A NOTE ON VARIATIONAL REPRESENTATIONS OF CAPACITIES FOR REVERSIBLE AND NON-REVERSIBLE MARKOV CHAINS

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Abstract. Recent progress in the understanding of variational principles for capacities in the reversible and non-reversible setting is reviewed and commented. A particular emphasis is on the clarification of the mechanism behind the Dirichlet and Thomson principle in the non-reversible setting.

Contents

1. Introduction

One of the fundamental problems in potential theory is the classical Dirichlet problem. It originates from the study of physical questions coming from electrostatics. The investigation in existence and uniqueness of solutions to it has a long and venerable history which can be traced back e.g. to the work of Dirichlet [10], Poincaré [30], Kellogg [23], Lebesgue [25].

A first probabilistic solution to the classical Dirichlet problem was given by Kakutani [21]. His pioneering work and the extensive study by Doob [11] and Hunt [18, 19, 20] established the profound connection between potential theory and Markov processes. There is now a large literature on (transient) potential theory and Markov processes, including books e.g. by Blumenthal and Getoor [5], Port and Stone [31], Karatzas and Shreve [22, chap. 4] and the comprehensive treatment by Doob [13].

In the context of Markov chains on finite or denumerable state spaces, the connection to (recurrent) potential theory was developed by Doob [12] and Kemeny,

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Knapp and Snell [24]. Nash-Williams first linked the property of transience or reccurence of an irreducible reversible Markov chain to structural properties of the underlying electric network [28]. He proved that a Markov chain is recurrent, if and only if, the effective resistance between the starting position and infinity of the corresponding electric network is infinite. Although the discrete potential theory has proven to be a robust tool to study properties of Markov chains, its application attracted new attention with the beautiful elementary book by Doyle and Snell [15]. Since that time various aspects of Markov chains have been studied exploiting the interdependence between probabilistic objects and its analytic counterparts and there is now a large literature on this topic including books e.g. by Woess [34], Telcs [33], Levin, Peres and Wilmer [26], Lyons and Peres [27].

The potential theoretic approach to metastability, systematically studied in the past 10 years is a further example of the fruitful interplay between probability and potential theory [8, 9, 6, 1, 2, 32]. This approach is based on the following three observations. First, most quantities of physical interest can be represented as solutions of certain *Dirichlet problems* with respect to the generator of the dynamics. Second, the corresponding solutions can be expressed in terms of *capacities* and *equilibrium potential*. Mind that the first two observations do not rely on the reversibility of the Markov process as it will be illustrated in the remaining part of this introductory section. Third, capacities satisfies *variational principles*. For reversible Markov processes, these variational principles allow us to derive reasonable upper and lower bounds in a quit flexible way.

To our best knowledge, a Dirichlet principle for capacities in the non-reversible setting was first derived by Doyle in an unpublished manuscript [14]. In contrast to the reversible setting, the Dirichlet principle in the non-reversible setting is a saddle-point problem. In a recent paper [16], Gaudillière and Landim gave an alternative proof of Doyle's result and extended it by rewriting the saddle-point problem into a pure minimization problem. Mind that such kind of dual formulation of a variational principle is well known in the context of differential operations.

In this note, we present an alternative and elementary proof of the Dirichlet principle both in the reversible and non-reversible setting. By identifying the mechanism on which the derivation is based on, we can establish in addition a version of Thomson's principle in the non-reversible setting.

1.1. **Setting.** Let us consider a discrete-time Markov chain $\{X(t) \colon t \in \mathbb{N}_0\}$, defined on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$, taking values in a finite state space $\mathcal{S}$. The corresponding discrete generator, L, acts on functions $f \colon \mathcal{S} \to \mathbb{R}$ as

$$\big(Lf\big)(x) \;=\; \sum_{y \in \mathcal{S}} p(x,y)\,\big(f(y) - f(x)\big). \tag{1.1}$$

Its transition probabilities are denoted by $P = \big(p(x,y) : x, y \in \mathcal{S}\big)$. We will assume that the dynamics is *irreducible* and admits a *unique invariant measure*, m. We write $\langle\,\cdot\,,\cdot\,\rangle_m$ for the scalar product in $l^2(m)$. We consider further the time-reverse Markov chain, $\{X^*(t) \colon t \in \mathbb{N}_0\}$ those transition probabilities, $p^*(x,y)$, are characterized by

$$p^*(x,y) \;=\; \frac{m(y)}{m(x)}\, p(y,x). \tag{1.2}$$

Mind that the corresponding generator, L^*, is the adjoint of L in $l^2(m)$. Further, we denote by $S = \frac{1}{2}\big(L + L^*\big)$ the symmetrized operator.

We denote by $\mathbb{P}_y$ the law of the Markov chain $\{X(t)\}$ starting in a single configuration y and by $\mathbb{E}_y$ its expectation with respect to $\mathbb{P}_y$. Analog, we introduce the notation $\mathbb{P}^*_\nu$ and $\mathbb{E}^*_\nu$ to denote the law and expectation of the time-reversed Markov chain $\{X^*(t)\}$. For any $A \subset \mathcal{S}$, let τ_A be the first hitting time of the set A *after* time zero, i.e.

$$\tau_A \;:=\; \inf\big\{t > 0 \;\big|\; X(t) \in A\big\}.$$

When the set A is a singleton $\{y\}$ we write simply τ_y instead of $\tau_{\{y\}}$.

1.2. **Equilibrium potential and capacity.** We turn now our attention to the discrete analog of the classical *Dirichlet boundary value problem*. That is, given a non-empty subset $D \subset \mathcal{S}$, measurable functions $g\colon D^c \to \mathbb{R}$ and $u\colon D \to \mathbb{R}$, the task is to find a (bounded) function $f\colon \mathcal{S} \to \mathbb{R}$ which satisfies

$$\begin{cases} \big(Lf\big)(x) \;=\; -g(x), & x \in D^c \\ \qquad f(x) \;=\; u(x), & x \in D, \end{cases} \tag{1.3}$$

where $D^c = \mathcal{S} \setminus D$. Provided that such a function f exists, it will be called *solution to the Dirichlet problem*. The probabilistic solution of (1.3) in the discrete-time setting is well established, see for instance [29]. It is given by

$$f(x) \;=\; \mathbb{E}_x\left[u\big(X(\tau_D)\big) \;+\; \sum_{s=0}^{\tau_D - 1} g\big(X(s)\big)\right], \qquad \forall\, x \in D^c \tag{1.4}$$

whereas $f \equiv u$ on D. Mind that (1.4) allows us to compute many interesting expectation values for Markov chains by means of solving appropriate Dirichlet problems.

