{\boldsymbol{z}\in\mathfrak{S}(A)} \frac{\mu(\boldsymbol{z})}{\sqrt{-\det \mathrm{Hess}\, F(\boldsymbol{z})}}\;.$$

The proof of this proposition is divided in several lemmas. The main point is that the capacities depend on the behavior of the function F around the saddle points of F.

Fix a saddle point $\boldsymbol{z}$ of F and denote by $\mathbb{M} = (\mathrm{Hess}\, F)(\boldsymbol{z})$ the Hessian of F at $\boldsymbol{z}$. Denote by $-\mu$ the negative eigenvalue of $\mathbb{M}$ and by $0 < \lambda_2 \le \cdots \le \lambda_d$ the positive eigenvalues. Let $\boldsymbol{v}$, $\boldsymbol{w}^i$, $2 \le i \le d$, be orthonormal eigenvectors associated to the eigenvalues $-\mu$, λ_i, respectively. We sometimes denote $\boldsymbol{v}$ by $\boldsymbol{w}^1$ and $-\mu$ by λ_1.

Let $\mathbb{V}$ the $(d \times d)$-matrix whose j-th column is the vector $\boldsymbol{w}^j$ and denote by $\mathbb{V}^*$ its transposition. Denote by $\mathbb{D}$ the diagonal matrix whose diagonal entries are λ_i so that $\mathbb{M} = \mathbb{V}\mathbb{D}\mathbb{V}^*$. Let $\mathbb{D}_\star$ be the matrix $\mathbb{D}$ in which we replaced the negative eigenvalue λ_1 by its absolute value μ and let

$$\mathbb{M}_\star \;=\; \mathbb{V}\,\mathbb{D}_\star\,\mathbb{V}^* \;. \tag{2.3.1}$$

Clearly, $\det \mathbb{M} = -\det \mathbb{M}_\star$.

Let $B_N = B_N^{\boldsymbol{z}}$ be a mesoscopic neighborhood of $\boldsymbol{z}$:

$$B_N = \Big\{ \boldsymbol{x} \in \Xi_N : |(\boldsymbol{x}-\boldsymbol{z})\cdot \boldsymbol{v}| \le \varepsilon_N \,,\; \max_{2\le j\le d} |(\boldsymbol{x}-\boldsymbol{z})\cdot \boldsymbol{w}^j| \le 2\sqrt{\mu/\lambda_j}\varepsilon_N \Big\}\;, \tag{2.3.2}$$

where $N^{-1} \ll \varepsilon_N \ll 1$ is a sequence of positive numbers to be chosen later. Unless needed, we omit the index $\boldsymbol{z}$ from the notation $B_N^{\boldsymbol{z}}$. Denote by ∂B_N the outer boundary of B_N defined by

$$\partial B_N = \{ \boldsymbol{x} \in \Xi_N \setminus B_N : \exists\, \boldsymbol{y} \in B_N \text{ s.t. } \|\boldsymbol{y}-\boldsymbol{x}\| = N^{-1} \}\;, \tag{2.3.3}$$

and let $\partial_- B_N$, $\partial_+ B_N$ be the pieces of the outer boundary of B_N defined by

$$\begin{aligned} \partial_- B_N &= \{ \boldsymbol{x} \in \partial B_N : (\boldsymbol{x}-\boldsymbol{z})\cdot \boldsymbol{v} < -\varepsilon_N \}\;, \\ \partial_+ B_N &= \{ \boldsymbol{x} \in \partial B_N : (\boldsymbol{x}-\boldsymbol{z})\cdot \boldsymbol{v} > \varepsilon_N \}\;. \end{aligned}$$

The Dirichlet forms in the sets B_N

Denote by $D_N(f; B_N)$ the piece of the Dirichlet form of a function $f : \Xi_N \to \mathbb{R}$ corresponding to the edges in the set B_N:

$$D_N(f;B_N) \;=\; \sum_{i=1}^{d} \sum_{\boldsymbol{x}\in B_N} \mu_N(\boldsymbol{x})\, R_N(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_i)\, [f(\boldsymbol{x}+\boldsymbol{e}_i) - f(\boldsymbol{x})]^2 \;,$$

where $\{\mathfrak{e}_1, \dots, \mathfrak{e}_d\}$ is the canonical basis of $\mathbb{R}^d$ and $\boldsymbol{e}_i = N^{-1}\mathfrak{e}_i$.

Let $\mu_N^{\boldsymbol{z}}$ be the measure on B_N given by

$$\mu_N^{\boldsymbol{z}}(\boldsymbol{x}) \;=\; \frac{1}{Z_N}\, e^{-NF(\boldsymbol{z})}\, e^{-(1/2)N(\boldsymbol{y}\cdot \mathbb{M}\boldsymbol{y})} \;,$$

where $\boldsymbol{y} = \boldsymbol{x} - \boldsymbol{z}$, and where $\boldsymbol{v} \cdot \boldsymbol{w}$ represents the scalar product between $\boldsymbol{v}$ and $\boldsymbol{w}$. Denote by $D^{\boldsymbol{z}}_N$ the Dirichlet form defined by

$$D^{\boldsymbol{z}}_N(f) \;=\; \sum_{i=1}^{d} \sum_{\boldsymbol{x} \in B_N} \mu^{\boldsymbol{z}}_N(\boldsymbol{x})\, [f(\boldsymbol{x} + \boldsymbol{e}_i) - f(\boldsymbol{x})]^2 \;. \tag{2.3.4}$$

The next assertion follows from an elementary computation and from assumption (H1).

Assertion 2.3.A. *For every function $f : \Xi_N \to \mathbb{R}$,*

$$D_N(f; B_N) \;=\; \big[1 + O(\varepsilon_N) + O(N\varepsilon_N^3)\big]\, D^{\boldsymbol{z}}_N(f) \;.$$

The equilibrium potential

We introduce in this subsection an approximation in the set B_N of the solution to the Dirichlet variational problem for the capacity. To explain the choice, consider a one-dimensional random walk on the interval $I_N = \{-K_N/N, \dots, (K_N - 1)/N, K_N/N\}$ whose Dirichlet form D_N is given by

$$D_N(f) \;=\; \sum_k e^{\mu N k^2}\, [f(k + N^{-1}) - f(k)]^2 \;,$$

where the sum is performed over $k \in I_N$, $k \neq K_N/N$. An elementary computation shows that the equilibrium potential $V(k/N) = P_{k/N}[H_{K_N/N} < H_{-K_N/N}]$ is given by

$$V(k/N) \;=\; \frac{\sum_{j=-K_N/N}^{(k-1)/N} e^{-\mu N j^2}}{\sum_{j=-K_N/N}^{(K_N-1)/N} e^{-\mu N j^2}} \;\sim\; \frac{\int_{-\infty}^{k/N} e^{-\mu N r^2}\, dr}{\int_{-\infty}^{\infty} e^{-\mu N r^2}\, dr} \;,$$

where the last approximation holds provided $\sqrt{N} \ll K_N \ll N$.

In view of the previous observation, let $f : \mathbb{R} \to \mathbb{R}_+$ be given by

$$f_N(r) \;=\; \frac{\int_{-\infty}^{r} e^{-(1/2)N\mu s^2}\, ds}{\int_{-\infty}^{\infty} e^{-(1/2)N\mu s^2}\, ds} \;=\; \sqrt{\frac{N\mu}{2\pi}} \int_{-\infty}^{r} e^{-(1/2)N\mu s^2}\, ds \;.$$

The function V_N defined below is an approximation on the set B_N for the equilibrium potential between $\partial_- B_N$ and $\partial_+ B_N$:

$$V_N(\boldsymbol{x}) \;=\; V^{\boldsymbol{z}}_N(\boldsymbol{x}) \;=\; f_N([\boldsymbol{x} - \boldsymbol{z}] \cdot \boldsymbol{v}) \;. \tag{2.3.5}$$

Assertion 2.3.B. *Assume that $N^{-1/2} \ll \varepsilon_N \ll N^{-1/3}$. Then,*

$$\frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NF(\boldsymbol{z})}\, D_N(V_N; B_N) \;=\; [1 + o_N(1)]\, \frac{\mu}{\sqrt{-\det \operatorname{Hess} F(\boldsymbol{z})}} \;.$$

Proof. By Assertion 2.3.A, it is enough to estimate $D_N^{\boldsymbol z}(V_N)$. By definition of the Dirichlet form $D_N^{\boldsymbol z}$,

$$Z_N\, e^{NF(\boldsymbol z)}\, D_N^{\boldsymbol z}(V_N) \;=\; \sum_{i=1}^{d} \sum_{\boldsymbol x\in B_N} e^{-(1/2)\,N\,(\boldsymbol y\cdot \mathbb M\,\boldsymbol y)}\,[V_N(\boldsymbol x+\boldsymbol e_i)-V_N(\boldsymbol x)]^2\;,$$

where $\boldsymbol y = \boldsymbol x - \boldsymbol z$. Denote by $\boldsymbol v_1,\dots,\boldsymbol v_d$ the coordinates of the vector $\boldsymbol v$ and recall that $\|\boldsymbol v\| = 1$. Recall the definition of the matrix $\mathbb M_\star$ introduced in (2.3.1). Since $(\boldsymbol y\cdot\mathbb M\,\boldsymbol y) = \sum_{1\le j\le d}\lambda_j(\boldsymbol y\cdot \boldsymbol w^j)^2$, by definition of V_N this sum is equal to

$$\begin{aligned}
&[1+o_N(1)]\,\frac{\mu}{2\pi N}\,\sum_{i=1}^{d}\boldsymbol v_i^2 \sum_{\boldsymbol x\in B_N} e^{-(1/2)\,N\,(\boldsymbol y\cdot\mathbb M\,\boldsymbol y)}\, e^{-\mu N(\boldsymbol y\cdot\boldsymbol v)^2}\\
&\quad=\;[1+o_N(1)]\,\frac{\mu}{2\pi N}\sum_{\boldsymbol x\in B_N} e^{-(1/2)\,N\,(\boldsymbol y\cdot\mathbb M_\star\,\boldsymbol y)}\;.
\end{aligned}$$

Let $\boldsymbol w = \sqrt N\boldsymbol y = \sqrt N[\boldsymbol x - \boldsymbol z]$ so that $\boldsymbol w\in N^{-1/2}\mathbb Z^d$, to rewrite the previous sum as

$$[1+o_N(1)]\,\frac{\mu}{2\pi N}\sum_{\boldsymbol w} e^{-(1/2)\,(\boldsymbol w\cdot\mathbb M_\star\,\boldsymbol w)}\;,$$

where the sum is performed over $\boldsymbol w$ such that $|\boldsymbol w\cdot\boldsymbol v| \le N^{1/2}\varepsilon_N$ and $|\boldsymbol w\cdot\boldsymbol w^j| \le 2\sqrt{\mu/\lambda_j}N^{1/2}\varepsilon_N$, $2\le j\le d$. Since, by assumption, $N^{1/2}\varepsilon_N\uparrow\infty$, this expression is equal to

$$[1+o_N(1)]\,\frac{\mu}{2\pi N}N^{d/2}\int_{\mathbb R^d} e^{-(1/2)\,(\boldsymbol w\cdot\mathbb M_\star\boldsymbol w)}d\boldsymbol w\;.$$

The previous integral is equal to $(2\pi)^{d/2}\{\det\mathbb M_\star\}^{-1/2} = (2\pi)^{d/2}\{-\det\mathbb M\}^{-1/2}$, which completes the proof of the assertion. □

We conclude the proof of Proposition 2.3.1 extending the definition of V_N to the entire set Ξ_N and estimating its Dirichlet form. We denote by $\partial^{\rm in}B_N$ the inner boundary of B_N, the set of points in B_N which have a neighbor in $\Xi_N\setminus B_N$. Let B_N^*, $\partial^{\rm in}_\pm B_N$ be the $(d-1)$-dimensional sections of the boundary ∂B_N, $\partial^{\rm in}B_N$:

$$\begin{aligned}
B_N^* \;&=\; \bigcup_{2\le j\le d}\Big\{\boldsymbol x\in\partial B_N : |(\boldsymbol x-\boldsymbol z)\cdot\boldsymbol w^j| > 2\sqrt{\mu/\lambda_j}\varepsilon_N\Big\}\;,\\
\partial^{\rm in}_\pm B_N &= \{\boldsymbol x\in\partial^{\rm in}B_N : \exists\,\boldsymbol y\in\partial_\pm B_N \text{ s.t. } \|\boldsymbol y-\boldsymbol x\| = N^{-1}\}\;.
\end{aligned}$$

Assertion 2.3.C. *For all N sufficiently large,*

$$\inf_{\boldsymbol x\in B_N^*} F(\boldsymbol x)\;\ge\; F(\boldsymbol z)\;+\;\mu\,\varepsilon_N^2\;.$$

Proof. Indeed, by a Taylor expansion of F around $\boldsymbol{z}$, for $\boldsymbol{x} \in B_N^*$,

$$F(\boldsymbol{x}) \;=\; F(\boldsymbol{z}) \;+\; (1/2)(\boldsymbol{x}-\boldsymbol{z})\cdot\mathbb{M}\,(\boldsymbol{x}-\boldsymbol{z}) \;+\; O(\varepsilon_N^3)\,.$$

The second term on the right hand side is equal to $(1/2)\sum_{1\le j\le d}\lambda_j\,[(\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{w}^j]^2$. Since $\lambda_1=-\mu$, $\lambda_j>0$ for $2\le j\le d$, and $\boldsymbol{x}$ belongs to B_N^*, for N sufficiently large the previous expression is bounded below by

$$F(\boldsymbol{z}) \;+\; \frac{3\,\mu}{2}\,\varepsilon_N^2 \;+\; O(\varepsilon_N^3) \;\ge\; F(\boldsymbol{z}) \;+\; \mu\,\varepsilon_N^2\;,$$

which proves the claim. □

Let $\vartheta = \min\{\mu(\boldsymbol{z}) : \boldsymbol{z}\in\mathfrak{S}(A)\}$. Denote by $\mathcal{U}$ the connected component of the set $\{\boldsymbol{x}\in\Xi : F(\boldsymbol{x}) < F(\boldsymbol{z})+\vartheta\,\varepsilon_N^2\}$ which contains a set W_a, $a\in A$, and let $\mathcal{U}_N=\mathcal{U}\cap\Xi_N$. The set $\mathcal{U}_N$ may be decomposed in disjoint sets. Let $\mathfrak{B}_N^{\boldsymbol{z}}=\mathcal{U}_N\cap B_N^{\boldsymbol{z}}$, $\boldsymbol{z}\in\mathfrak{S}(A)$, $\mathcal{V}_N=\mathcal{U}_N\setminus\cup_{\boldsymbol{z}\in\mathfrak{S}(A)}\mathfrak{B}_N^{\boldsymbol{z}}$ so that

$$\mathcal{U}_N \;=\; \mathcal{V}_N \,\cup \bigcup_{\boldsymbol{z}\in\mathfrak{S}(A)} \mathfrak{B}_N^{\boldsymbol{z}}\;.$$

Figure 2.4 represents the sets $\mathcal{U}_N$ and $B_N^{\boldsymbol{z}}$. By Assertion 2.3.C, the set $\mathcal{V}_N$ is formed by several connected components separated by the sets $B_N^{\boldsymbol{z}}$, $\boldsymbol{z}\in\mathfrak{S}(A)$. In Figure 2.4, for example, the set $\mathcal{V}_N$ is composed of 4 connected components. Let $\mathcal{V}_N^A$ be the union of all connected components of $\mathcal{V}_N$ which contains a point in W_a, $a\in A$, and let $\mathcal{V}_N^B=\mathcal{V}_N\setminus\mathcal{V}_N^A$.