A fundamental quantity is the *equilibrium potential*, $h_{A,B}$, of a *capacitor*, (A, B), build up by two non-empty disjoint subsets $A, B \subset \mathcal{S}$. It is the unique solution of the following boundary value problem

$$\begin{cases} \big(Lf\big)(x) \;=\; 0, & x \in (A \cup B)^c \\ \qquad f(x) \;=\; \mathbb{1}_A(x), & x \in \;A \cup B. \end{cases} \tag{1.5}$$

In view of (1.4), the equilibrium potential has a natural interpretation in terms of *hitting probabilities*, i.e. $h_{A,B}(x) = \mathbb{P}_x\left[\tau_A < \tau_B\right]$, $x \notin A \cup B$. A related quantity is the *equilibrium measure*, $e_{A,B}$, on A which is defined through

$$e_{A,B}(x) \;:=\; -\big(Lh_{A,B}\big)(x) \;=\; \mathbb{P}_x\big[\tau_B < \tau_A\big], \qquad \forall\, x \in A. \tag{1.6}$$

Analog, we denote by $h^*_{A,B}$ and $e^*_{A,B}$ the equilibrium potential and equilibrium measure with respect to L^*, i.e. $h^*_{A,B}(x) = \mathbb{P}^*_x\left[\tau_A < \tau_B\right]$, $x \notin A \cup B$.

The key object we will work with is the *capacity* of a capacitor (A, B) with potential one on A and zero on B. It is defined as

$$\operatorname{cap}(A,B) \;:=\; \sum_{x \in A} m(x)\, e_{A,B}(x), \qquad \operatorname{cap}^*(A,B) \;:=\; \sum_{x \in A} m(x)\, e^*_{A,B}(x). \tag{1.7}$$

The *energy* associated to the pair (P, m) is defined by $\mathcal{E}(f) := \langle f, -Lf \rangle_m$ for any $f \in l^2(m)$. As a consequence of the fact that $h_{A,B}$ and $h^*_{A,B}$ satisfy the same boundary conditions, it holds that

$$\operatorname{cap}(A,B) \;=\; \langle h^*_{A,B}, -L h_{A,B} \rangle_m \;=\; \langle -L^* h^*_{A,B}, h_{A,B} \rangle_m \;=\; \operatorname{cap}^*(A,B). \tag{1.8}$$

Moreover, an application of Green's first identity which is just a summation by parts yields

$$\operatorname{cap}(A,B) \;=\; \frac{1}{2} \sum_{x,y \in \mathcal{S}} m(x)\, p^s(x,y)\, \big(h_{A,B}(x) - h_{A,B}(y)\big)^2 \tag{1.9}$$

where $p^s(x,y) = \frac{1}{2}\big(p(x,y) + p^*(x,y)\big)$ denotes the symmetrized transition matrix.

Remark 1.1. Suppose that the cardinality of both set A and B is larger than one. In such a situation let us define a new Markov chain on the state space $\mathfrak{S}$ in which the sets A and B are collapsed to a singleton ξ_A and ξ_B, i.e. $\mathfrak{S} = \mathcal{S} \setminus (A \cup B) \cup \xi_A \cup \xi_B$.

Consider a map $\rho \colon \mathcal{S} \to \mathfrak{S}$,

$$x \;\longmapsto\; \rho(x) \;:=\; \begin{cases} x, & \text{if } x \notin A \cup B, \\ \xi_A, & \text{if } x \in A, \\ \xi_B, & \text{if } x \in B. \end{cases}$$

and define the induced measure and transitions probabilities on $\mathfrak{S}$ via

$$\mathfrak{m} \;:=\; m \circ \rho^{-1} \qquad \text{and} \qquad \mathfrak{p}(s,s') \;=\; \frac{1}{\mathfrak{m}(s)} \sum\nolimits_{x \in \rho^{-1}(s)} m(x) \sum\nolimits_{y \in \rho^{-1}(s')} p(x,y).$$

Notice that $\mathfrak{m}$ is the invariant measure with respect to $\mathfrak{p}$. Then, for every $f, g \colon \mathcal{S} \to \mathbb{R}$ which are constant on A and B, it holds that

$$\langle f, -Lg \rangle_m \;=\; \langle \mathfrak{f}, -\mathfrak{L}\, \mathfrak{g} \rangle_{\mathfrak{m}}, \tag{1.10}$$

where $\mathfrak{L}$ denote the discrete generator corresponding to $\mathfrak{p}$ and $\mathfrak{f} \colon \mathfrak{S} \to \mathbb{R}$ denotes the projection of f onto $\mathfrak{S}$, i.e. $\mathfrak{f}$ coincides with f on $(A \cup B)^c$ whereas on ξ_A and ξ_B it assumes the corresponding values of f on A and B, respectively. In particular,

$$\operatorname{cap}(A,B) \;=\; \langle h_{A,B}, -L h_{A,B} \rangle_m \;=\; \langle \mathfrak{h}_{A,B}, -\mathfrak{L}\, \mathfrak{h}_{A,B} \rangle_{\mathfrak{m}}. \tag{1.11}$$

1.3. **Relation between capacity and mean hitting times.** The first important ingredient of the potential theoretic approach to metastability is a formula for the average mean hitting time when starting the Markov chain in the so called *last exit biased distribution* on a set A that connects it to the capacity and the equilibrium potential. For any two disjoint subsets $A, B \subset \mathcal{S}$ this distribution is defined through

$$\nu^*_{A,B}(x) \;=\; \frac{m(x)\; \mathbb{P}^*_x\big[\tau_B < \tau_A\big]}{\sum_{y \in A} m(y)\; \mathbb{P}^*_y\big[\tau_B < \tau_A\big]} \;=\; \frac{m(x)\, e^*_{A,B}(x)}{\operatorname{cap}(A,B)} \qquad \forall\, x \in A. \tag{1.12}$$

Notice that $\nu^*_{A,B}$ is concentrated on those starting configurations $y \in A$ that are at the boundary of this set.