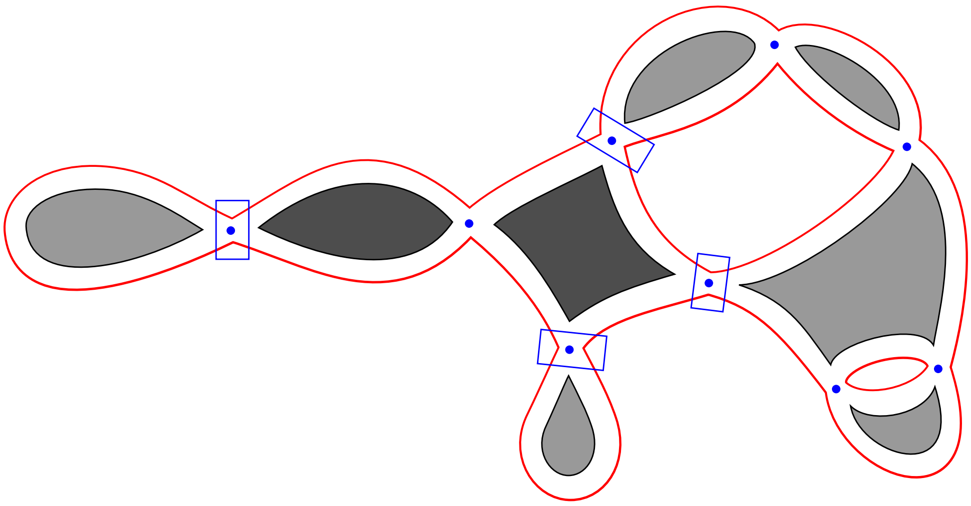

Figure 2.4: In red the boundary of the set $\mathcal{U}_N$. In dark gray the wells W_b^ϵ, $b\in A$. In blue the boxes $B_N^{\boldsymbol{z}}$, $\boldsymbol{z}\in\mathfrak{S}(A)$.

For each $\boldsymbol{z}\in\mathfrak{S}(A)$, choose an orthonormal basis of $(\mathrm{Hess}\,F)(\boldsymbol{z})$ in such a way that the eigenvector $\boldsymbol{v}(\boldsymbol{z})$ points to the direction of $\mathcal{E}_N(A)$. Define $V_N^A:\Xi_N\to[0,1]$

by

$$V_N^A(\boldsymbol{x}) \;=\; \begin{cases} 0 & \boldsymbol{x}\in\mathcal{V}_N^B\,, \\ 1 & \boldsymbol{x}\in\mathcal{V}_N^A\,, \end{cases} \qquad V_N^A(\boldsymbol{x}) \;=\; \begin{cases} V_N^{\boldsymbol{z}}(\boldsymbol{x}) & \boldsymbol{x}\in\mathfrak{B}_N^{\boldsymbol{z}}\,, \\ (1/2) & \text{otherwise,} \end{cases}$$

where $V_N^{\boldsymbol{z}}$ is the function defined in (2.3.5).

Assertion 2.3.D. *Let ε_N be a sequence such that $N\varepsilon_N^3\to 0$, $\exp\{-N\varepsilon_N^2\}$ converges to 0 faster than any polynomial. Then,*

$$\frac{Z_N}{(2\pi N)^{d/2}}\,2\pi N\,e^{NF(\boldsymbol{z})}\,D_N(V_N^A)\;\le\;[1+o_N(1)]\sum_{\boldsymbol{z}\in\mathfrak{S}(A)}\frac{\mu(\boldsymbol{z})}{\sqrt{-\det\operatorname{Hess}F(\boldsymbol{z})}}\;.$$

Proof. We estimate the Dirichlet form of V_N^A inside the sets $\mathfrak{B}_N^{\boldsymbol{z}}$, $\boldsymbol{z}\in\mathfrak{S}(A)$, at the boundary of $\mathcal{U}_N$, and at the boundary of $B_N^{\boldsymbol{z}}$ which is contained in $\mathcal{U}_N$.

Denote by $\partial\mathcal{U}_N$ the outer boundary of $\mathcal{U}_N$. The contribution to the Dirichlet form $D_N(V_N^A)$ of the edges in $\partial\mathcal{U}_N$ is less than or equal to

$$\sum_{i=1}^{d}\sum_{\boldsymbol{x}\in\partial\mathcal{U}_N}\mu_N(\boldsymbol{x})[R_N(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)+R_N(\boldsymbol{x},\boldsymbol{x}-\boldsymbol{e}_i)]\le\frac{C_0}{Z_N}e^{-NF(\boldsymbol{z})}\sum_{x\in\partial\mathcal{U}_N}e^{-\vartheta N\varepsilon_N^2},$$

where C_0 denotes a finite constant which does not depend on N and whose value may change from line to line. The sum on the right hand side is bounded by $C_0N^{d-1}e^{-\vartheta N\varepsilon_N^2}$, which vanishes as $N\uparrow\infty$ in view of our choice of ε_N.

Let $R_N^{\pm}(\boldsymbol{z}) = \partial_{\pm}^{\rm in}B_N^{\boldsymbol{z}}\cap\mathcal{U}_N$, $\boldsymbol{z}\in\mathfrak{S}(A)$. we estimate the contribution to the Dirichlet form $D_N(V_N^A)$ of the edges in $R_N^-(\boldsymbol{z})$, the one of $R_N^+(\boldsymbol{z})$ being analogous. By the definition of V_N^A this contribution is bounded by

$$\begin{aligned}&\sum_{i=1}^{d}\sum_{\boldsymbol{x}\in R_N^-(\boldsymbol{z})}\mu_N(\boldsymbol{x})\,[R_N(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)+R_N(\boldsymbol{x},\boldsymbol{x}-\boldsymbol{e}_i)]\,V_N^{\boldsymbol{z}}(\boldsymbol{x})^2\,,\\ &\qquad\le\;\frac{C_0}{Z_N}e^{-NF(\boldsymbol{z})}\sum_{\boldsymbol{x}\in R_N^-(\boldsymbol{z})}e^{-(1/2)N(\boldsymbol{y}\cdot\mathbb{M}^{\boldsymbol{z}}\boldsymbol{y})}V_N^{\boldsymbol{z}}(\boldsymbol{x})^2\,,\end{aligned}\tag{2.3.6}$$

where $\boldsymbol{y}=\boldsymbol{x}-\boldsymbol{z}$. In the remainder of this paragraph we omit the dependence on $\boldsymbol{z}$ in the notation. Since $\boldsymbol{x}$ belongs to B_N, $\exp\{-(1/2)N(\boldsymbol{y}\cdot\mathbb{M}\boldsymbol{y})\}$ is less than or equal to $\exp\{(1/2)\mu N\varepsilon_N^2\}\exp\{-(1/2)N\sum_{2\le j\le d}\lambda_j(\boldsymbol{y}\cdot\boldsymbol{w}^j)^2\}$. On the other hand, by a change of variables,

$$V_N(\boldsymbol{x})^2=\Big(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{(N\mu)^{1/2}(\boldsymbol{y}\cdot\boldsymbol{v})}e^{-r^2/2}\,dr\Big)^2\,.$$

Since $\boldsymbol{x}$ belongs to $\partial_-^{\rm in}B_N$, $\boldsymbol{y}\cdot\boldsymbol{v}\le-\varepsilon_N+C_0N^{-1}$. The previous expression is therefore less than or equal to $(C_0/N\varepsilon_N^2)\exp\{-\mu N\varepsilon_N^2\}$ because $\int_{(-\infty,A]}\exp\{-(1/2)r^2\}dr\le$

$|A|^{-1}\exp\{-(1/2)A^2\}$ for $A < 0$. This proves that the sum appearing in (2.3.6) is less than or equal to $C_0 N^{d-1}\exp\{-(1/2)\mu N\varepsilon_N^2\}$, which vanishes as $N \uparrow \infty$, in view of the definition of ε_N.

Since, for each $\boldsymbol{z} \in \mathfrak{S}(A)$, the set $\mathfrak{B}_N^{\boldsymbol{z}}$ is contained in $B_N^{\boldsymbol{z}}$, the contribution to the Dirichlet form of the bonds in the set $\mathfrak{B}_N^{\boldsymbol{z}}$ is less than or equal to $D_N(V_N; B_N^{\boldsymbol{z}})$. To conclude the proof it remains to recall Assertion 2.3.B. □

2.4 Lower bound for the capacities

We prove in this section the lower bound of Theorem 2.2.1. The proof is based on the arguments presented in [10, 11].

Proposition 2.4.1. *For every proper subset A of $\{1, \dots, \ell\}$,*

$$\liminf_{N\to\infty} \frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NF(\boldsymbol{z})}\, \mathrm{cap}_N(\mathcal{E}_N(A), \mathcal{E}_N(A^c)) \;\ge\; \sum_{\boldsymbol{z}\in\mathfrak{S}(A)} \frac{\mu(\boldsymbol{z})}{\sqrt{-\det \mathrm{Hess}\, F(\boldsymbol{z})}}\;.$$

The idea of the proof is quite simple. It is based on Thomson's principle [30, Proposition 3.2.2] which expresses the inverse of the capacity as an infimum over divergence free, unitary flows. The construction of a unitary flow from $\mathcal{E}_N(A)$ to $\mathcal{E}_N(A^c)$ will be done in two steps. We first construct a unitary flow from $\mathcal{E}_N(A)$ to $\mathcal{E}_N(A^c)$ for each saddle point $\boldsymbol{z} \in \mathfrak{S}(A)$. Then, we define a unitary flow from $\mathcal{E}_N(A)$ to $\mathcal{E}_N(A^c)$ as a convex combination of the unitary flows defined in the first step.

Step 1: Flows associated to saddle points. The main difficulty of the proof of Proposition 2.4.1 consists in defining unitary flows associated to saddle points. Fix $\boldsymbol{z} \in \mathfrak{S}(A)$ and two wells W_a, W_b such that $a \in A$, $b \in A^c$, $\boldsymbol{z} \in W_a \cap W_b$. Assume, without loss of generality, that all coordinates of the vector $\boldsymbol{v}$ are non-negative. Let B_N be the subset defined by

$$B_N \;=\; \Big\{\boldsymbol{x} \in \Xi_N : |(\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{v}| \le \varepsilon_N\,,\ \max_{2\le j\le d} |(\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{w}^j| \le \varepsilon_N\Big\}\,,$$

where ε_N is a sequence such that $N\varepsilon_N^3 \to 0$, $\exp\{-N\varepsilon_N^2\}$ converges to 0 faster than any polynomial. Note that the definition of the set B_N changed with respect to the one of the previous section.

Keep in mind that we assumed $\boldsymbol{v}$ to be a vector with non-negative coordinates. Denote by $N(\boldsymbol{v})$ the set of positive coordinates of $\boldsymbol{v}$, $N(\boldsymbol{v}) = \{j : \boldsymbol{v}_j > 0\}$. Let Q_N^o be the cone $Q_N^o = \{\boldsymbol{x} \in N^{-1}\mathbb{Z}^d : \boldsymbol{x}_j \ge 0\,,\ j \in N(\boldsymbol{v}) \text{ and } \boldsymbol{x}_j = 0\,,\ j \notin N(\boldsymbol{v})\}$, and let $Q_N^{\boldsymbol{x}}$, $\boldsymbol{x} \in N^{-1}\mathbb{Z}^d$, be the cone Q_N^o translated by $\boldsymbol{x}$, $Q_N^{\boldsymbol{x}} = \{\boldsymbol{x}+\boldsymbol{x}' : \boldsymbol{x}' \in Q_N^o\}$.

Denote by $\partial_-^{\mathrm{in}} B_N$ the inner boundary of B_N, defined as $\partial_-^{\mathrm{in}} B_N = \{\boldsymbol{x} \in B_N : \exists\, j \text{ s.t. } [\boldsymbol{x}-\boldsymbol{z}-\boldsymbol{e}_j]\cdot\boldsymbol{v} < -\varepsilon_N\}$. Denote by Q_N^+ the set of all cones with root in $\partial_-^{\mathrm{in}} B_N$, $Q_N^+ = \cup_{\boldsymbol{x}\in\partial_-^{\mathrm{in}} B_N} Q_N^{\boldsymbol{x}}$, and let

$$Q_N \;=\; \big\{\boldsymbol{x} \in Q_N^+ : (\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{v} \le \varepsilon_N\big\}\,.$$

Note that $B_N \subset Q_N$. Figure 2.5 represents the sets B_N, Q_N.

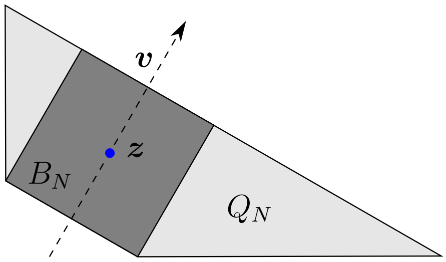

Figure 2.5: The vector $\boldsymbol{v}$, the set B_N in dark gray, and the set Q_N in light gray.

There exists a finite constant C_0, independent of N, such that for all $N \geq 1$,

$$\max_{2\leq k\leq d} \max_{\boldsymbol{x}\in Q_N} |\,(\boldsymbol{x}-\boldsymbol{z})\cdot \boldsymbol{w}^k\,| \;\leq\; C_0\,\varepsilon_N\;. \tag{2.4.1}$$

Indeed, if $\boldsymbol{x}$ belongs to Q_N, $\boldsymbol{x} = \boldsymbol{x}' + \boldsymbol{x}''$, where $\boldsymbol{x}' \in \partial_-^{\text{in}} B_N$ and $\boldsymbol{x}'' \in Q_N^o$. On the one hand, $\boldsymbol{x}' \in B_N$ so that $|\,(\boldsymbol{x}'-\boldsymbol{z})\cdot \boldsymbol{w}^k\,| \;\leq\; \varepsilon_N$ for all k and N. On the other hand, $\boldsymbol{x}''\cdot\boldsymbol{v} = [\boldsymbol{x}-\boldsymbol{z}]\cdot\boldsymbol{v} - [\boldsymbol{x}'-\boldsymbol{z}]\cdot\boldsymbol{v}$. The first term is bounded by ε_N because $\boldsymbol{x}$ belongs to Q_N. As $\boldsymbol{x}' \in B_N$, the second term is absolutely bounded by ε_N. This proves that $\boldsymbol{x}''_j \leq C_0\,\varepsilon_N$ for all $j \in N(\boldsymbol{v})$. The inequality holds trivially for $j \notin N(\boldsymbol{v})$ from what we conclude that there exists C_0 such that $\boldsymbol{x}''_j \;\leq\; C_0\,\varepsilon_N$ for all j and N. Assertion (2.4.1) follows from this bound and from the bounds obtained on $\boldsymbol{x}'$.