Proposition 1.2. *Let $A, B \subset \mathcal{S}$ with $A \cap B = \emptyset$. Then*

$$\sum_{x \in A} \nu^*_{A,B}(x)\, \mathbb{E}_x[\tau_B] \;=\; \frac{1}{\mathrm{cap}(A,B)} \sum_{x \notin B} m(x)\, h^*_{A,B}(x). \tag{1.13}$$

In the sequel, we will give two different proofs of this Proposition. The first one use purely probabilistic arguments, while the second one relies on analytic considerations.

Proof of Proposition 1.2 via probabilistic methods. First, let us define the last exit time $L_{A,B}$ from A before hitting B as

$$L_{A,B} \;:=\; \sup\big\{0 \le t < \tau_B \;\big|\; X(t) \in A\big\}. \tag{1.14}$$

Then we have for all $y \notin B$,

$$\begin{aligned} m(y)\, \mathbb{P}^*_y\big[\tau_A < \tau_B\big] \;&=\; m(y)\, \mathbb{P}^*_y\big[L_{A,B} > 0\big] \\ &=\; \sum_{t=1}^{\infty} \sum_{x \in A} m(y)\, \mathbb{P}^*_y\big[L_{A,B} = t,\, X(t) = x\big] \\ &=\; \sum_{t=1}^{\infty} \sum_{x \in A} m(y)\, \mathbb{P}^*_y\big[X(t) = x, t < \tau_B\big]\, \mathbb{P}^*_x\big[\tau_B < \tau_A\big], \end{aligned} \tag{1.15}$$

where we used the Markov property in the last step. By time reversal, we have that

$$m(y)\, \mathbb{P}^*_y\big[X(t) = x, t < \tau_B\big] \;=\; m(x)\, \mathbb{P}_x\big[X(t) = y, t < \tau_B\big]. \tag{1.16}$$

In view of (1.12), this implies that

$$\mathbb{E}_{\nu^*_{A,B}}\left[\sum_{t=0}^{\tau_B - 1} \mathbb{1}_{X(t)=y}\right] - \frac{m(y)\, \mathbb{P}^*_y\big[\tau_B < \tau_A\big]}{\mathrm{cap}(A,B)}\, \mathbb{1}_{y \in A} \;=\; \frac{m(y)\, \mathbb{P}^*_y\big[\tau_A < \tau_B\big]}{\mathrm{cap}(A,B)} \tag{1.17}$$

By summing over all configurations y outside B, we obtain (1.13). □

Proof of Proposition 1.2 via analytic methods. Recall that the mean hitting time of a set B starting the Markov chain in a configuration $x \notin B$ solves the Dirichlet problem (1.3) with the choice $D = B$, $u \equiv 0$ and $g \equiv 1$. But,

$$\begin{aligned} \textstyle\sum_{x \in A} m(x)\, e^*_{A,B}(x)\, w_B(x) \;&=\; \langle -L^* h^*_{A,B}, w_B \rangle_m \\ &=\; \langle h^*_{A,B}, -L w_B \rangle_m \;=\; \textstyle\sum_{x \notin B} m(x)\, h^*_{A,B}(x). \end{aligned}$$

Normalizing the measure on the left-hand side immediately yields the assertion. □

2. The Dirichlet and Thomson principle: a dual variational principle

As it can be seen from (1.9), the capacity has a representation in terms of a positive-definite quadratic form. Whenever a object of interests can be expressed as a positive-definite quadratic form, it is often possible to establish dual variational principles from which upper and lower bound for it can be constructed. Notice that many variational methods are based on this tool. In the context of reversible Markov processes, our presentation follows in parts the one given by Lieberstein [17] in the context of partial differential equations.

2.1. **Reversible setting.** In order to clarify the mechanism that is behind the proof of both the Dirichlet and Thomson, we will first considered the case of a reversible Markov chain, i.e. $\{X(t)\}$ satisfies the *detailed balance* condition

$$m(x)\, p(x,y) \;=\; m(y)\, p(y,x). \tag{2.1}$$

The bilinear form $\mathcal{E}(f,g)$ associated to the Dirichlet form $\mathcal{E}(f)$ is given by

$$\mathcal{E}(f,g) \;=\; \frac{1}{2} \sum_{x,y\in\mathcal{S}} m(x)\, p^s(x,y) \big(f(x)-f(y)\big)\big(g(x)-g(y)\big), \qquad \forall\, f,g \in l^2(m). \tag{2.2}$$

Let us stress the fact that due to the reversibility, it holds that $\mathcal{E}(f,g) = \langle f, -L\, g\rangle_m$. Moreover, Cauchy-Schwarz's inequality yields

$$\mathcal{E}(f,g)^2 \;\le\; \mathcal{E}(f)\, \mathcal{E}(g) \tag{2.3}$$

which serves as the starting point to derive

Proposition 2.1 (Dirichlet and Thomson principle). *For any non-empty disjoint sets $A, B \subset \mathcal{S}$,*

(i) the Dirichlet principle holds, that is

$$\operatorname{cap}(A,B) \;=\; \min_{f\in\mathcal{H}_{A,B}} \mathcal{E}(f) \tag{2.4}$$

where $\mathcal{H}_{A,B} := \big\{f\colon \mathcal{S}\to[0,1] \;\big|\; f|_A \equiv 1,\; f|_B \equiv 0\big\}$.

(ii) the Thomson principle holds, that is

$$\operatorname{cap}(A,B) \;=\; \max_{f\in\mathfrak{H}_{A,B}} \frac{\Big(\sum_{x\in A} m(x)\,\big(-Lf\big)(x)\Big)^2}{\mathcal{E}(f)}. \tag{2.5}$$

where $\mathfrak{H}_{A,B} := \big\{f\colon \mathcal{S}\to[0,1] \;\big|\; (Lf)(y) \le 0,\; \forall\, y \notin B\big\}$.

Remark 2.2. An immediate corollary of the Dirichlet principle is *Rayleigh's monotonicity law*. It allows to derive a lower bound for capacities by using the monotonicity of the Dirichlet form in the transition probabilities to compare the original process with a simplified one. This is well known in the language of electrical networks, see [15].

Proof. Starting point for the proof of both Dirichlet and Thomson principle is the equation (2.3) with $g \equiv h_{A,B}$, i.e.

$$\mathcal{E}(f, h_{A,B})^2 \;\le\; \mathcal{E}(f,f)\, \operatorname{cap}(A,B). \tag{2.6}$$

(i) Consider $f \in \mathcal{H}_{A,B}$, i.e. f coincides on the set $A\cup B$ with the function $h_{A,B}$. Since L is assumed to be symmetric, we obtain immediately that

$$\mathcal{E}(f,\, h_{A,B}) \;=\; \langle f, -Lh_{A,B}\rangle_m \;=\; \sum_{x\in A} m(x)\, e_{A,B}(x) \;=\; \operatorname{cap}(A,B). \tag{2.7}$$

In view of (2.6), we get immediately that $\operatorname{cap}(A,B) \le \mathcal{E}(f)$. Since the minimum is attained f being the equilibrium potential, (2.4) follows.

(ii) Instead of considering a function f which coincides with $h_{A,B}$ on $A \cup B$, suppose that f is super-harmonic on B^c, i.e. $\big(Lf\big)(x) \leq 0$ for all $x \in B^c$. Then

$$\mathcal{E}(f,\, h_{A,B}) \;=\; \langle -Lf, h_{A,B}\rangle_m \;\geq\; \sum_{y \in A} m(x)\,\big(-Lf\big)(x) \;\geq\; 0. \tag{2.8}$$

where we used in the second step that on $(A \cup B)^c$ the equilibrium potential is non-negative. Hence, from (2.6), we get that

$$\operatorname{cap}(A,B) \;\geq\; \frac{\Big(\sum_{x \in A} m(x)\,\big(-Lf\big)(x)\Big)^2}{\mathcal{E}(f)}. \tag{2.9}$$

Since $h_{A,B}$ is harmonic on $(A \cup B)^c$ and $(-Lh_{A,B})(x) = \mathbb{P}_x[\tau_B < \tau_A] \geq 0$ for all $x \in A$, it follows that $h_{A,B} \in \mathfrak{H}_{A,B}$. Thus, together with the definition of the capacity, (2.5) is immediate. □

The Thomson principle is well known in the context of random walks and electrical networks. However, in that language it is differently formulated in terms of unit flows, see [15, 27]. For this reason, we will briefly discuss the connection between these formulations. To start with, we recall the definition of discrete flows.

Definition 2.3 (Discrete flow)**.** Given two non-empty disjoint sets $A, B \subset \mathcal{S}$ and consider a map $\varphi\colon \mathcal{S} \times \mathcal{S} \to \mathbb{R}$. We call φ compatible to p^s, if for all $x, y \in \mathcal{S}$ for which $p^s(x,y) = 0$ implies that $\varphi(x,y) = 0$.

(a) The map φ is called *flow*, if it is antisymmetric, compatible to p^s and satisfies *Kirchoff's law*, that is

$$(\operatorname{div}\varphi)(x) \;:=\; \sum_y \varphi(x,y) \;=\; 0, \quad \forall\, x \in S. \tag{2.10}$$

If φ satisfies Kirchoff's law only for all $x \in (A \cup B)^c$, it is called a *AB-flow*.

(b) The map φ is an *unit AB-flow*, if it is a AB-flow and the *strength* of φ is 1

$$\sum_{x \in A} (\operatorname{div}\varphi)(x) \;=\; 1 \;=\; -\sum_{x \in B} (\operatorname{div}\varphi)(x); \tag{2.11}$$

We denote the set of unit AB-flows by $\mathfrak{U}^1_{A,B}$.

(c) A *divergence free AB-flow* is a AB-flow with strength 0. We denote the set of AB-flows with vanishing divergence by $\mathfrak{U}^0_{A,B}$.

Let us now define a bilinear form for flows from A to B. Given two maps φ, ψ that are compatible with respect to p^s, we set

$$\mathcal{D}(\varphi,\psi) \;:=\; \frac{1}{2} \sum_{x,y \in \mathcal{S}} \frac{1}{m(x)\,p^s(x,y)}\,\varphi(x,y)\,\psi(x,y), \qquad \mathcal{D}(\varphi) \;:=\; \mathcal{D}(\varphi,\varphi). \tag{2.12}$$

Mind that an application of Cauchy-Schwarz inequality yields

$$\mathcal{D}(\varphi,\psi)^2 \;\leq\; \mathcal{D}(\varphi)\,\mathcal{D}(\psi). \tag{2.13}$$

An important unit AB-flow in the reversible setting is the *harmonic unit flow*, $\varphi_{A,B}$, which is defined in terms of the equilibrium potential, $h_{A,B}$,

$$\varphi_{A,B}(x,y) \;:=\; \frac{m(x)\,p^s(x,y)}{\operatorname{cap}(A,B)}\,\Big(h_{A,B}(x) - h_{A,B}(y)\Big). \tag{2.14}$$

With the notations introduced above, Thomson's principle can be reformulated in the following way

Proposition 2.4 (Thomson principle in terms of flows)**.** *For any non-empty disjoint sets $A, B \subset \mathcal{S}$,*

$$\operatorname{cap}(A,B) \;=\; \max_{\varphi\in\mathfrak{U}^1_{A,B}} \frac{1}{\mathcal{D}(\varphi)}, \tag{2.15}$$

where the maximum is attained for the harmonic flow, $\varphi_{A,B}$.