Denote by ∂B_N the external boundary of the set B_N, the set of sites which do not belong to B_N and which have a neighbor in B_N: $\partial B_N = \{\boldsymbol{x} \notin B_N : \exists\, j \text{ s.t. } \boldsymbol{x} + \boldsymbol{e}_j \text{ or } \boldsymbol{x} - \boldsymbol{e}_j \in B_N\}$. Two pieces of the external boundary of B_N play an important role in the proof of the lower bound for the capacity. Denote by $\partial_\pm B_N$ the sets

$$\partial_- B_N = \Big\{\boldsymbol{x} \in \partial B_N : (\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{v} < -\varepsilon_N\Big\}\,, \quad \partial_+ B_N = \Big\{\boldsymbol{x} \in \partial B_N : (\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{v} > \varepsilon_N\Big\}\,.$$

Denote by $\partial_+ Q_N$ the outer boundary of Q_N defined by $\partial_+ Q_N = \{\boldsymbol{x} \in \Xi_N : [\boldsymbol{x}-\boldsymbol{z}]\cdot\boldsymbol{v} > \varepsilon_N \text{ and } \exists\, j \text{ s.t. } \boldsymbol{x}-\boldsymbol{e}_j \in Q_N\}$. We shall construct a divergence free, unitary flow from $\mathcal{E}_N^a$ to $\partial_- B_N$, one from $\partial_- B_N$ to $\partial_+ Q_N$ and a third one from $\partial_+ Q_N$ to $\mathcal{E}_N^b$. The more demanding one is the flow from $\partial_- B_N$ to $\partial_+ Q_N$.

1.A. Sketch of the proof. To explain the idea of the proof of this part, we first consider the case where the eigenvector $\boldsymbol{v}$ associated to the negative eigenvalue of $(\text{Hess}\, F)(\boldsymbol{z})$ is $\mathfrak{e}_1$, the first vector of the canonical basis. In this case the cone Q_N^o introduced in the previous section is just a “straight line”: $Q_N^o = \{(k/N, 0, \dots, 0) : k \geq 0\}$ and $\partial_+ Q_N$ coincides with $\partial_+ B_N$.

We know that the optimal unitary flow from $\partial_- B_N$to $\partial_+ B_N$ is given by $\widehat{\Phi}(\boldsymbol{x},\boldsymbol{y}) = c(\boldsymbol{x},\boldsymbol{y})[\widehat{V}(\boldsymbol{x}) - \widehat{V}(\boldsymbol{y})]/\text{cap}(\partial_- B_N, \partial_+ B_N)$, where $c(\boldsymbol{x},\boldsymbol{y}) = \mu_N(\boldsymbol{x})\,R_N(\boldsymbol{x},\boldsymbol{y})$ is the conductance between the vertices $\boldsymbol{x}$ and $\boldsymbol{y}$ and $\widehat{V}$ is the equilibrium potential between $\partial_- B_N$ and $\partial_+ B_N$. We introduced in (2.3.5) an approximation V of the equilibrium potential $\widehat{V}$. A calculation shows that the flow $\Phi(\boldsymbol{x},\boldsymbol{y}) = c(\boldsymbol{x},\boldsymbol{y})[V(\boldsymbol{x}) - V(\boldsymbol{y})]$ is almost constant along the $\boldsymbol{v}$ direction. Hence, in the case where $\boldsymbol{v} = \mathfrak{e}_1$, a natural candidate is a flow constant along the $\mathfrak{e}_1$ direction. Denote a point $\boldsymbol{x} \in \Xi_N$ as $(\hat{\boldsymbol{x}}, \check{\boldsymbol{x}})$ where $\hat{\boldsymbol{x}} \in N^{-1}\mathbb{Z}$ and $\check{\boldsymbol{x}} \in N^{-1}\mathbb{Z}^{d-1}$, and let $\check{B}_N = \{\check{\boldsymbol{x}} \in N^{-1}\mathbb{Z}^{d-1} : \exists x \in N^{-1}\mathbb{Z} \text{ s.t. } (x, \check{\boldsymbol{x}}) \in B_N\}$,

$$\Phi(\boldsymbol{x},\boldsymbol{y}) \;=\; \begin{cases} \Phi(\check{\boldsymbol{x}}) & \text{if } \boldsymbol{y} = \boldsymbol{x} + \boldsymbol{e}_1,\, \boldsymbol{x} \in B_N \cup \partial_- B_N, \\ 0 & \text{otherwise,} \end{cases}$$

where $\Phi : \check{B}_N \to \mathbb{R}_+$ is such that $\sum_{\boldsymbol{x}\in \check{B}_N} \Phi(\check{\boldsymbol{x}}) = 1$.

By Thomson's principle, the inverse of the capacity is bounded above by the energy dissipated by the flow Φ:

$$\frac{1}{\text{cap}_N(\partial_- B_N, \partial_+ B_N)} \;\le\; \|\Phi\|^2 \;:=\; \sum_{\boldsymbol{x}\in B_N \cup \partial_- B_N} \frac{1}{c(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_1)}\, \Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_1)^2 \;, \quad (2.4.2)$$

By definition of the flow and by a second order Taylor expansion, the previous sum is equal to

$$[1+o_N(1)]\, Z_N\, e^{NF(\boldsymbol{z})} \sum_{\boldsymbol{x}\in B_N \cup \partial_- B_N} e^{(N/2)\,(\boldsymbol{y}\cdot \mathbb{M}\boldsymbol{y})}\, \Phi(\check{\boldsymbol{x}})^2 \;,$$

provided $N\varepsilon_N^3 \to 0$. In this equation, $\boldsymbol{y} = \boldsymbol{x} - \boldsymbol{z}$. Recall from (2.3.1) the definition of the matrices $\mathbb{V}$, $\mathbb{D}$. Let $\check{\mathbb{D}}$ be the diagonal matrix in which the entry $\lambda_1 = -\mu$ has been replaced by 0, and let $\check{\mathbb{M}}$ be the symmetric matrix $\check{\mathbb{M}} = \mathbb{V}\check{\mathbb{D}}\mathbb{V}^*$. In particular, for any vector $\boldsymbol{y}$, $\boldsymbol{y}\cdot\check{\mathbb{M}}\boldsymbol{y} = \sum_{2\le k\le d} \lambda_k (\boldsymbol{y}\cdot\boldsymbol{w}^k)^2$, and $\boldsymbol{y}\cdot\mathbb{M}\boldsymbol{y} = \boldsymbol{y}\cdot\check{\mathbb{M}}\boldsymbol{y} - \mu\hat{\boldsymbol{y}}^2$. With this notation, and since $\boldsymbol{y}\cdot\check{\mathbb{M}}\boldsymbol{y}$ depends on $\boldsymbol{y}$ only as a function of $\check{\boldsymbol{y}}$, we may rewrite the previous sum as

$$[1+o_N(1)]\, Z_N\, e^{NF(\boldsymbol{z})} \sum_{\check{\boldsymbol{x}}\in \check{B}_N} e^{(N/2)\,(\boldsymbol{y}\cdot \check{\mathbb{M}}\boldsymbol{y})}\, \Phi(\check{\boldsymbol{x}})^2 \sum_k e^{-\mu(N/2)k^2} \;,$$

where the second sum is performed over all $k \in N^{-1}\mathbb{Z}$ such that $-\varepsilon_N - N^{-1} \le k \le \varepsilon_N$. The optimal choice of Φ satisfying $\sum_{\boldsymbol{x}\in \check{B}_N} \Phi(\check{\boldsymbol{x}}) = 1$ is

$$\Phi(\check{\boldsymbol{x}}) \;=\; e^{-(N/2)\,(\boldsymbol{y}\cdot \check{\mathbb{M}}\boldsymbol{y})} \Big/ \sum_{\boldsymbol{x}\in \check{B}_N} e^{-(N/2)\,(\boldsymbol{y}\cdot \check{\mathbb{M}}\boldsymbol{y})} \;.$$

With this choice the previous sum becomes

$$[1+o_N(1)]\, Z_N\, e^{NF(\boldsymbol{z})} \frac{\sum_k e^{-\mu(N/2)k^2}}{\sum_{\check{\boldsymbol{x}}\in \check{B}_N} e^{-(N/2)\,(\boldsymbol{y}\cdot \check{\mathbb{M}}\boldsymbol{y})}} \;.$$

At this point we may repeat the arguments presented at the end of the proof of Assertion 2.3.B to conclude that the previous expression is equal to

$$[1+o_N(1)]\, Z_N\, e^{NF(\boldsymbol{z})} \frac{(2\pi N)\sqrt{-\det \mathbb{M}/\mu}}{(2\pi N)^{d/2}\sqrt{\mu}} \;=\; [1+o_N(1)]\, Z_N\, e^{NF(\boldsymbol{z})} \frac{(2\pi N)\sqrt{-\det \mathbb{M}}}{(2\pi N)^{d/2}\mu} \;,$$

In conclusion, we constructed a divergence free, unitary flow Φ from $\partial_- B_N$ to $\partial_+ B_N$ whose dissipated energy, $\|\Phi\|^2$, defined in (2.4.2) satisfies

$$\lim_{N\to\infty} \frac{(2\pi N)^{d/2}}{Z_N} \frac{1}{2\pi N} e^{-NF(\boldsymbol{z})} \|\Phi\|^2 \;=\; \frac{\sqrt{-\det[(\mathrm{Hess}\, F)(\boldsymbol{z})]}}{\mu} \;.$$

1.B. A unitary flow from $\partial_- B_N$ to $\partial_+ Q_N$. We turn now to the general case. We learned from the previous example that the optimal flow is

$$\Phi(\boldsymbol{x},\boldsymbol{y}) = M_N^{-1}\, c(\boldsymbol{x},\boldsymbol{y})[V(\boldsymbol{x}) - V(\boldsymbol{y})],$$

where V is the function introduced in (2.3.5) and M_N a constant which turns the flow unitary. We thus propose the flow

$$\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j) \;=\; \frac{\sqrt{-\det \mathbb{M}/\mu}}{(2\pi N)^{(d-1)/2}}\, \boldsymbol{v}_j\, e^{-(N/2)\boldsymbol{y}\cdot\check{\mathbb{M}}\boldsymbol{y}} \;. \tag{2.4.3}$$

We claim that Φ is an essentially unitary flow:

$$\sum_{j=1}^{d} \sum_{\boldsymbol{x}\in\partial_{j,-}B_N} \Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j) \;=\; [1+o_N(1)] \;, \tag{2.4.4}$$

where $\partial_{j,-}B_N$ represents the set of points $\boldsymbol{x}\in\partial_- B_N$ such that $\boldsymbol{x}+\boldsymbol{e}_j \in B_N$. We have to show that

$$\sum_{j=1}^{d} \boldsymbol{v}_j \sum_{\boldsymbol{x}\in\partial_{j,-}B_N} e^{-(N/2)\boldsymbol{y}\cdot\check{\mathbb{M}}\boldsymbol{y}} \;=\; [1+o_N(1)]\, \frac{(2\pi N)^{(d-1)/2}\sqrt{\mu}}{\sqrt{-\det\mathbb{M}}} \;. \tag{2.4.5}$$

Fix $1\le j\le d$, and let $V = \{\boldsymbol{x}\in\mathbb{R}^d : [\boldsymbol{x}-\boldsymbol{z}]\cdot\boldsymbol{v} = -\varepsilon_N\}$. Denote by $\delta(\boldsymbol{x})$, $\boldsymbol{x}\in\partial_{j,-}B_N$, the amount needed to translate $\boldsymbol{x}$ in the $\boldsymbol{e}_j$-direction for $\boldsymbol{x}$ to belong to V: $\boldsymbol{x}+\delta(\boldsymbol{x})\boldsymbol{e}_j\in V$. Observe that $\delta(\boldsymbol{x})\in(0,1]$. Let $T(\boldsymbol{x}) = \boldsymbol{x}+\delta(\boldsymbol{x})\boldsymbol{e}_j$, $\boldsymbol{x}\in\partial_{j,-}B_N$. Since $\delta(\boldsymbol{x})$ is absolutely bounded by 1,

$$\sum_{\boldsymbol{x}\in\partial_{j,-}B_N} e^{-(N/2)\boldsymbol{y}\cdot\check{\mathbb{M}}\boldsymbol{y}} \;=\; [1+o_N(1)] \sum_{\boldsymbol{x}\in\partial_{j,-}B_N} \exp\Big\{-(N/2)\sum_{k=2}^{d}\lambda_k\{[T(\boldsymbol{x})-\boldsymbol{z}]\cdot\boldsymbol{w}^k\}^2\Big\}$$

Replacing $\boldsymbol{x}$ by $\sqrt{N}\boldsymbol{x}$, and approximating the sum appearing on the right hand side by a Riemann integral, the previous term becomes

$$\begin{aligned} &[1+o_N(1)]\, \boldsymbol{v}_j\, N^{(d-1)/2} \prod_{k=2}^{d} \int_{-\sqrt{N}\varepsilon_N}^{\sqrt{N}\varepsilon_N} e^{-(1/2)\lambda_k r^2}\, dr \\ &\quad=\; [1+o_N(1)]\, \boldsymbol{v}_j\, (2\pi N)^{(d-1)/2} \frac{\sqrt{\mu}}{\sqrt{-\det\mathbb{M}}} \;, \end{aligned}$$

where $\boldsymbol{v}_j$ appeared to take into account the tilt of the hypersurface V. Multiplying the last term by $\boldsymbol{v}_j$ and summing over j we get (2.4.5) because $\|\boldsymbol{v}\| = 1$. This proves that the flow Φ is essentially unitary, as stated in (2.4.4).

1.C. Turning the flow divergence free. In this subsection, we add a correction R to the flow Φ to turn it divergence free. We start with an estimate on the divergence of the flow Φ. Denote by $(\text{div } \Phi)(\boldsymbol{x})$ the divergence of the flow Φ at $\boldsymbol{x}$:

$$(\text{div } \Phi)(\boldsymbol{x}) \;=\; \sum_{j=1}^{d} \{\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j) - \Phi(\boldsymbol{x}-\boldsymbol{e}_j, \boldsymbol{x})\} \;.$$

We claim that there exists a finite constant C_0, independent of N, such that

$$\max_{i\in N(\boldsymbol{v})} \max_{\boldsymbol{x}\in Q_N} \Big| \frac{(\text{div } \Phi)(\boldsymbol{x})}{\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_i)} \Big| \;\le\; C_0 \varepsilon_N^2 \;. \tag{2.4.6}$$

Fix $i \in N(\boldsymbol{v})$, $\boldsymbol{x} \in Q_N$, and recall the definition of the flow Φ. By (2.4.1), by definition of the matrix $\check{\mathbb{M}}$ and by a second order Taylor expansion, for each $1 \le i \le d$,

$$\begin{aligned} \sum_{j=1}^{d} \frac{\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j) - \Phi(\boldsymbol{x}-\boldsymbol{e}_j, \boldsymbol{x})}{\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_i)} \;&=\; \sum_{j=1}^{d} \frac{\boldsymbol{v}_j}{\boldsymbol{v}_i} \sum_{k=2}^{d} \lambda_k(\mathfrak{e}_j \cdot \boldsymbol{w}^k)([\boldsymbol{x}-\boldsymbol{z}]\cdot \boldsymbol{w}^k) + O(\varepsilon_N^2) \\ &=\; \frac{1}{\boldsymbol{v}_i} \sum_{k=2}^{d} \lambda_k(\boldsymbol{v} \cdot \boldsymbol{w}^k)([\boldsymbol{x}-\boldsymbol{z}]\cdot \boldsymbol{w}^k) + O(\varepsilon_N^2) \;. \end{aligned}$$

The first term on the right hand side vanishes because $\boldsymbol{v}$ is orthogonal to $\boldsymbol{w}^k$, which proves (2.4.6).