Proof. To simplify notations, we set $\Psi_g(x,y) = m(x)\, p^s(x,y)\big(g(x) - g(y)\big)$. Mind that $\Psi_{h_{A,B}}$ is a AB-flow in the reversible setting. In particular, $\mathcal{D}(\Psi_{h_{A,B}}) = \operatorname{cap}(A,B)$ and $\varphi_{A,B} \in \mathfrak{U}^1_{A,B}$. On the other hand, for any $\psi \in \mathfrak{U}^1_{A,B}$, a simple computation shows that

$$\mathcal{D}(\Psi_{h_{A,B}}, \psi) \;=\; \frac{1}{2}\sum_{x,y\in\mathcal{S}} \big(h_{A,B}(x) - h_{A,B}(y)\big)\,\psi(x,y) \;=\; \sum_{x\in A} (\operatorname{div}\psi)(x) \;=\; 1.$$

Thus, in view of (2.13), we get that $\operatorname{cap}(A,B) \geq 1/\mathcal{D}(\psi)$ for every $\psi \in \mathfrak{U}^1_{A,B}$ whereas equality holds for the particular choice $\psi = \varphi_{A,B}$. This completes the proof. □

2.2. **Non-reversible setting.** What prevents us deriving variational principles for non-reversible Markov chains in a similar way as described above, is the fact that $\mathcal{E}(f,g) = \langle f, -Lg\rangle$ if and only if the Markov chains is reversible. For this reason, we proceed differently.

First, we define the following norms

$$\|f\|^2_{H^1(m)} \;:=\; \langle f, -Lf\rangle_m \qquad \text{and} \qquad \|f\|^2_{H^{-1}(m)} \;:=\; \sup_g \Big(2\langle f,g\rangle_m - \|g\|^2_{H^1(m)}\Big).$$

Since $\{X(t)\}_t$ is assumed to be irreducible, the Theorem of Perron-Frobenius implies that $0 \in \operatorname{spec}\{-L\}$ is a simple eigenvalue. Hence, $\|f\|_{H^{-1}(m)} < \infty$, if and only if, $\langle f, 1\rangle_m = 0$. Provided that $\langle f, 1\rangle_m = 0$, the supremum in the definition of the $H^{-1}(m)$-norm is actually attained for any g solving the equation $Lg = -f$.

These both definitions allow for a simple interpolation estimate by an application of Cauchy-Schwarz inequality

$$\big|\langle f, g\rangle_m\big| \;\leq\; \|g\|_{H^1(m)}\, \|f\|_{H^{-1}(m)} \tag{2.16}$$

for all functions f, g with $\langle f, 1\rangle_m = 0$. In later applications, we would like to take advantage of (2.16) in order to obtain an upper bound for $\big|\langle -L^*f, g\rangle_m\big|$ for all functions f, g having the property of being constant on both the set A and B. As an immediate consequence of Remark 1.1, we obtain

$$\langle -L^*f, g\rangle^2_m \;\leq\; \|g\|^2_{H^1(m)} \sup_{h\in\mathcal{G}_{A,B}} \Big(2\langle -L^*f, h\rangle_m - \|h\|^2_{H^1(m)}\Big), \tag{2.17}$$

where $\mathcal{G}_{A,B} := \big\{h : \mathcal{S} \to [0,1] \;\big|\; h|_A \equiv cst,\; h|_B \equiv cst\big\}$. Now, we are prepared to prove

Proposition 2.5 (Dirichlet and Thomson principle)**.** *For any non-empty disjoint sets $A, B \subset \mathcal{S}$,* *(i) the Dirichlet principle holds, that is*

$$\operatorname{cap}(A,B) \;=\; \min_{f\in\mathcal{H}_{A,B}} \sup_{h\in\mathcal{G}_{A,B}} \Big(2\langle -L^* f, h\rangle_m - \|h\|^2_{H^1(m)}\Big). \tag{2.18}$$

The optimum is attained for $f = \frac{1}{2}\big(h_{A,B} + h^*_{A,B}\big)$.

(ii) the Thomson principle holds, that is

$$\operatorname{cap}(A,B) \;=\; \max_{f\in\mathfrak{H}_{A,B}\cap G_{A,B}} \frac{\Big(\sum_{x\in A} m(x)\,\big(-Lf\big)(x)\Big)^2}{\mathcal{E}(f)}, \tag{2.19}$$

where $\mathfrak{H}_{A,B} := \big\{f\colon \mathcal{S}\to[0,1] \;\big|\; (Lf)(y)\le 0,\ \forall\, y\notin B\big\}$.

Proof. (i) Starting point for the proof of the Dirichlet principle is the equation (2.17) with $g\equiv h_{A,B}$, i.e.

$$\langle -L^* f, h_{A,B}\rangle_m^2 \;\le\; \operatorname{cap}(A,B) \sup_{h\in\mathcal{G}_{A,B}} \Big(2\langle -L^* f, h\rangle_m - \|h\|^2_{H^1(m)}\Big) \tag{2.20}$$

Since, $\langle -L^* f, h_{A,B}\rangle_m = \operatorname{cap}(A,B)$ for every $f\in\mathcal{H}_{A,B}$, we get

$$\operatorname{cap}(A,B) \;\le\; \inf_{f\in\mathcal{H}_{A,B}} \sup_{h\in\mathcal{G}_{A,B}} \Big(2\langle -L^* f, h\rangle_m - \|h\|^2_{H^1(m)}\Big). \tag{2.21}$$

Hence, it remains to show that the infimum is actually attained. For this purpose, let us consider the function $f = \frac{1}{2}\big(h_{A,B} + h^*_{A,B}\big)$. Then, the supremum of the right-hand side of (2.21) reads

$$\begin{aligned}
\sup_{h\in\mathcal{G}_{A,B}} \langle h_{A,B} + h^*_{A,B} - h, -Lh\rangle_m \;&=\; \sup_{h\in\mathcal{G}_{A,B}} \langle h^*_{A,B} + h, -L(h_{A,B} - h)\rangle_m\\
&=\; \operatorname{cap}(A,B) \;-\; \inf_{h\in\mathcal{G}_{A,B}} \langle h, -Lh\rangle\\
&=\; \operatorname{cap}(A,B),
\end{aligned} \tag{2.22}$$

where we used step in the second step that $\operatorname{cap}(A,B) = \operatorname{cap}^*(A,B)$. This concludes the proof.