We now define a correction R to the flow Φ to turn it divergence free. Let $G_0 = \partial_- B_N$, G for generation. Define recursively the sets G_k, $k \ge 1$, by

$$G_{k+1} \;=\; \Big\{ \boldsymbol{x} \in Q_N : \boldsymbol{x} - \boldsymbol{e}_j \in \bigcup_{\ell=0}^{k} G_\ell \cup Q_N^c \text{ for all } j \in N(\boldsymbol{v}) \Big\} \;, \quad k \ge 0 \;.$$

The first three generations are illustrated in Figure 2.6. Denote by K_N the smallest integer k such that $Q_N \subset \cup_{1\le \ell\le k} G_\ell$. Clearly, $K_N \le C_0 \varepsilon_N^{-1}$ for some finite constant C_0.

The flow R is also defined recursively. For all $\boldsymbol{x} \in G_1$, define $R(\boldsymbol{x}-\boldsymbol{e}_j, \boldsymbol{x}) = 0$, $1 \le j \le d$, and let

$$R(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j) \;=\; p_j \Big\{ \sum_{i=1}^{d} R(\boldsymbol{x}-\boldsymbol{e}_i, \boldsymbol{x}) \;-\; (\text{div } \Phi)(\boldsymbol{x}) \Big\} \;, \tag{2.4.7}$$

where $p_j = \boldsymbol{v}_j / \sum_{1\le i\le d} \boldsymbol{v}_i$. Note that $R(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j) = 0$ if $j \notin N(\boldsymbol{v})$ and that we may restrict the sum over i to the set $N(\boldsymbol{v})$. On the other hand, by construction, $(\text{div } R)(\boldsymbol{x}) = -(\text{div } \Phi)(\boldsymbol{x})$ for all $\boldsymbol{x} \in \cup_{1\le \ell\le K_N} G_\ell$.

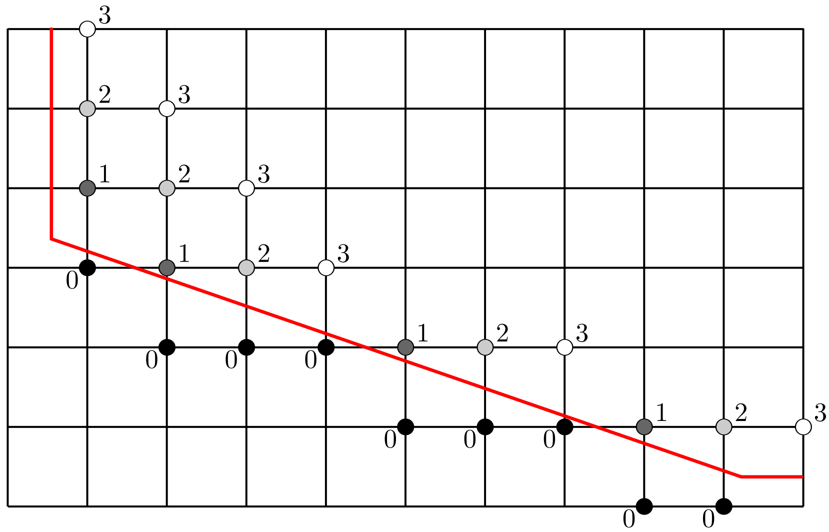

Figure 2.6: The first three generations. The red line represents the boundary of the set Q_N, and the numbers the generation of each point.

There exists a finite constant C_0 such that

$$\max_{i\in N(\boldsymbol{v})}\max_{\boldsymbol{x}\in G_k}\Big|\frac{R(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)}{\Phi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)}\Big| \;\le\; C_0\, k\, \varepsilon_N^2 \tag{2.4.8}$$

for all $1\le k\le K_N$. This assertion is proved by induction. Since $R(\boldsymbol{x}-\boldsymbol{e}_j,\boldsymbol{x})=0$ for $\boldsymbol{x}\in G_1$, by (2.4.6), $\max_{i\in N(\boldsymbol{v})}\max_{\boldsymbol{x}\in G_1}|\,R(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)/\Phi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)\,|\le C_1\,\varepsilon_N^2$, where C_1 is the constant C_0 appearing on the right hand side of (2.4.6).

Suppose that $\max_{i\in N(\boldsymbol{v})}\max_{\boldsymbol{x}\in G_j}|\,R(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)/\Phi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)|\le C_j\,\varepsilon_N^2$ for all $1\le j\le k$, where C_j is an increasing sequence. Fix $i\in N(\boldsymbol{v})$ and $\boldsymbol{x}\in G_{k+1}$. By definition of R, by (2.4.6), and by the induction hypothesis,

$$\Big|\frac{R(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)}{\Phi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)}\Big|\le C_k\,\varepsilon_N^2\,p_i\sum_{j\in N(\boldsymbol{v})}\frac{\Phi(\boldsymbol{x}-\boldsymbol{e}_j,\boldsymbol{x})}{\Phi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_i)}\;+\;C_0\,\varepsilon_N^2\;.$$

The computations performed to prove (2.4.6) yield that the first term on the right hand side is bounded by

$$\begin{aligned}&C_k\,\varepsilon_N^2\,p_i\sum_{j\in N(\boldsymbol{v})}\frac{\boldsymbol{v}_j}{\boldsymbol{v}_i}\Big\{1+\sum_{m=2}^{d}\lambda_m(\mathfrak{e}_j\cdot\boldsymbol{w}^m)(\boldsymbol{y}\cdot\boldsymbol{w}^m)+C_0\varepsilon_N^2\Big\}\\&\quad=\;C_k\,\varepsilon_N^2\,\big\{1+C_0\varepsilon_N^2\big\}\;\le\;C_k\,\varepsilon_N^2\,e^{C_0\varepsilon_N^2}\;.\end{aligned}$$

The identity has been derived using the definition of p_j, the orthogonality of $\boldsymbol{v}$ and $\boldsymbol{w}^k$, and summing first over j. We have thus obtained the recursive relation $C_{k+1}\le[C_0+C_k e^{C_0\varepsilon_N^2}]$ from which it follows that $C_k\le C_0 k e^{C_0 k\varepsilon_N^2}$. Since $k\le K_N\le C_0\varepsilon_N^{-1}$, (2.4.8) holds.

1.D. A divergence free unitary flow. We construct in this subsection a divergence-free, unitary flow from $\partial_- B_N$ to $\partial_+ Q_N$ whose energy dissipated is given by the right hand side of (2.4.9).

Let Ψ be the flow from $\partial_- B_N$ to $\partial_+ Q_N$ defined by $\Psi = \Phi + R$, where Φ is introduced in (2.4.3) and R in (2.4.7). By (2.4.4) and by construction of R, Ψ is a unitary flow. Since $(\text{div } R)(\boldsymbol{x}) = -(\text{div } \Phi)(\boldsymbol{x})$ for all $\boldsymbol{x} \in \cup_{0\le \ell\le K_N} G_\ell$, Ψ is divergence-free. It remains to show that the energy dissipated by Ψ satisfies

$$\begin{aligned} &\sum_{j=1}^{d} \sum_{\boldsymbol{x}} \frac{1}{c(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)}\, \Psi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)^2 \\ &\quad = [1+o_N(1)]\, \frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NF(\boldsymbol{z})}\, \frac{\sqrt{-\det[(\text{Hess } F)(\boldsymbol{z})]}}{\mu}\;. \end{aligned} \tag{2.4.9}$$

A second order expansion of $F(\boldsymbol{x})$ at $\boldsymbol{z}$ taking advantage of (2.4.1) and of the fact that $N\varepsilon_N^3 \to 0$ permits to write the left hand side of the previous equation as

$$[1+o_N(1)]\, Z_N\, e^{NF(\boldsymbol{z})} \sum_{j=1}^{d} \sum_{\boldsymbol{x}} e^{(N/2)(\boldsymbol{y}\cdot \mathbb{M}\cdot \boldsymbol{y})}\, \Psi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)^2\;,$$

where, as before, $\boldsymbol{y} = \boldsymbol{x} - \boldsymbol{z}$. We may bound $\Psi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)^2$ by $(1+\varepsilon_N)\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)^2 + (1+\varepsilon_N^{-1})R(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)^2$, and apply (2.4.8) together with the fact that $k \le K_N \le C_0 \varepsilon_N^{-1}$ to estimate the previous sum by $[1+O(\varepsilon_N)]\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)^2$. The previous displayed equation is therefore equal to the same sum with Ψ replaced by Φ. Replacing $\Phi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)$ by its value (2.4.3) the previous sum becomes

$$[1+o_N(1)]\, Z_N\, e^{NF(\boldsymbol{z})}\, \frac{1}{(2\pi N)^{d-1}}\, \frac{\det \mathbb{M}}{-\mu} \sum_{j=1}^{d} \boldsymbol{v}_j^2 \sum_{\boldsymbol{x}} e^{-(N/2)(\boldsymbol{y}\cdot \mathbb{M}_\star \cdot \boldsymbol{y})}\;,$$

where $\mathbb{M}_\star$ is the matrix introduced in (2.3.1). At this point it remains to recall that $\boldsymbol{v}$ is a normal vector and to repeat the calculations performed in the proof of the upper bound of the capacity to retrieve (2.4.9).

1.E. A unitary flow from $\mathcal{E}_N^a$ to $\partial_- B_N$. We extend in this section the flow Ψ from $\partial_- B_N$ to $\mathcal{E}_N^a$. The same arguments permit to extend the flow Ψ from $\partial_+ Q_N$ to $\mathcal{E}_N^b$. The idea is quite simple. For each bond $(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)$, $\boldsymbol{x} \in \partial_- B_N$, $\boldsymbol{x}+\boldsymbol{e}_j \in B_N$, we construct a path of nearest neighbor sites $(\boldsymbol{x} = \boldsymbol{x}^0, \boldsymbol{x}^1, \dots, \boldsymbol{x}^n)$, $\boldsymbol{x}^n \in \mathcal{E}_N^a$, from $\boldsymbol{x}$ to $\mathcal{E}_N^a$, and we define the flow $\Psi_{\boldsymbol{x},\boldsymbol{e}_j}$ from $\boldsymbol{x}$ to $\mathcal{E}_N^a$ by $\Psi_{\boldsymbol{x},\boldsymbol{e}_j}(\boldsymbol{x}^k, \boldsymbol{x}^{k+1}) = -\Psi(\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{e}_j)$. Adding all flows $\Psi_{\boldsymbol{x},\boldsymbol{e}_j}$ we obtain a divergence free, unitary flow from $\partial_- B_N$ to $\mathcal{E}_N^a$ whose dissipated energy is easily estimated.

We start defining the paths. For $\boldsymbol{y} \in \mathbb{R}^d$, denote by $[\boldsymbol{y}]$ the vector whose j-th coordinate is $[\boldsymbol{y}_j N]/N$, where $[a]$ stands for the largest integer less than or equal to $a \in \mathbb{R}$. Fix $\boldsymbol{x} \in \partial_- B_N$. Denote by $\boldsymbol{x}(t)$ the solution of the ODE $\dot{\boldsymbol{x}}(t) = -\nabla F(\boldsymbol{x}(t))$

with initial condition $\boldsymbol{x}(0) = \boldsymbol{x}$. Since $[\boldsymbol{x} - \boldsymbol{z}] \cdot \boldsymbol{v} < 0$, $\boldsymbol{x}(t)$ converges, as $t \to \infty$, to one of the local minima of F in W_a. Let $T = \inf\{t > 0 : \boldsymbol{x}(t) \in W_a^o\}$, where W_a^o is an open set whose closure is contained in W_a^ϵ, the set introduced in (2.2.2). Let $\boldsymbol{y}^0 = \boldsymbol{x}, \boldsymbol{y}^1, \dots, \boldsymbol{y}^m$ be the sequence of points in Ξ_N visited by the trajectory $[\boldsymbol{x}(t)]$, $0 \le t \le T$. If necessary, add points to this sequence in order to obtain a sequence $\boldsymbol{x}^0 = \boldsymbol{x}, \boldsymbol{x}^1, \dots, \boldsymbol{x}^{m'}$ such that $\|\boldsymbol{x}^k - \boldsymbol{x}^{k+1}\| = N^{-1}$. Remove from this sequence the loops and denote by n the length of the path. Since $F(\boldsymbol{x}(t))$ does not increase in time, and since for all k there exists some $0 \le t \le T$ such that $\|\boldsymbol{x}^k - \boldsymbol{x}(t)\| \le d/N$, there exists a finite constant C_0 such that

$$F(\boldsymbol{x}^k) \;\le\; F(\boldsymbol{x}) \;+\; \frac{C_0}{N} \text{ for all } 0 \le k \le n\,. \tag{2.4.10}$$

Fix a bond $(\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{e}_j)$, $\boldsymbol{x} \in \partial_- B_N$, $\boldsymbol{x} + \boldsymbol{e}_j \in B_N$. Define the flow $\Psi_{\boldsymbol{x},\boldsymbol{e}_j}$ from $\boldsymbol{x}$ to $\mathcal{E}_N^a$ by $\Psi_{\boldsymbol{x},\boldsymbol{e}_j}(\boldsymbol{x}^k, \boldsymbol{x}^{k+1}) = -\Psi(\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{e}_j)$, $0 \le k < n$. We claim that there exists a finite constant C_0 and a positive constant c_0 such that

$$\|\Psi_{\boldsymbol{x},\boldsymbol{e}_j}\|^2 \;\le\; C_0 N Z_N e^{NF(\boldsymbol{z})} e^{-c_0 N \varepsilon_N^2}\,. \tag{2.4.11}$$

The proof of this assertion is simple. Since $\Psi(\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{e}_j) = \Phi(\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{e}_j)$ is given by (2.4.3), by (2.4.10) and by definition of the set A_N^1,

$$\|\Psi_{\boldsymbol{x},\boldsymbol{e}_j}\|^2 \;\le\; C_0 Z_N \sum_{k=0}^{n-1} e^{NF(\boldsymbol{x}^k)} \Phi(\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{e}_j)^2 \;\le\; \frac{C_0 Z_N n}{N^{d-1}} e^{NF(\boldsymbol{x})} e^{-N(\boldsymbol{y} \cdot \check{\mathbb{M}} \boldsymbol{y})}\,.$$

By a second order Taylor expansion, $\exp N\{F(\boldsymbol{x}) - (\boldsymbol{y} \cdot \check{\mathbb{M}} \boldsymbol{y})\}$ is less than or equal to $C_0 \exp\{NF(\boldsymbol{z})\} \exp\{-(1/2)\mu N \varepsilon_N^2\}$ because $N\varepsilon_N^3 \to 0$ and $[\boldsymbol{x} - \boldsymbol{z}] \cdot \boldsymbol{v} < -\varepsilon_N$. This proves (2.4.11) because $n \le |\Xi_N|$.

Let $\Psi = \sum_{\boldsymbol{x},j} \Psi_{\boldsymbol{x},\boldsymbol{e}_j}$, where the sum is carried over all $\boldsymbol{x}$, j such that $\boldsymbol{x} \in \partial_- B_N$, $\boldsymbol{x} + \boldsymbol{e}_j \in B_N$. Ψ is a unitary, divergence free flow from $\partial_- B_N$ to $\mathcal{E}_N^a$. Moreover, by Schwarz inequality and by (2.4.11),

$$\|\Psi\|^2 \;\le\; M \sum_{\boldsymbol{x},j} \|\Psi_{\boldsymbol{x},\boldsymbol{e}_j}\|^2 \;\le\; C_0 N^{d+1} Z_N e^{NF(\boldsymbol{z})} e^{-c_0 N \varepsilon_N^2}\,,$$

where M represents the number of flows $\Psi_{\boldsymbol{x},\boldsymbol{e}_j}$.

Choosing ε_N appropriately and juxtaposing the flow just constructed with the one obtained in Section 1.D and a flow from $\partial_+ Q_N$ to $\mathcal{E}_N^b$, similar to the one described in this section, yields a divergence free, unitary flow from $\mathcal{E}_N^a$ to $\mathcal{E}_N^b$, denoted by Φ_z, such that

$$\lim_{N\to\infty} \frac{(2\pi N)^{d/2}}{Z_N} \frac{1}{2\pi N} e^{-NF(\boldsymbol{z})} \|\Phi_z\|^2 \;=\; \frac{\sqrt{-\det[(\operatorname{Hess} F)(\boldsymbol{z})]}}{\mu(\boldsymbol{z})}\,. \tag{2.4.12}$$

Step 2. Conclusion. Up to this point, for each saddle point z separating $\mathcal{E}_N(A)$ from $\mathcal{E}_N(A^c)$ we constructed a divergence free, unitary flow Φ_z from $\mathcal{E}_N(A)$ to $\mathcal{E}_N(A^c)$

for which (2.4.12) holds. Denote the right hand side of (2.4.12) by $a(z)$ and observe that $F(\boldsymbol{z})$ is constant for $\boldsymbol{z} \in \mathfrak{S}(A)$.

Let Φ be a convex combination of the previous flows: $\Phi = \sum_{\boldsymbol{z}\in\mathfrak{S}(A)} \theta_{\boldsymbol{z}} \Phi_{\boldsymbol{z}}$, where $\theta_{\boldsymbol{z}} \geq 0$, $\sum_{\boldsymbol{z}\in\mathfrak{S}(A)} \theta_{\boldsymbol{z}} = 1$. By construction, Φ is a flow from $\mathcal{E}_N(A)$ to $\mathcal{E}_N(A^c)$. On the other hand, since the saddle points are isolated and since the main contribution of the flow Φ_z occurs in a small neighborhood of z

$$\limsup_{N\to\infty} \frac{(2\pi N)^{d/2}}{Z_N} \frac{1}{2\pi N} e^{-NF(\boldsymbol{z})} \|\Phi\|^2 \;\leq\; \sum_{\boldsymbol{z}\in\mathfrak{S}(A)} \theta_{\boldsymbol{z}}^2 \, a(\boldsymbol{z}) \; .$$

The optimal choice for θ is $\theta_z = a(\boldsymbol{z})^{-1}/\sum_{\boldsymbol{z}'} a(\boldsymbol{z}')^{-1}$. With this choice the right hand side of the previous equation becomes $(\sum_{\boldsymbol{z}\in\mathfrak{S}(A)} a(\boldsymbol{z})^{-1})^{-1}$. Proposition 2.4.1 follows from Thomson's principle and from the previous bound for the flow Φ. □

2.5 Proof of Theorem 2.2.2

Theorem 2.2.2 follows from Propositions 2.5.1 and 2.5.2 below. Throughout this section $1 \leq i \leq i_0$ and $1 \leq j \leq \ell_i$ are fixed and dropped from the notation.

Proposition 2.5.1. *For every disjoint subsets A, B of S,*

$$\mathrm{cap}_N(\mathcal{E}_N(A), \mathcal{E}_N(B)) \;\leq\; [1 + o_N(1)] \, \frac{(2\pi N)^{d/2}}{Z_N} \, \frac{e^{-NH_i}}{2\pi N} \, \mathrm{cap}_{\mathbb{G}}(A, B) \; .$$

The proof of this proposition is similar to the one of Proposition 2.3.1 up to Assertion 2.3.C. Recall the definition of the set $\mathcal{U}_N$. Denote by $\mathfrak{S}_{i,j}$ the set of all saddle points in Ω^i_j, and let $\mathfrak{B}^{\boldsymbol{z}}_N = \mathcal{U}_N \cap B^{\boldsymbol{z}}_N$, $\boldsymbol{z} \in \mathfrak{S}_{i,j}$, $\mathcal{V}_N = \mathcal{U}_N \setminus \cup_{\boldsymbol{z}\in\mathfrak{S}_{i,j}} \mathfrak{B}^{\boldsymbol{z}}_N$ so that

$$\mathcal{U}_N \;=\; \mathcal{V}_N \cup \bigcup_{\boldsymbol{z}\in\mathfrak{S}_{i,j}} \mathfrak{B}^{\boldsymbol{z}}_N \; .$$

In contrast with Section 2.3, we define a set $\mathfrak{B}^{\boldsymbol{z}}_N$ around each saddle point $\boldsymbol{z}$. By Assertion 2.3.C, the set $\mathcal{V}_N$ is formed by several connected components separated by the sets $\mathfrak{B}^{\boldsymbol{z}}_N$, $\boldsymbol{z} \in \mathfrak{S}_{i,j}$. Let $\mathcal{V}^a_N$ be the connected component of $\mathcal{V}_N$ which contains a point in W_a, $a \in S$.

Fix two disjoint subsets A, B of S and denote by $V_{A,B}$ the equilibrium potential between A and B for the graph $\mathbb{G}$. Fix a saddle point $\boldsymbol{z} \in \mathfrak{S}_{i,j}$ and assume that $\boldsymbol{z} \in W_a \cap W_b$. Recall the definition of the function $V^{\boldsymbol{z}}_N$ introduced in (2.3.5) and assume without loss of generality that $\partial_- B_N \cap W_a \neq \varnothing$ so that $\partial_+ B_N \cap W_b \neq \varnothing$. Define $W^{\boldsymbol{z}}_N : \mathfrak{B}^{\boldsymbol{z}}_N \to [0, 1]$ as

$$W^{\boldsymbol{z}}_N(\boldsymbol{x}) \;=\; V_{A,B}(a) \;+\; [V_{A,B}(b) - V_{A,B}(a)] \, V^{\boldsymbol{z}}_N(\boldsymbol{x}) \; .$$

Let $V_N^{A,B} : \Xi_N \to [0,1]$ by

$$V_N^{A,B}(\boldsymbol{x}) \;=\; \begin{cases} V_{A,B}(a) & \boldsymbol{x} \in \mathcal{V}_N^a\ , \\ W_N^{\boldsymbol{z}}(\boldsymbol{x}) & \boldsymbol{x} \in \mathfrak{B}_N^{\boldsymbol{z}}\ , \\ (1/2) & \text{otherwise.} \end{cases}$$

Assertion 2.5.A. *Let ε_N be a sequence such that $N\varepsilon_N^3 \to 0$, $\exp\{-N\varepsilon_N^2\}$ converges to 0 faster than any polynomial. Then,*

$$\frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NF(\boldsymbol{z})}\, D_N(V_N^{A,B}) \;\le\; [1 + o_N(1)]\, D_{\mathbb{G}}(V_{A,B})\ ,$$

where $D_{\mathbb{G}}(V_{A,B})$ represents the Dirichlet form of $V_{A,B}$ with respect to the graph $\mathbb{G}$.

The proof of this assertion is similar to the one of Assertion 2.3.D. Proposition 2.5.1 follows from the last assertion and from the fact that $\mathrm{cap}_{\mathbb{G}}(A,B) = D_{\mathbb{G}}(V_{A,B})$.

We conclude the section with the proof of the lower bound.

Proposition 2.5.2. *For every disjoint subsets A, B of S,*

$$\mathrm{cap}_N(\mathcal{E}_N(A), \mathcal{E}_N(B)) \;\ge\; [1 + o_N(1)]\, \frac{(2\pi N)^{d/2}}{Z_N}\, \frac{e^{-NH_i}}{2\pi N}\, \mathrm{cap}_{\mathbb{G}}(A,B)\ .$$

Proof. Fix two disjoint subsets A, B of S. We construct below a divergence-free, unitary flow Ψ from $\mathcal{E}_N(A)$ to $\mathcal{E}_N(B)$.

Recall that we denote by $V_{A,B}$ the equilibrium potential between A and B in the graph $\mathbb{G}$. Denote by $\varphi = \varphi_{A,B}$ the flow from A to B in the graph $\mathbb{G}$ given by $\varphi(a,b) = \boldsymbol{c}(a,b)[V_{A,B}(a) - V_{A,B}(b)]/\mathrm{cap}_{\mathbb{G}}(A,B)$, and observe that $\varphi(a,b) = 0$ if a, b belong to A or if a, b belong to B. By [30, Proposition 3.2.2],

$$\frac{1}{\mathrm{cap}_{\mathbb{G}}(A,B)} \;=\; \frac{1}{2} \sum_{a,b\in S} \frac{1}{\boldsymbol{c}(a,b)}\, \varphi_{A,B}(a,b)^2 \;=:\; \|\varphi_{A,B}\|^2\ . \tag{2.5.1}$$

Assume first that each pair of wells has at most one saddle point separating them, that is, assume that the sets $W_a \cap W_b$ are either empty or singletons. In this case, each edge (a,b) of the graph $\mathbb{G}$ corresponds to a unique saddle point $\boldsymbol{z}$.

Denote by $\Phi_{a,b}$, $a \ne b \in S$, $\boldsymbol{c}(a,b) > 0$, the flow $\Phi_{\boldsymbol{z}}$ constructed just above (2.4.12) from $\mathcal{E}_N^a$ to $\mathcal{E}_N^b$, where $\boldsymbol{z} \in W_a \cap W_b$ is the saddle point separating W_a and W_b. Note that $\Phi_{a,b} \ne -\Phi_{b,a}$. We may assume that the flow $\Phi_{a,b}$ is a flow from $\boldsymbol{x}^a$ to $\boldsymbol{x}^b$, where $\boldsymbol{x}^c$, $c \in S$, are points in $\mathcal{E}_N^c$. Define the flow Ψ by

$$\Psi(\boldsymbol{x},\boldsymbol{y}) \;=\; \sum_{a,b} \varphi(a,b)\, \Phi_{a,b}(\boldsymbol{x},\boldsymbol{y})\ , \quad \boldsymbol{x}\,,\, \boldsymbol{y} \,\in\, \Xi_N\ ,$$

where the sum is carried out over all $a \neq b \in S$ such that $\varphi(a,b) > 0$. We claim that Ψ is a unitary, divergence-free flow from $\mathcal{E}_N(A)$ to $\mathcal{E}_N(B)$.

Clearly,

$$\sum_{\boldsymbol{x}\in\mathcal{E}_N(A),\boldsymbol{y}\notin\mathcal{E}_N(A)} \Psi(\boldsymbol{x},\boldsymbol{y}) \;=\; \sum_{a,b}\varphi(a,b) \sum_{\boldsymbol{x}\in\mathcal{E}_N(A),\boldsymbol{y}\notin\mathcal{E}_N(A)} \Phi_{a,b}(\boldsymbol{x},\boldsymbol{y})\;.$$

The flows $\Phi_{a,b}$ which cross $\mathcal{E}_N(A)$ are the ones starting or ending at $\mathcal{E}_N(A)$. Since, in addition, $\varphi(a,b) = 0$ if a, $b \in A$, and $\varphi(a,b) < 0$ if $a \notin A$, $b \in A$, the previous expression is equal to

$$\sum_{a\in A,b\notin A}\varphi(a,b) \sum_{\boldsymbol{x}\in\mathcal{E}_N(A),\boldsymbol{y}\notin\mathcal{E}_N(A)} \Phi_{a,b}(\boldsymbol{x},\boldsymbol{y}) \;=\; \sum_{a\in A,b\notin A}\varphi(a,b)\;,$$

where the last identity follows from the fact that $\Phi_{a,b}$ is a unitary flow from $\mathcal{E}_N^a$ to $\mathcal{E}_N^b$. As φ is a unitary flow from A to B, the last sum is equal to 1, proving that Ψ is unitary.

To prove that Ψ is divergence-free, fix a site $\boldsymbol{x} \notin \{\boldsymbol{x}^c : c \in A\cup B\}$. If $\boldsymbol{x} \notin \{\boldsymbol{x}^c : c \in S\setminus[A\cup B]\}$, Ψ has no divergence at $\boldsymbol{x}$ because it is the convex combination of flows which have no divergence at $\boldsymbol{x}$. If $\boldsymbol{x} = \boldsymbol{x}^c$, $c \notin A\cup B$, the flows $\Phi_{a,b}$, a, $b \neq c$, have no divergence at $\boldsymbol{x}^c$, while the divergence of $\Phi_{a,c}$ (resp. $\Phi_{c,a}$) at $\boldsymbol{x}^c$ is equal to -1 (resp. 1) because these flows are unitary and end (resp. start) at $\boldsymbol{x}^c$. Therefore, the divergence of Ψ at $\boldsymbol{x}^c$ is equal to

$$(\operatorname{div}\Psi)(\boldsymbol{x}^c) \;=\; \sum_{a,b}\varphi(a,b)\,(\operatorname{div}\Phi_{a,b})(\boldsymbol{x}^c) \;=\; -\sum_{a:\varphi(a,c)>0}\varphi(a,c) \;+\; \sum_{a:\varphi(c,a)>0}\varphi(c,a)\;.$$

Since φ is a divergence-free flow in the graph $\mathbb{G}$, this sum vanishes, which proves that Ψ is also divergence-free at $\boldsymbol{x}^c$, $c \in S\setminus[A\cup B]$.