(ii) Set $f\equiv\frac{1}{2}(h_{A,B} + h^*_{A,B})$. As a consequence of the computation above,

$$\sup_{h\in G_{A,B}} \Big(2\langle f, h\rangle_m - \|h\|^2_{H^1(m)}\Big) \;\le\; \operatorname{cap}(A,B).$$

Hence,

$$\bigg(\sum_{x\in A} m(x)\,\big(-Lg\big)(x)\bigg)^2 \;\le\; \frac{1}{2}\,\langle h_{A,B} + h^*_{A,B}, -Lg\rangle_m^2 \;\le\; \mathcal{E}(g)\,\operatorname{cap}(A,B).$$

for all $g\in\mathfrak{H}_{A,B}\cap G_{A,B}$. Solving this equation for $\operatorname{cap}(A,B)$ yields the assertion. ☐

One major achievement in [16] was to rewrite the saddle-point problem (2.18) into a minimization problem. In what follows, we give an elementary proof of their result and establish in addition a Thomson principle in terms of flows. Recall the definition of the anti-symmetric map $\Psi_g(x,y) = m(x)\,p^s(x,y)\big(g(x)-g(y)\big)$ and set

$$\Phi_f(x,y) \;=\; m(x)\,p(x,y)\,f(x) - m(y)\,p(y,x)\,f(y).$$

Proposition 2.6 (Dirichlet and Thomson principle in terms of flows)**.** *Suppose that $A, B \subset \mathcal{S}$ are non-empty and disjoint. Then,*

(i) the Dirichlet principle holds, that is

$$\operatorname{cap}(A,B) \;=\; \min_{f \in \mathcal{H}_{A,B}} \min_{\psi \in \mathfrak{U}^0_{A,B}} \mathcal{D}(\Phi_f - \psi), \tag{2.23}$$

where the minimum is attained for $f = \frac{1}{2}(h_{A,B} + h^*_{A,B})$ and $\psi = \Phi_f - \Psi_{h_{A,B}}$.

(ii) the Thomson principle holds, that is

$$\operatorname{cap}(A,B) \;=\; \max_{\varphi \in \mathfrak{U}^1_{A,B}} \max_{g \in G^0_{A,B}} \frac{1}{\mathcal{D}(\varphi - \Phi_g)}, \tag{2.24}$$

where $G^0_{A,B}$ denotes the set of functions that vanishes on $A \cup B$. The maximum is attained for $\varphi = \varphi_{A,B} + \Phi_g$ where $\varphi_{A,B}$ is the harmonic flow and $g = \frac{1}{2}(h^*_{A,B} - h_{A,B}) / \operatorname{cap}(A,B)$.

Proof. (i) First of all notice that $\mathcal{D}(\Psi_f, \psi) = 0$ for every $f \in \mathcal{H}_{A,B}$ and $\psi \in \mathfrak{U}^0_{A,B}$. Thus,

$$\mathcal{D}(\Phi_f - \psi, \Psi_{h_{A,B}}) \;=\; \mathcal{D}(\Phi_f, \Psi_{h_{A,B}}) \;=\; \langle -L^* f, h_{A,B} \rangle_m \;=\; \operatorname{cap}(A,B). \tag{2.25}$$

Since $\mathcal{D}(\Psi_{h_{A,B}}) = \operatorname{cap}(A,B)$, (2.13) yields that $\operatorname{cap}(A,B) \leq \mathcal{D}(\Phi_f - \psi)$ for all $f \in \mathcal{H}_{A,B}$ and $\varphi \in \mathfrak{U}^0_{A,B}$. In order to establish (2.23), we are left with showing that $\psi = \Phi_f - \Psi_{h_{A,B}}$ with $f = \frac{1}{2}(h_{A,B} + h^*_{A,B})$ is a divergence-free AB-flow. But,

$$(\operatorname{div} \psi)(x) \;=\; \frac{m(x)}{2} \Big((L h_{A,B})(x) \;-\; (L^* h^*_{A,B})(x) \Big).$$

Hence, $\psi \in \mathfrak{U}^0_{A,B}$.

(ii) For every $g \in G^0_{A,B}$ and $\varphi \in \mathfrak{U}^1_{A,B}$ it holds that

$$\mathcal{D}(\varphi - \Phi_g, \Psi_{h_{A,B}}) \;=\; \sum_{x \in A} (\operatorname{div} \varphi)(x) \;-\; \langle -L^* g, h_{A,B} \rangle \;=\; 1. \tag{2.26}$$

In view of (2.13) it is immediate that $\operatorname{cap}(A,B) \geq 1/\mathcal{D}(\varphi - \Phi_g)$ for every unit AB-flow, φ, and for every function g that vanishes on $A \cup B$. Thus, (2.24) follows ones we have shown that the maximum is attained. For this purpose, consider $\varphi = \varphi_{A,B} + \Phi_g$ with $g = \frac{1}{2}(h^*_{A,B} - h_{A,B}) / \operatorname{cap}(A,B)$. Since,

$$(\operatorname{div} \varphi)(x) \;=\; \frac{m(x)}{2 \operatorname{cap}(A,B)} \Big(\big(- L h_{A,B} \big)(x) \;+\; \big(- L^* h^*_{A,B} \big)(x) \Big) \tag{2.27}$$

ϕ is a unit AB-flow and $\mathcal{D}(\varphi - \Phi_g) = \mathcal{D}(\varphi_{A,B}) = 1/\operatorname{cap}(A,B)$. This concludes the proof. □

3. Berman-Konsowa principle

The variational principles, we have presented in the previous section, rely on an application of the Cauchy-Schwarz inequality. In the context of reversible Markov chains, We will now describe a little-known variational principles for capacities that does not use (2.3). It was first proven by Berman and Konsowa in [3]. Our presentation will follow the arguments first given in [4] and then in [7].

Definition 3.1. Consider a map $\varphi\colon \mathcal{S}\times\mathcal{S}\to[0,\infty)$ which is compatible to $p^s\equiv p$. We call φ a *loop-free non-negative unit AB-flow*, if it satisfies the following properties

(i) if $\varphi(x,y)>0$ then $\varphi(y,x)=0$,
(ii) φ satisfies Kirchhoff's law on $(A\cup B)^c$,
(iii) the strength of φ is equal to 1,
(iv) any path, γ, from A to B such that $\varphi(x,y)>0$ for all $(x,y)\in\gamma$ is self-avoiding.