We claim that the energy dissipated by the flow Ψ is given by

$$\|\Psi\|^2 \;=\; [1+o_N(1)]\,\frac{Z_N}{(2\pi N)^{d/2}}\,2\pi N\,e^{NH_i}\,\frac{1}{\operatorname{cap}_{\mathbb{G}}(A,B)}\;. \tag{2.5.2}$$

Indeed, by definition,

$$\|\Psi\|^2 \;=\; \sum_{j=1}^{d}\sum_{\boldsymbol{x}}\frac{1}{c(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_j)}\Psi(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_j)^2\;,$$

where the second sum is performed over all $\boldsymbol{x} \in \Xi_N$ such that $\boldsymbol{x}+\boldsymbol{e}_j \in \Xi_N$. By definition of the flow Ψ, the previous sum is equal to

$$\sum_{a,b}\varphi(a,b)^2\sum_{j=1}^{d}\sum_{\boldsymbol{x}}\frac{1}{c(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_j)}\Phi_{a,b}(\boldsymbol{x},\boldsymbol{y})^2 \tag{2.5.3}$$

$$+\;\sum_{(a,b)\neq(a',b')}\varphi(a,b)\varphi(a',b')\sum_{j=1}^{d}\sum_{\boldsymbol{x}}\frac{1}{c(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_j)}\Phi_{a,b}(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_j)\Phi_{a',b'}(\boldsymbol{x},\boldsymbol{x}+\boldsymbol{e}_j)\;.$$

By (2.4.9), the first line is equal to

$$[1 + o_N(1)]\, \frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NH_i} \sum_{a,b} \varphi(a,b)^2\, \frac{\sqrt{-\det[(\text{Hess}\, F)(\boldsymbol{z}_{a,b})]}}{\mu(\boldsymbol{z}_{a,b})}\ ,$$

where $\boldsymbol{z}_{a,b}$ stands for the saddle point in $W_a \cap W_b$ and $-\mu(\boldsymbol{z}_{a,b})$ for the negative eigenvalue of $(\text{Hess}\, F)(\boldsymbol{z}_{a,b})$. By (2.2.4) and by (2.5.1), the previous sum is equal to

$$\sum_{a,b} \frac{1}{\boldsymbol{c}(a,b)}\, \varphi(a,b)^2 \;=\; \frac{1}{\text{cap}_{\mathbb{G}}(A,B)}\ .$$

We turn to the second line of (2.5.3). We have seen in the proof of Proposition 2.2.4 that the contribution of the bonds which do not belong to a mesoscopic neighborhood of the saddle point $\boldsymbol{z}_{a,b}$ to the total energy dissipated by the flow $\Phi_{a,b}$ is negligible. We may therefore restrict our attention in the second line of (2.5.3) to the points $\boldsymbol{x}$ which belong to one of these neighborhoods. Since the flow $\Phi_{\boldsymbol{z}}$ vanishes in a neighborhood of a saddle point $\boldsymbol{z}' \neq \boldsymbol{z}$, the product $\Phi_{a,b}(\boldsymbol{x},\boldsymbol{y})\Phi_{a',b'}(\boldsymbol{x},\boldsymbol{y})$ vanishes for all for $(a,b) \neq (a',b')$ and all $\boldsymbol{x}$ in a neighborhood of some saddle point $\boldsymbol{z}$. In particular, the second line of (2.5.3) is of order

$$o_N(1)\, \frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NH_i}\ .$$

Assertion (2.5.2) follows from the estimates of the two lines of (2.5.3).

Since Ψ is a divergence-free unitary flow from $\mathcal{E}^N(A)$ to $\mathcal{E}^N(B)$, by Thomson's principle, and by (2.5.2),

$$\frac{1}{\text{cap}_N(\mathcal{E}^N(A), \mathcal{E}^N(B))} \;\le\; \|\Psi\|^2 \;=\; [1 + o_N(1)]\, \frac{Z_N}{(2\pi N)^{d/2}}\, 2\pi N\, e^{NH_i} \frac{1}{\text{cap}_{\mathbb{G}}(A,B)}\ .$$

This completes the proof of the proposition in the case where there is at most one saddle point between two wells.

In the general case, one has to change the definition of Ψ as follows. For each a, $b \in S$ such that $\varphi(a,b) > 0$, denote by $\boldsymbol{z}^1_{a,b}, \dots, \boldsymbol{z}^n_{a,b}$ the set of saddle points between W_a and W_b: $W_a \cap W_b = \{\boldsymbol{z}^1_{a,b}, \dots, \boldsymbol{z}^n_{a,b}\}$, where $n = n_{a,b}$. Set

$$\Psi \;=\; \sum_{a,b} \varphi(a,b) \sum_{k=1}^{n} \theta_k(a,b)\, \Phi_{\boldsymbol{z}^k_{a,b}}\ ,$$

where the sum is carried out over all $a \neq b \in S$ such that $\varphi(a,b) > 0$, where $\Phi_{\boldsymbol{z}^k_{a,b}}$ is the flow constructed just above (2.4.12) from $\mathcal{E}^a_N$ to $\mathcal{E}^b_N$ passing through the saddle point $\boldsymbol{z}^k_{a,b}$, and where

$$\theta_k(a,b) \;=\; \frac{\mu(\boldsymbol{z}^k_{a,b})}{\sqrt{-\det[(\text{Hess}\, F)(\boldsymbol{z}^k_{a,b})]}}\, \frac{1}{\boldsymbol{c}(a,b)}\ .$$

Note that $\sum_k \theta_k(a,b) = 1$. The arguments presented above for the case where there is at most one saddle point separating the wells can be easily adapted to the present case. □

2.6 Proof of Theorem 2.2.4

According to [33, Theorem 5.1], Theorem 2.2.4 follows from Proposition 2.6.1 below.

Recall the notation introduced in Section 2.2. Fix $1 \le i \le i_0$ and $1 \le j \le \ell_i$, which are dropped out from the notation. Fix a connected component $\Omega = \Omega^i_j$, $1 \le m \le n = n_{i,j}$ and denote by $\mathcal{E}_{m,N}$ the union of the wells $\mathcal{E}^a_N$, $a \in S_m$, $\mathcal{E}_{m,N} = \cup_{a\in S_m} \mathcal{E}^a_N$. As m is fixed throughout this section, it will sometimes be omitted from the notation.

Denote by $\{T_{m,N}(t) : t \ge 0\}$ the additive functional

$$T_{m,N}(t) \;=\; \int_0^t \mathbf{1}\{X_N(s) \in \mathcal{E}_{m,N}\}\, ds\;,$$

and by $S_{m,N}(t)$ its generalized inverse: $S_{m,N}(t) = \sup\{s \ge 0 : T_{m,N}(s) \le t\}$. The time-change process $X^{m,\mathrm{T}}_N(t) := X_N(S_{m,N}(t))$ is called the trace process of $X_N(t)$ on $\mathcal{E}_{m,N}$. The process $X^{m,\mathrm{T}}_N(t)$ is a $\mathcal{E}_{m,N}$-valued, continuous-time Markov chain. We refer to [3] for a summary of its properties.

Denote by $R^{m,\mathrm{T}}_N(\boldsymbol{x},\boldsymbol{y})$, $\boldsymbol{x}$, $\boldsymbol{y} \in \mathcal{E}_N$, the jump rates of the trace process. According to [3, Proposition 6.1],

$$R^{m,\mathrm{T}}_N(\boldsymbol{x},\boldsymbol{y}) \;=\; \lambda_N(\boldsymbol{x})\,\mathbf{P}_{\boldsymbol{x}}\big[\,H^+_{\mathcal{E}_{m,N}} = H_{\boldsymbol{y}}\,\big]\;, \quad \boldsymbol{x}\,,\, \boldsymbol{y} \in \mathcal{E}_{m,N}\,,\; \boldsymbol{x} \ne \boldsymbol{y}\,.$$

Denote by $r^m_N(a,b)$ the average rate at which the trace process jumps from $\mathcal{E}^a_N$ to $\mathcal{E}^b_N$, a, $b \in S_m$:

$$r^m_N(a,b) \;:=\; \frac{1}{\mu_N(\mathcal{E}^a_N)} \sum_{\boldsymbol{x}\in\mathcal{E}^a_N} \mu_N(\boldsymbol{x}) \sum_{\boldsymbol{y}\in\mathcal{E}^b_N} R^{m,\mathrm{T}}_N(\boldsymbol{x},\boldsymbol{y})\;. \tag{2.6.1}$$

Recall the definition of the projection Ψ^m_N introduced in (2.2.7). Denote by $\boldsymbol{X}^{m,\mathrm{T}}_N(t)$ the projection by Ψ^m_N of the trace process $X^{m,\mathrm{T}}_N(t)$, $\boldsymbol{X}^{m,\mathrm{T}}_N(t) = \Psi^m_N(X^{\mathrm{T}}_N(t))$.

Proposition 2.6.1. *Fix $1 \le i \le i_0$, $1 \le j \le \ell_i$, $1 \le m \le n_{i,j}$, $a \in S_m$ and a sequence of configurations $\boldsymbol{x}_N$ in $\mathcal{E}^a_N$. Under $\mathbf{P}_{\boldsymbol{x}_N}$, the time re-scaled projection of the trace $\mathbb{X}^{m,\mathrm{T}}_N(t) = \boldsymbol{X}^{m,\mathrm{T}}_N(t\beta_m)$ converges in the Skorohod topology to a S_m-valued continuous-time Markov chain $\mathbb{X}^m(t)$ whose jump rates are given by (2.2.9). Moreover, in the time scale β_m, the time spent by the original chain $X_N(t)$ outside $\mathcal{E}_{m,N}$ is negligible: for all $t > 0$,*

$$\lim_{N\to\infty} \mathbf{E}_{\boldsymbol{x}_N}\Big[\int_0^t \mathbf{1}\{X_N(s\beta_m) \notin \mathcal{E}_{m,N}\}\, ds\Big] \;=\; 0\;. \tag{2.6.2}$$

Proof. By [3, Theorem 2.7], the first assertion of the proposition follows by Lemmata 2.6.2 and 2.6.3 below. We turn to the proof of the second assertion of the proposition.

Fix $\delta > 0$ such that $\delta < H_{i+1} - H_i$ and let $\widetilde{\Omega}^i_\delta = \{\boldsymbol{x} \in \Xi : F(\boldsymbol{x}) \le H_i + \delta\}$. Denote by $\widetilde{\Omega}_\delta = \widetilde{\Omega}^{i,j}_\delta$ the connected component which contains Ω^i_j and let $A_N = \widetilde{\Omega}_\delta \cap \Xi_N$.

By the large deviations principle for the chain $X_N(t)$, for every $T > 0$ and every sequence $\boldsymbol{x}_N \in \mathcal{E}_{1,N}$,

$$\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N}\big[H_{A_N^c} \le T\beta_m\big] \;=\; 0 \;.$$

This statement can be proved as Theorem 4.2 of Chapter 4, or Theorem 6.2 of Chapter 6 in [28]. It is therefore enough to prove (2.6.2) for the chain $X_N(t)$ reflected at A_N, the chain obtained by removing all jumps between A_N and A_N^c.

Denote the reflected chain by $\tilde{X}_N(t)$, by $\tilde{\mu}_N$ its stationary state, and by $\tilde{\mathbf{P}}_{\boldsymbol{x}}$ the measure on the path space $D(\mathbb{R}_+, A_N)$ induced by the chain $\tilde{X}_N(t)$ starting from $\boldsymbol{x} \in A_N$. Expectation with respect to $\tilde{\mathbf{P}}_{\boldsymbol{x}}$ is represented by $\tilde{\mathbf{E}}_{\boldsymbol{x}}$. We have to prove (2.6.2) with $X_N(t)$, $\mathbf{E}_{\boldsymbol{x}_N}$ replaced by $\tilde{X}_N(t)$, $\tilde{\mathbf{E}}_{\boldsymbol{x}}$, respectively. Equation (2.6.2) with these replacements is represented as (2.6.2 $*$).

Let $\Delta_{m,N} = A_N \setminus \mathcal{E}_{m,N}$. By definition of the sets $\mathcal{E}^a_N$, for $a \in S_1$, $\tilde{\mu}_N(\Delta_{1,N})/\tilde{\mu}_N(\mathcal{E}^a_N)$ is at most of the order $\exp\{-N(\theta_1 - \epsilon)\}$, where ϵ has been introduced right before (2.2.2). For each fixed $1 < m \le n$, $a \in S_m$, $\tilde{\mu}_N(\Delta_{m,N})/\tilde{\mu}_N(\mathcal{E}^a_N)$ is at most of the order $\exp\{-N(\theta_m - \theta_{m-1} - \epsilon)\}$. Therefore, for every $1 \le m \le n$, $a \in S_m$,

$$\lim_{N\to\infty} \frac{\tilde{\mu}_N(\Delta_{m,N})}{\tilde{\mu}_N(\mathcal{E}^a_N)} \;=\; 0 \;. \tag{2.6.3}$$

Fix $1 \le m < n$, $a \in S_{m+1}$ and a sequence $\boldsymbol{x}_N \in \mathcal{E}^a_N$. By the large deviations principle for the chain $\tilde{X}_N(t)$, for every $T > 0$,

$$\lim_{N\to\infty} \tilde{\mathbf{P}}_{\boldsymbol{x}_N}\big[H_{(\mathcal{E}^a_N)^c} \le T\beta_m\big] \;=\; 0 \;. \tag{2.6.4}$$

By [3, Theorem 2.7], assertion (2.6.2 $*$) follows from the first part of this proposition and from (2.6.3), (2.6.4), which concludes the proof. □

Recall that we denoted by $\{\boldsymbol{m}_{a,1}, \dots, \boldsymbol{m}_{a,q}\}$, $q = q_a$, the deepest local minima of F which belong to W_a.

Lemma 2.6.2. *Under the hypotheses of Proposition 2.6.1, for every $a \in S_m$,*

$$\lim_{N\to\infty} \sup_{\boldsymbol{y}\in\mathcal{E}^a_N} \frac{\mathrm{cap}_N(\mathcal{E}^a_N, \cup_{b\in S_m, b\neq a}\mathcal{E}^b_N)}{\mathrm{cap}_N(\{\boldsymbol{y}\}, \{\boldsymbol{m}_{a,1}\})} \;=\; 0 \;.$$

Proof. Fix $a \in S_m$, $\boldsymbol{y} \in \mathcal{E}^a_N$. We estimate $\mathrm{cap}_N(\{\boldsymbol{y}, \{\boldsymbol{m}_{a,1}\})$ through Thomson's principle. Let $(\boldsymbol{y} = \boldsymbol{x}_0, \boldsymbol{x}_1, \dots, \boldsymbol{x}_m = \boldsymbol{m}_{a,1})$ be a path γ from $\boldsymbol{y}$ to $\boldsymbol{m}_{a,1}$ so that $\|\boldsymbol{x}_i - \boldsymbol{x}_{i+1}\| = 1/N$. By Thomson's principle,

$$\frac{1}{\mathrm{cap}_N(\{\boldsymbol{y}\}, \{\boldsymbol{m}_{a,1}\})} \;\le\; \sum_{j=0}^{m-1} \frac{1}{\mu_N(\boldsymbol{x}_j)\, R_N(\boldsymbol{x}_j, \boldsymbol{x}_{j+1})} \;.$$

In view of the explicit formulas for the measure μ_N and the rates R_N, there exists a finite constant C_0 such that

$$\frac{1}{\mu_N(\boldsymbol{x}_j)\, R_N(\boldsymbol{x}_j, \boldsymbol{x}_{j+1})} \;\le\; C_0\, Z_N\, e^{NF(\boldsymbol{x}_i)}\ .$$

It follows from the definition (2.2.2) of the set W_a^ϵ that the path γ can be chosen in such a way that $F(\boldsymbol{x}_j) \le H_i - \epsilon$. The previous sum is thus bounded above by $C_0\, Z_N\, N\, \exp N\{H_i - \epsilon\}$, where N has been introduced to take care of the length of the path. This estimate is uniform over $\boldsymbol{y} \in \mathcal{E}_N^a$. To conclude the proof of the lemma, it remains to recall the assertion of Theorem 2.2.2. □

Lemma 2.6.3. *Under the hypotheses of Proposition 2.6.1, for every a, $b \in S_m$,*

$$\lim_{N\to\infty} \beta_m\, r_N^m(a,b) \;=\; \boldsymbol{r}_m(a,b)\ ,$$

where the rates $\boldsymbol{r}_m(a,b)$ are given by (2.2.9).