We denote the set of loop-free non-negative unit AB-flows by $\mathfrak{U}^+_{A,B}$.

Now, we will show that each loop-free non-negative unit flow f give rise to a probability measure $\mathbb{P}^f$ on self-avoiding paths. Mind that, for every $\varphi\in\mathfrak{U}^+_{A,B}$, its divergence, $(\operatorname{div}\varphi)(x)$, is positive for all $x\notin B$. Let $\mathbb{P}^\varphi$ be the law of a Markov chain $\{\xi(t)\}$ that is stopped at the arrival of B with initial distribution $\mathbb{P}^\varphi\big[\xi(0)=x\big]=(\operatorname{div}\varphi)(x)\,\mathbb{1}_A(x)$ and transition probabilities

$$q^\varphi(x,y)\;=\;\frac{\varphi(x,y)}{(\operatorname{div}\varphi)(y)},\qquad x\notin B. \tag{3.1}$$

Hence, for a path $\gamma=\big(x^0,\dots,x^r\big)$ with $x^0\in A$, $x^r\in B$ and $x^k\in\mathcal{S}\setminus(A\cup B)$, $\forall\,k=1,\dots r-1$ we have

$$\mathbb{P}^\varphi\big[\xi=\gamma\big]\;=\;(\operatorname{div}\varphi)(x^0)\prod_{k=0}^{r-1}\frac{\varphi(x^k,x^{k+1})}{(\operatorname{div}\varphi)(x^k)} \tag{3.2}$$

where we used the convention that $0/0=0$. Using Kirchhoff's law, we obtain the following representation for the probability that $\{\xi(t)\}$ passes through an edge (x,y)

$$\mathbb{P}^\varphi\big[\xi\ni(x,y)\big]\;=\;\sum_\gamma\mathbb{P}^\varphi\big[\xi=\gamma\big]\,\mathbb{1}_{(x,y)\in\gamma}\;=\;\varphi(x,y). \tag{3.3}$$

The equation (3.3) gives rise to the following *partition of unity*

$$\mathbb{1}_{\varphi(x,y)>0}\;=\;\sum_\gamma\mathbb{P}^\varphi\big[\xi=\gamma\big]\,\frac{1}{\varphi(x,y)}\,\mathbb{1}_{(x,y)\in\gamma}. \tag{3.4}$$

Employing this representation, we can bound the Dirichlet form for every $h\in\mathcal{H}_{A,B}$ from below by

$$\begin{aligned}\mathcal{E}(h)\;&\ge\;\sum_{(x,y)}m(x)\,p(x,y)\big(h(x)-h(y)\big)^2\,\mathbb{1}_{\varphi(x,y)>0}\\&=\;\sum_\gamma\mathbb{P}^\varphi\big[\xi=\gamma\big]\sum_{(x,y)\in\gamma}\frac{m(x)\,p(x,y)}{\varphi(x,y)}\,\big(h(x)-h(y)\big)^2\end{aligned} \tag{3.5}$$

Let us now minimize the expression above over all functions h with $h|_A=1$ and $h|_B=0$. By interchanging the minimum and the sum on the right-hand side of (3.5), we are left with the task to solve optimization problems along one-dimensional paths from A to B whose minimizer are explicitly known [6]. As a result, we get

$$\operatorname{cap}(A,B)\;\ge\;\sum_\gamma\mathbb{P}^\varphi\big[\xi=\gamma\big]\left(\sum\nolimits_{(x,y)\in\gamma}\frac{\varphi(x,y)}{m(x)\,p(x,y)}\right)^{-1}. \tag{3.6}$$

An important non-negative loop-free unit flow is the *harmonic flow*, $\varphi^{+}_{A,B}$, which is defined in terms of the equilibrium potential

$$\varphi^{+}_{A,B}(x,y) \;:=\; \frac{m(x)\,p(x,y)}{\mathrm{cap}(A,B)} \Big[h_{A,B}(x) - h_{A,B}(y)\Big]_{+}. \tag{3.7}$$

It is easy to verify that $\varphi^{+}_{A,B}$ satisfies the conditions (i)–(iv). While, (i) is obvious, (ii) is a consequence of the fact that $h_{A,B}$ is harmonic in $(A \cup B)^c$ and (iii) follows from (1.7). Condition (iv) exploits that the harmonic flow only moves in directions where $h_{A,B}$ decreases. Since $\mathbb{P}^{\varphi}$-a.s. equality is obtained in (3.6) for $\varphi^{+}_{A,B}$, this proves

Proposition 3.2. *(Berman-Konsowa principle) Let $A, B \subset \mathcal{S}$ be disjoint. Then, with the notations introduced above,*

$$\mathrm{cap}(A,B) \;=\; \max_{\varphi \in \mathcal{U}^{+}_{A,B}} \mathbb{E}^{\varphi}\left[\left(\sum\nolimits_{(x,y)\in\gamma} \frac{\varphi(x,y)}{m(x)\,p(x,y)}\right)^{-1}\right]. \tag{3.8}$$

where the maximum is attained for $\varphi^{+}_{A,B}$.

Remark 3.3. For $\varphi \in \mathcal{U}^{+}_{A,B}$, Jensen's inequality implies

$$\mathbb{E}^{\varphi}\left[\left(\sum\nolimits_{(x,y)\in\gamma} \frac{\varphi(x,y)}{m(x)\,p(x,y)}\right)^{-1}\right] \;\geq\; \left(\mathbb{E}^{\varphi}\left[\sum\nolimits_{(x,y)\in\gamma} \frac{\varphi(x,y)}{m(x)\,p(x,y)}\right]\right)^{-1} \;=\; \frac{1}{\mathcal{D}(\varphi)}. \tag{3.9}$$

Since the Thomson principle, see Proposition 2.4, can also be established for loop-free non-negative unit flows, this shows that the lower bound on the capacity obtained by the Berman-Konsowa principle provides, in principle, a better approximation compared to the Thomson principle.