Proof. By [3, Lemma 6.8],

$$\begin{aligned} r_N^m(a,b) \;=\; \frac{1}{2}\,\frac{1}{\mu_N(\mathcal{E}_N^a)} \Big\{ &\mathrm{cap}_N(\mathcal{E}_N^a, \mathcal{E}_{m,N}\setminus \mathcal{E}_N^a) \;+\; \mathrm{cap}_N(\mathcal{E}_N^b, \mathcal{E}_{m,N}\setminus \mathcal{E}_N^b) \\ &-\; \mathrm{cap}_N(\mathcal{E}_N^a\cup \mathcal{E}_N^b, \mathcal{E}_{m,N}\setminus [\mathcal{E}_N^a\cup \mathcal{E}_N^b]) \Big\}\ . \end{aligned}$$

By (2.2.3),

$$\mu_N(\mathcal{E}_N^a) \;=\; [1+o_N(1)]\,\frac{(2\pi N)^{d/2}}{Z_N}\,\frac{e^{-NH_i}}{2\pi N}\,\beta_m\,\boldsymbol{\mu}(a)\ .$$

The assertion of the lemma follows from this equation, Theorem 2.2.2 and the definition of $\boldsymbol{c}_m$ given just above (2.2.9). □

We conclude this section with a calculation which provides an estimation for the measure of the wells. Denote by $\boldsymbol{m}^1, \dots, \boldsymbol{m}^r$ the global minima of F on Ξ. We claim that

$$\lim_{N\to\infty} \frac{e^{NF(\boldsymbol{m}^1)}}{(2\pi N)^{d/2}}\, Z_N \;=\; \sum_{k=1}^{r} \frac{1}{\sqrt{\det[(\mathrm{Hess}\, F)(\boldsymbol{m}^k)]}}\ \cdot \tag{2.6.5}$$

A similar argument yields (2.2.3).

Indeed, fix a sequence ε_N such that $\lim_{N\to\infty} N\varepsilon_N^3 = 0$ and for which $\exp\{-N\varepsilon_N^2\}$ vanishes faster than any polynomial. Fix $1 \le k \le r$ and denote by $\boldsymbol{w}^1, \dots, \boldsymbol{w}^d$ the eigenvectors of $(\mathrm{Hess}\, F)(\boldsymbol{m}^k)$ and by $0 < \lambda_1 \le \cdots \le \lambda_d$ the eigenvalues. Consider the neighborhood B_N of $\boldsymbol{m}^k$ defined by

$$B_N \;=\; \big\{\boldsymbol{x} \in \Xi_N : |(\boldsymbol{x} - \boldsymbol{m}^k)\cdot \boldsymbol{w}^i| \le \varepsilon_N\, ,\, 1 \le i \le d\big\}\ .$$

It follows from the assumptions on ε_N and on F, from a second-order Taylor expansion of F around $\boldsymbol{m}^k$, and from a simple calculation that

$$\lim_{N\to\infty} \frac{e^{NF(\boldsymbol{m}^1)}}{(2\pi N)^{d/2}} \sum_{\boldsymbol{x}\in B_N} e^{-NF(\boldsymbol{x})} \;=\; \frac{1}{\sqrt{\det[(\operatorname{Hess} F)(\boldsymbol{m}^k)]}} \;.$$

Denote by $B_N^{(2)}$ the neighborhood of $\boldsymbol{m}^k$ defined by

$$B_N^{(2)} \;=\; \big\{\boldsymbol{x}\in\Xi_N : \|\boldsymbol{x}-\boldsymbol{m}^k\| \le \lambda_1/(4C_1)\big\}\;,$$

where C_1 is the Lipschitz constant introduced in assumption (H1). Clearly, on $B_N^{(2)}$, $F(\boldsymbol{x})-F(\boldsymbol{m}^1) \ge (1/2)\lambda_1\|\boldsymbol{x}-\boldsymbol{m}^k\|^2 - C_1\|\boldsymbol{x}-\boldsymbol{m}^k\|^3 \ge (\lambda_1/4)\|\boldsymbol{x}-\boldsymbol{m}^k\|^2$. Therefore, as $\|\boldsymbol{x}-\boldsymbol{m}^k\|^2 \ge \varepsilon_N^2$ on B_N^c and as $N\,\varepsilon_N^2\to\infty$,

$$\lim_{N\to\infty} \frac{e^{NF(\boldsymbol{m}^1)}}{(2\pi N)^{d/2}} \sum_{\boldsymbol{x}\in B_N^{(2)}\setminus B_N} e^{-NF(\boldsymbol{x})} \;=\; 0\;.$$

On the complement of the union of all $B_N^{(2)}$-neighborhoods of the global minima $\boldsymbol{m}^k$, $F(\boldsymbol{x})-F(\boldsymbol{m}^1)\ge\delta$ for some $\delta>0$. In particular the contribution to Z_N of the sum over this set is negligible. Putting together all previous estimates we obtain (2.6.5).

2.7 Proof of Theorem 2.2.7

We prove in this section Theorem 2.2.7. Recall the notation introduced in Subsection 2.2.D. Herafter, C_0 represents a finite constant independent of N which may change from line to line. We start with some preliminary results.

Lemma 2.7.1. *Fix $1\le i\le i_0$, $1\le j\le \ell_i$, and $a\in S=\{1,\dots \ell_j^i\}$. Let $\mathcal{B}_a = \cup_{\boldsymbol{z}\in\mathfrak{S}_a}\mathcal{D}_{\boldsymbol{z}}$. For any sequence $\{\boldsymbol{x}_N : N\ge 1\}$, $\boldsymbol{x}_N\in\mathcal{E}_N^a$,*

$$\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N}\Big[H_{\mathcal{D}_a} = H_{\mathcal{B}_a}\Big] \;=\; 1\;.$$

Proof. By [7, Lemma 4.3],

$$\mathbf{P}_{\boldsymbol{x}_N}[H_{\mathcal{D}_a} < H_{\mathcal{B}_a}] \;\le\; \frac{\operatorname{cap}_N(\boldsymbol{x}_N,\mathcal{D}_a\setminus\mathcal{B}_a)}{\operatorname{cap}_N(\boldsymbol{x}_N,\mathcal{D}_a)}\;.$$

Let $V:\Xi_N\to[0,1]$ be the indicator of the set $\mathcal{D}_a\setminus\mathcal{B}_a$. By the Dirichlet principle and a straightforward computation,

$$\operatorname{cap}_N(\boldsymbol{x}_N,\mathcal{D}_a\setminus\mathcal{B}_a) \le D_N(V) \le C_0 Z_N^{-1} N^d \exp\{-N(H_i+\delta_N)\}.$$

On the other hand, it is not difficult to construct a divergence-free, unitary flow Φ from $\mathcal{B}_a$ to $\boldsymbol{x}_N$, similar to the one presented in the proof of Lemma 2.6.2, such that $\|\Phi\|^2 \le C_0 Z_N N\exp\{NH_i\}$. Therefore, by Thomson's principle, $\operatorname{cap}_N(\boldsymbol{x}_N,\mathcal{D}_a)^{-1}$ is bounded by $C_0 Z_N N\exp\{NH_i\}$, which proves the lemma in view of the definition of the sequence δ_N. □

Fix $\boldsymbol{z} \in \mathfrak{S}_a$ and recall that we denote by $\boldsymbol{v} = \boldsymbol{w}^1$, $\boldsymbol{w}^j$, $2 \le j \le d$, a basis of eigenvectors of $\operatorname{Hess} F(\boldsymbol{z})$, where $\boldsymbol{v}$ is the one associated to the unique negative eigenvalue $-\mu$. Let $B_N = B_N^{\boldsymbol{z}}$ be a mesoscopic neighborhood of $\boldsymbol{z}$:

$$B_N = \Big\{ \boldsymbol{x} \in \Xi_N : |(\boldsymbol{x} - \boldsymbol{z}) \cdot \boldsymbol{v}| \le a\, \varepsilon_N \,,\ \max_{2 \le j \le d} |(\boldsymbol{x} - \boldsymbol{z}) \cdot \boldsymbol{w}^j| \le \varepsilon_N \Big\}\,, \tag{2.7.1}$$

where $a = \max\{1, \mu^{-1}(1 + \sum_{2\le j \le d} \lambda_j)\}$, and ε_N is a sequence of positive numbers such that $N^{-2} \ll \varepsilon_N^4 \ll N^{-3/2}$, $\varepsilon_N^2 \gg \delta_N$. The sets $D_{\boldsymbol{z}}$, $\boldsymbol{z} \in \mathfrak{S}_a$, are contained in B_N because, by (2.2.11) and (2.2.12),

$$\sup_{\boldsymbol{x} \in D_{\boldsymbol{z}}} \|\boldsymbol{x} - \boldsymbol{z}\|^2 \ \le\ (4/\lambda_2)\, \delta_N\,. \tag{2.7.2}$$

Recall from (2.3.3) the definition of the outer boundary ∂B_N of B_N, and let $\partial_- B_N$, $\partial_+ B_N$ be the pieces of the outer boundary of B_N defined by

$$\begin{aligned} \partial_- B_N &= \{ \boldsymbol{x} \in \partial B_N : (\boldsymbol{x} - \boldsymbol{z}) \cdot \boldsymbol{v} < -a\, \varepsilon_N \}\,, \\ \partial_+ B_N &= \{ \boldsymbol{x} \in \partial B_N : (\boldsymbol{x} - \boldsymbol{z}) \cdot \boldsymbol{v} > a\, \varepsilon_N \}\,. \end{aligned}$$

A Taylor expansion of F around $\boldsymbol{z}$ shows that

$$\max_{\boldsymbol{x} \in \partial_- B_N \cup \partial_+ B_N} F(\boldsymbol{x}) \ \le\ H_i \ -\ \frac{1}{2}\, \varepsilon_N^2 \big(1 + O(\varepsilon_N)\big)\,. \tag{2.7.3}$$

Denote by H_N the hitting time of the boundary ∂B_N, and by $H_N^{\pm}$ the hitting time of the sets $\partial_\pm B_N$.

Proposition 2.7.2. *For every $\boldsymbol{z} \in \mathfrak{S}_a$,*

$$\lim_{N\to\infty} \max_{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}} \Big| \mathbf{P}_{\boldsymbol{x}}\big[H_N = H_N^{\pm}\big] \ -\ \frac{1}{2} \Big| \ =\ 0\,.$$

Corollary 2.7.3. *Let $\{\boldsymbol{x}_N^c : N \ge 1\}$, $c \in S$, be a sequence of points in $\mathcal{E}_N^c$ and let $\hat{S} = \hat{S}_N = \{\boldsymbol{x}_N^c : c \in S\}$. Fix $a \ne b \in S$ and $\boldsymbol{z} \in \mathfrak{S}_{a,b}$. Then,*

$$\lim_{N\to\infty} \max_{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}} \Big| \mathbf{P}_{\boldsymbol{x}}\big[H_{\hat{S}} = H_{\boldsymbol{x}_N^c}\big] \ -\ q(c) \Big| \ =\ 0\,,$$

where $q(a) = q(b) = 1/2$ and $q(c) = 0$ for $c \in S \setminus \{a, b\}$.

Proof. Fix $a \ne b \in S$, $c \in S$, $\boldsymbol{z} \in \mathfrak{S}_{a,b}$ and $\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}$. Since $H_N \le H_{\hat{S}}$, by the strong Markov property,

$$\mathbf{P}_{\boldsymbol{x}}\big[H_{\hat{S}} = H_{\boldsymbol{x}_N^c}\big] \ =\ \mathbf{E}_{\boldsymbol{x}}\Big[\mathbf{P}_{X_N(H_N)}\big[H_{\hat{S}} = H_{\boldsymbol{x}_N^c}\big]\Big]\,.$$

By the proposition, the previous expression is equal to

$$\sum_{\boldsymbol{y} \in \partial_\pm B_N} \mathbf{P}_{\boldsymbol{x}}\big[X_N(H_N) = \boldsymbol{y}\big] \mathbf{P}_{\boldsymbol{y}}\big[H_{\hat{S}} = H_{\boldsymbol{x}_N^c}\big] \ +\ R_N(\boldsymbol{x})\,,$$

where $\lim_{N\to\infty} \max_{\boldsymbol{x}\in\mathfrak{D}_{\boldsymbol{z}}} |R_N(\boldsymbol{x})| = 0$.

Let $\boldsymbol{x}(t)$, $0 \le t \le 1$, be a continuous path from $\boldsymbol{x}_N^a$ to $\boldsymbol{x}_N^b$ for which there exists $0 < t_0 < 1$ such that $F(\boldsymbol{x}(t)) < H_i$ for all $t \neq t_0$ and $\boldsymbol{x}(t_0) = \boldsymbol{z}$. Assume that this path crosses B_N only at $\partial_\pm B_N$ and assume, without loss of generality, that it crosses $\partial_- B_N$ before $\partial_+ B_N$. In this case, an argument similar to the one presented in the proof of Lemma 2.7.1 yields that

$$\lim_{N\to\infty} \min_{\boldsymbol{y}\in\partial_+ B_N} \mathbf{P}_{\boldsymbol{y}}\big[H_{\hat{S}} = H_{\boldsymbol{x}_N^b}\big] \;=\; 1\;, \quad \lim_{N\to\infty} \min_{\boldsymbol{y}\in\partial_- B_N} \mathbf{P}_{\boldsymbol{y}}\big[H_{\hat{S}} = H_{\boldsymbol{x}_N^a}\big] \;=\; 1\;.$$

In the proof of this assertion, instead of using an indicator function to bound from above the capacity, as we did in the proof of Lemma 2.7.1, we use the function constructed in Section 2.3. Note also that if the continuous path from $\boldsymbol{x}_N^a$ to $\boldsymbol{x}_N^b$ crosses first $\partial_+ B_N$ and then $\partial_- B_N$, one has to interchange a and b in the previous displayed formula.