References

[1] J. Beltrán and C. Landim. Tunneling and metastability of continuous time markov chains. *J. Stat. Phys.*, 140(6), 2010. 2

[2] J. Beltrán and C. Landim. Tunneling and metastability of continuous time markov chains ii, the nonreversible case. *arXiv:1205.0445*, pages 1–19, 2012. 2

[3] K.A. Berman and M.H. Konsowa. Random-paths and cuts, electrical networks, and reversible Markov-chains. *SIAM J. Discrete Math.*, 3(3):311–319, Aug 1990. 10

[4] A. Bianchi, A. Bovier, and D. Ioffe. Sharp asymptotics for metastability in the random field Curie-Weiss model. *Elect. J. Probab.*, 14:1541–1603, Jul 2009. 10

[5] R.M. Blumenthal and R.K. Getoor. *Markov Processes and Potential Theory*, volume 29 of *Pure and Applied Mathematics*. Academic Press, 1 edition, 1968. 1

[6] A. Bovier. Metastability. In *Methods of Contemporary Mathematical Statistical Physics*, volume 1970 of *Lecture Notes in Mathematics*, pages 177–221. Springer-Verlag, 2009. 2, 11

[7] A. Bovier, F. den Hollander, and C. Spitoni. Homogenous nucleation for Glauber and Kawasaki dynamics in large volumens at low temperatures. *Ann. Probab.*, 38(2):661–713, Mar 2010. 10

[8] A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein. Metastability in stochastic dynamics of disordered mean-field models. *Probab. Theory Rel. Fields*, 119(1):99–161, Jan 2001. 2

[9] A. Bovier, M. Eckhoff, V. Gayrard, and M. Klein. Metastability and low lying spectra in reversible Markov chains. *Commun. Math. Phys.*, 228(2):219–255, Jun 2002. 2

[10] P.G.L. Dirichlet. Über einen neuen Ausdruck zur Bestimmung der Dichtigkeit einer unendlich dünnen Kugelschale, wenn der Werth des Potentials derselben in jedem Punkt ihrer Oberfläche gegeben ist. *Königl. Akad. d. Wiss.*, 1850:99–116, 1852. 1

[11] J.L. Doob. Semimartingales and subharmonic functions. *Trans. Amer. Math. Soc.*, 77(1):86–121, 1954. 1

[12] J.L. Doob. Discrete potential theory and boundaries. *J. Math. Mech.*, 8(3):433–458; erratum 993, 1959. 1

[13] J.L. Doob. *Classical Potential Theory and Its Probabilistic Counterpart*, volume 262 of *Grundlehren der mathematischen Wissenschaften*. Springer-Verlag, 1 edition, 1984. 1

[14] P. Doyle. Energy for Markov chains. *Preprint*, available at `http://math.dartmouth.edu/~doyle/`:1–6, 1994. 2

[15] P.G. Doyle and J.L. Snell. *Random Walks and Electric Networks*, volume 22 of *Carus Mathematical Monographs*. Mathematical Association of America, 1 edition, 1984. 2, 6, 7

[16] A. Gaudillière and C. Landim. A dirichlet principle for non reversible Markov chains and some recurrence theorems. *arXiv:1111.2445*, pages 1–27, 2012. 2, 9

[17] Lieberstein H.M. *Theory of Partial Differential Equations*, volume 93 of *Mathematics in Science and Engineering*. Academic Press, 1 edition, 1972. 5

[18] G.A. Hunt. Markoff processes and potentials. I. *Illinois J. Math.*, 1(1):44–93, 1957. 1

[19] G.A. Hunt. Markoff processes and potentials. II. *Illinois J. Math.*, 1(3):316–369, 1957. 1

[20] G.A. Hunt. Markoff processes and potentials. III. *Illinois J. Math.*, 2(2):151–213, 1958. 1

[21] S. Kakutani. Two-dimensional Brownian motion and harmonic functions. *Proc. Imp. Acad. Tokyo*, 20(10):706–714, Dec 1944. 1

[22] I. Karatzas and S.E. Shreve. *Brownian Motion and Stochastic Calculus*, volume 113 of *Graduate texts in mathematics*. Springer-Verlag, 2 edition, 1991. 1

[23] O.D. Kellogg. *Foundations of Potential Theory*, volume 31 of *Grundlehren der mathematische Wissenschaften*. Springer-Verlag, 1 edition, 1929. 1

[24] J.G. Kemeny, J.L. Snell, and A.W. Knapp. *Denumerable Markov Chains*, volume 40 of *Graduate texts in Mathematics*. Springer-Verlag, 2 edition, 1976. 2

[25] H. Lebesgue. Conditions de régularité, conditions d'irrégularité, conditions d'impossibilité dans le problème de Dirichlet. *Comp. Rendue Acad. Sci.*, 178(1):349–254, 1924. 1

[26] D.A. Levin, Y. Peres, and E.L. Wilmer. *Markov Chain and Mixing Times*. American Mathematical Society, 1 edition, 2008. 2

[27] R. Lyons and Y. Peres. *Probability on Trees and Networks*. Cambridge University Press, 2011. In preparation. Current version available at `http://mypage.iu.edu/~rdlyons/`. 2, 7

[28] C.St.J.A. Nash-Williams. Random walk and electric currents in networks. *Proc. Cambridge Philos. Soc.*, 55(2):181–194, 1959. 2

[29] J.R. Noris. *Markov Chains*. Cambridge University Press, 1 edition, 1997. 3

[30] H. Poincaré. *Théorie du Potentiel Newtonien*. Carré & Naud, 1 edition, 1899. 1

[31] S.C. Port and C.J. Stone. *Brownian Motion and Classical Potential Theory*, volume 29. Academic Press, 1 edition, 1978. 1

[32] M. Slowik. *Contribution to the potential theoretic approach with applications to the random field Curie-Weiss-Potts model*. PhD thesis, Technische Universität Berlin, 2012. 2

[33] A. Telcs. *The Art of Random Walks*, volume 1885 of *Lecture Notes in Mathematics*. Springer-Verlag, 1 edition, 2006. 2

[34] W. Woess. *Random Walks on Infinite Graphs and Groups*, volume 138 of *Cambridge Tracts in Mathematics*. Cambridge University Press, 1 edition, 2000. 2

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