Up to this point we showed that

$$\mathbf{P}_{\boldsymbol{x}}\big[H_{\hat{S}} = H_{\boldsymbol{x}_N^c}\big] \;=\; \mathbf{P}_{\boldsymbol{x}}\big[H_N = H_N^-\big]\mathbf{1}\{c=a\} \;+\; \mathbf{P}_{\boldsymbol{x}}\big[H_N = H_N^+\big]\mathbf{1}\{c=b\} \;+\; R_N'(\boldsymbol{x})\,,$$

where $R_N'(\boldsymbol{x})$ is a new sequence with the same properties as the previous one. To complete the proof it remains to recall the statement of the proposition. □

The proof of Proposition 2.7.2 is based on the fact that in a neighborhood of radius $N^{-1/2}$ around a saddle point $\boldsymbol{z}$ the re-scaled chain $\sqrt{N}X_N(tN)$ behaves as a diffusion. More precisely, let $g:\mathbb{R}^d \to \mathbb{R}$ be a three times continuously differentiable function and let $G(\boldsymbol{x}) = g(\sqrt{N}(\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{w}^1, \dots, \sqrt{N}(\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{w}^d)$. A Taylor expansion of the potential F around $\boldsymbol{z}$ gives that for $\boldsymbol{x}\in B_N$,

$$(L_N G)(\boldsymbol{x}) \;=\; \frac{1}{N}\sum_{j=1}^d \Big\{ -\lambda_j \boldsymbol{u}_j\,(\partial_{\boldsymbol{x}_j} g)(\boldsymbol{u}) + (\partial^2_{\boldsymbol{x}_j} g)(\boldsymbol{u})\Big\} \;+\; \frac{R_N}{N}\;, \tag{2.7.4}$$

where $\boldsymbol{u}_j = \sqrt{N}(\boldsymbol{x}-\boldsymbol{z})\cdot\boldsymbol{w}^j$, and R_N is an error term satisfying

$$|R_N| \;\le\; C_0\, N\varepsilon_N^2 \Big\{\frac{C_1(g)}{\sqrt{N}} \;+\; \frac{C_2(g)}{N}\Big\} \;+\; C_0\,\frac{C_3(g)}{\sqrt{N}}\;.$$

In this formula, $C_1(g) = \max_{1\le j\le d} \sup_{\boldsymbol{u}, \|\boldsymbol{u}\|\le a\sqrt{N}\varepsilon_N} |(\partial_{\boldsymbol{x}_j} g)(\boldsymbol{u})|$, with a similar definition for $C_2(g)$ and $C_3(g)$, replacing first derivates by second and thirds. Identity (2.7.4) asserts that the process $(\sqrt{N}(X_N(tN)-\boldsymbol{z})\cdot\boldsymbol{w}^1, \dots, \sqrt{N}(X_N(tN)-\boldsymbol{z})\cdot\boldsymbol{w}^d)$ is close to a diffusion whose coordinates evolve independently. The first coordinate has a drift towards $\pm\infty$ proportional to its distance to the origin, while the other coordinates are Ornstein-Uhlenbeck processes.

Lemma 2.7.4. *There exists a finite constant C_0 such that for every $\boldsymbol{z}\in\mathfrak{S}_a$,*

$$\max_{\boldsymbol{x}\in\mathfrak{D}_{\boldsymbol{z}}} \mathbf{E}_{\boldsymbol{x}}\big[H_N\big] \;\le\; C_0 N^{3/2}\varepsilon_N\;.$$

Proof. Let $g : \mathbb{R} \to \mathbb{R}$ be given by $g(x) = \int_0^x \exp\{-\mu y^2/2\} \int_0^y \exp\{\mu z^2/2\} dz dy$. It is clear that g solves the differential equation $\mu x g'(x) + g''(x) = 1$, $x \in \mathbb{R}$. By Dynkin's formula, for every $t > 0$, $\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}$,

$$\mathbf{E}_{\boldsymbol{x}}\Big[G\big(X_N(t \wedge H_N)\big) - G(\boldsymbol{x}) - \int_0^{t\wedge H_N} (L_N G)(X_N(s))\, ds\Big] \;=\; 0\;, \qquad (2.7.5)$$

where $G(\boldsymbol{x}) = g(N^{1/2}[\boldsymbol{x} - \boldsymbol{z}] \cdot \boldsymbol{v})$. By (2.7.4) and since $|g'(x)| \le C_0$, $|g''(x)| \le C_0|x|$, $|g'''(x)| \le C_0 x^2$, on B_N, $N(L_N G)(x) - 1$ is absolutely bounded by $C_0\sqrt{N}\varepsilon_N^2$. Therefore,

$$\big(1 - C_0\sqrt{N}\varepsilon_N^2\big)\mathbf{E}_{\boldsymbol{x}}\big[t \wedge H_N\big] \;\le\; N\,\mathbf{E}_{\boldsymbol{x}}\Big[G\big(X_N(t \wedge H_N)\big)\Big]\;.$$

Since $|g(x)| \le C_0|x|$, $\sup_{\boldsymbol{x}\in B_N} |G(\boldsymbol{x})| \le C_0\sqrt{N}\varepsilon_N$. To complete the proof of the lemma, it remains to observe that $\sqrt{N}\varepsilon_N^2 \to 0$ and to let $t \uparrow \infty$. □

Lemma 2.7.5. *For every $\boldsymbol{z} \in \mathfrak{S}_a$,*

$$\lim_{N\to\infty} \max_{\boldsymbol{x}\in\mathcal{D}_{\boldsymbol{z}}} \mathbf{P}_{\boldsymbol{x}}\big[H_N < H_N^+ \wedge H_N^-\big] \;=\; 0\;.$$

Proof. The proof is similar to the one of the previous lemma. Fix $2 \le j \le d$ and let $g : \mathbb{R} \to \mathbb{R}$ be given by $g(x) = x^2$. By Dynkin's formula, for every $t > 0$, $\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}$, (2.7.5) holds with $G(\boldsymbol{x}) = g(N^{1/2}[\boldsymbol{x} - \boldsymbol{z}] \cdot \boldsymbol{w}^j)$. By (2.7.4), $(L_N G)(\boldsymbol{x}) \le (2 + R_N)/N$ and $R_N/N \le C_0\varepsilon_N^3$. Therefore, letting $t \uparrow \infty$, by Lemma 2.7.4 we get that

$$\begin{aligned}\mathbf{E}_{\boldsymbol{x}}\Big[G\big(X_N(H_N)\big)\Big] \;&\le\; G(\boldsymbol{x}) \;+\; \Big(\frac{2}{N} + C_0\varepsilon_N^3\Big)\,\mathbf{E}_{\boldsymbol{x}}\big[H_N\big]\\ &\le\; G(\boldsymbol{x}) \;+\; C_0\Big(\frac{1}{N} + C_0\varepsilon_N^3\Big)N^{3/2}\varepsilon_N\;.\end{aligned}$$

The event $\mathcal{A}_N = \{|\,(X_N(H_N) - \boldsymbol{z}) \cdot \boldsymbol{w}^j\,| > \varepsilon_N\}$ corresponds to the event that the process $X_N(t)$ reaches the boundary of B_N by hitting the set $\{\boldsymbol{x} \in B_N : [\boldsymbol{x} - \boldsymbol{z}] \cdot \boldsymbol{w}^j = \pm\varepsilon_N\}$. On this event the function G is equal to $N\varepsilon_N^2$. Since G is nonnegative,

$$N\varepsilon_N^2\,\mathbf{P}_{\boldsymbol{x}}[\mathcal{A}_N] \;\le\; \mathbf{E}_{\boldsymbol{x}}\Big[G\big(X_N(H_N)\big)\Big]\;.$$

On the other hand, by Schwarz inequality and by (2.7.2), on the set $\mathcal{D}_{\boldsymbol{z}}$, $G(\boldsymbol{x})$ is absolutely bounded by $C_0 N\delta_N$. Putting together the previous two estimates, we get that

$$\max_{\boldsymbol{x}\in\mathcal{D}_{\boldsymbol{z}}} \mathbf{P}_{\boldsymbol{x}}[\mathcal{A}_N] \;\le\; C_0\Big(\frac{\delta_N}{\varepsilon_N^2} \;+\; \frac{1}{\sqrt{N}\,\varepsilon_N} \;+\; \sqrt{N}\,\varepsilon_N^2\Big)\;.$$

This completes the proof of the lemma in view of the definition of the sequence ε_N. □

Proof of Proposition 2.7.2. The proof is similar to the one of the two previous lemmas. Let $g(x) = \int_0^x \exp\{-\mu y^2/2\} dy$. By Dynkin's formula, for every $t > 0$, $\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}$, (2.7.5) holds for $G(\boldsymbol{x}) = g(N^{1/2}[\boldsymbol{x} - \boldsymbol{z}] \cdot \boldsymbol{v})$. Since $g''(x) + \mu x g'(x) = 0$, and since the first three derivative of g are uniformly bounded, by Lemma 2.7.4 and by (2.7.4),

$$\max_{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}} \Big| \mathbf{E}_{\boldsymbol{x}} \big[G\big(X_N(H_N)\big)\big] - G(\boldsymbol{x}) \Big| \;\le\; C_0\, \varepsilon_N^3\, N \;\to\; 0 \;.$$

On $D_{\boldsymbol{z}}$, the function G vanishes. On the other hand, on the event $\{H_N = H_N^{\pm}\}$, $G(X_N(H_N)) = \pm(2\pi/\mu)^{1/2} + o_N(1)$. Therefore, by Lemma 2.7.5,

$$\lim_{N\to\infty} \max_{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{z}}} \Big| \mathbf{P}_{\boldsymbol{x}} \big[H_N = H_N^+ \big] \;-\; \mathbf{P}_{\boldsymbol{x}} \big[H_N = H_N^- \big] \Big| \;=\; 0 \;.$$

This completes the proof of the proposition in view of Lemma 2.7.5. □

Proof of Theorem 2.2.7. Fix $1 \le i \le i_0$, $1 \le j \le \ell_i$. For each $a \in S$, fix a sequence $\{\boldsymbol{x}_a^N : N \ge 1\}$ of points in $\mathcal{E}_N^a$. Denote by $\hat{R}_N(a,b)$, $a \ne b \in S$, the jump rates of the trace of $X_N(t)$ on the set $\{\boldsymbol{x}_N^a : a \in S\}$. By [3, Lemma 6.8],

$$\begin{aligned} \mu_N(\boldsymbol{x}_N^a)\, \hat{R}_N(a,b) \;=\; \frac{1}{2}\Big\{ & \mathrm{cap}_N(\{\boldsymbol{x}_N^a\}, \hat{S} \setminus \{\boldsymbol{x}_N^a\}) \;+\; \mathrm{cap}_N(\{\boldsymbol{x}_N^b\}, \hat{S} \setminus \{\boldsymbol{x}_N^b\}) \\ & -\; \mathrm{cap}_N(\{\boldsymbol{x}_N^a, \boldsymbol{x}_N^b\}, \hat{S} \setminus \{\boldsymbol{x}_N^a, \boldsymbol{x}_N^b\}) \Big\} \;, \end{aligned}$$

where $\hat{S} = \{\boldsymbol{x}_N^c : c \in S\}$. By Remark 2.2.3, equation (2.2.8), and the fact that $\boldsymbol{c}_1(a', b') = \boldsymbol{c}(a', b')$, for $a \ne b \in S$,

$$\lim_{N\to\infty} \frac{\hat{R}_N(a,b)}{\sum_{c \in S, c \ne a} \hat{R}_N(a,c)} \;=\; p(a,b) \;,$$

where $p(a,b)$ has been introduced in (2.2.6).

On the other hand, by [3, Proposition 6.1], for $a \ne b \in S$,

$$\hat{R}_N(a,b) \;=\; \lambda_N(\boldsymbol{x}_N^a)\, \mathbf{P}_{\boldsymbol{x}_N^a} \big[H_{\boldsymbol{x}_N^b} = H_{\hat{S}}^+ \big] \;,$$

and by the strong Markov property,

$$\mathbf{P}_{\boldsymbol{x}_N^a}[H_{\boldsymbol{x}_N^b} = H_{\hat{S}}^+] \;=\; \mathbf{P}_{\boldsymbol{x}_N^a}[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}]\, \mathbf{P}_{\boldsymbol{x}_N^a}[H_{\hat{S}}^+ < H_{\boldsymbol{x}_N^a}^+] \;.$$

It follows from the last three displayed equations that

$$\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N^a}[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}] \;=\; p(a,b) \;, \quad a \ne b \in S \;. \tag{2.7.6}$$

Since any continuous path from $\boldsymbol{x}_N^a$ to $\hat{S} \setminus \{\boldsymbol{x}_N^a\}$ must cross D_a, $H_{\mathcal{D}_a} < H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}$ $\mathbf{P}_{\boldsymbol{x}_N^a}$-almost surely. Hence, by the strong Markov property,

$$\mathbf{P}_{\boldsymbol{x}_N^a}[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}] \;=\; \mathbf{E}_{\boldsymbol{x}_N^a}\Big[\mathbf{P}_{X_N(H_{\mathcal{D}_a})}\big[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}\big] \Big] \;.$$

By Lemma 2.7.1,

$$\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N^a}[H_{\mathfrak{D}_a} < H_{\mathfrak{B}_a}] \;=\; 0\;. \tag{2.7.7}$$

Therefore,

$$\begin{aligned}
&\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N^a}[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}] \\
&\quad = \lim_{N\to\infty} \sum_{\boldsymbol{z}\in\mathfrak{S}_a} \sum_{\boldsymbol{y}\in\mathfrak{D}_{\boldsymbol{z}}} \mathbf{P}_{\boldsymbol{x}_N^a}\big[H_{\mathfrak{D}_a} = H_{\boldsymbol{y}}\big]\, \mathbf{P}_{\boldsymbol{y}}\big[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}\big]\;.
\end{aligned}$$

By the strong Markov property at time $H_{\hat{S}}$, the previous expression is equal to

$$\lim_{N\to\infty} \sum_{\boldsymbol{z}\in\mathfrak{S}_a} \sum_{\boldsymbol{y}\in\mathfrak{D}_{\boldsymbol{z}}} \sum_{c\in S} \mathbf{P}_{\boldsymbol{x}_N^a}\big[H_{\mathfrak{D}_a} = H_{\boldsymbol{y}}\big]\, \mathbf{P}_{\boldsymbol{y}}\big[H_{\boldsymbol{x}_N^c} = H_{\hat{S}}\big]\, \mathbf{P}_{\boldsymbol{x}_N^c}\big[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}\big]\;.$$

By Corollary 2.7.3, this limit is equal to

$$\begin{aligned}
&\frac{1}{2}\lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N^a}\big[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}\big]\, \mathbf{P}_{\boldsymbol{x}_N^a}\big[H_{\mathfrak{D}_a} = H_{\mathfrak{B}_a}\big] \\
&\quad + \frac{1}{2}\lim_{N\to\infty} \sum_{\boldsymbol{z}\in\mathfrak{S}_{a,b}} \mathbf{P}_{\boldsymbol{x}_N^a}\big[H_{\mathfrak{D}_a} = H_{\mathfrak{D}_{\boldsymbol{z}}}\big]\;.
\end{aligned}$$

By (2.7.7), we may replace in the first line $\mathbf{P}_{\boldsymbol{x}_N^a}[H_{\mathfrak{D}_a} = H_{\mathfrak{B}_a}]$ by 1.

In conclusion, in view of (2.7.6), we have shown that

$$p(a,b) \;=\; \lim_{N\to\infty} \mathbf{P}_{\boldsymbol{x}_N^a}[H_{\boldsymbol{x}_N^b} = H_{\hat{S}\setminus\{\boldsymbol{x}_N^a\}}] \;=\; \lim_{N\to\infty} \sum_{\boldsymbol{z}\in\mathfrak{S}_{a,b}} \mathbf{P}_{\boldsymbol{x}_N^a}\big[H_{\mathfrak{D}_a} = H_{\mathfrak{D}_{\boldsymbol{z}}}\big]\;.$$

This completes the proof of the theorem in the case where the set $\mathfrak{S}_{a,b}$ is a singleton. It is not difficult to modify this argument to handle the case with more than one saddle point between two wells. Indeed, since the proof does not depend on the behavior of the function F on W_a^c, we can modify F on $W_a^c \setminus [\cup_{\boldsymbol{z}\in\mathfrak{S}_a} B_\epsilon(\boldsymbol{z})]$, for some $\epsilon > 0$, creating new wells of height H_i, and turning each saddle point $\boldsymbol{z} \in \mathfrak{S}_a$ the unique saddle point between the well W_a and new well $W'_{\boldsymbol{z}}$. □

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