Diffusion processes, electrical networks and entropic switching

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5th Spring School on Evolution Equations

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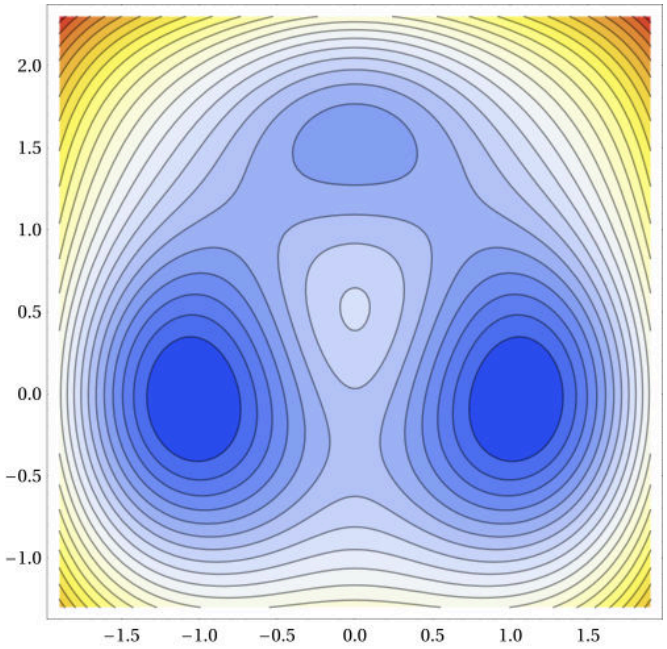
Introduction

Overdamped Langevin dynamics in a 3 hole potential

Hamiltonian $H : \mathbb{R}^2 \to \mathbb{R}$ *specific potential:*



Dynamic at temperature $\varepsilon > 0$ small

$$\mathrm{d}X_t = -\nabla H(X_t)\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}W_t$$

Fokker-Planck evolution of law $X_t = \varrho_t$

$$\partial_t \varrho_t = \nabla \cdot (\varepsilon \nabla \varrho_t + \varrho_t \nabla H)$$

Gibbs measure $\mu(\mathrm{d}x) = \frac{1}{Z_\mu} \exp\left(-\varepsilon^{-1} H\right) \mathrm{d}x$,
Z_μ partition sum

Generator evolution of density $f_t = \varrho_t/\mu$

$$\partial_t f_t = L f_t := \varepsilon \Delta f_t - \nabla H \cdot \nabla f_t.$$

Features

- two global minima a, b
- additional local minimum c
- saddle points $s_{a,b}$, $s_{a,c}$, $s_{c,b}$

degenerated $|H(s_{a,b}) - H(s_{a,c})| = \delta$ small

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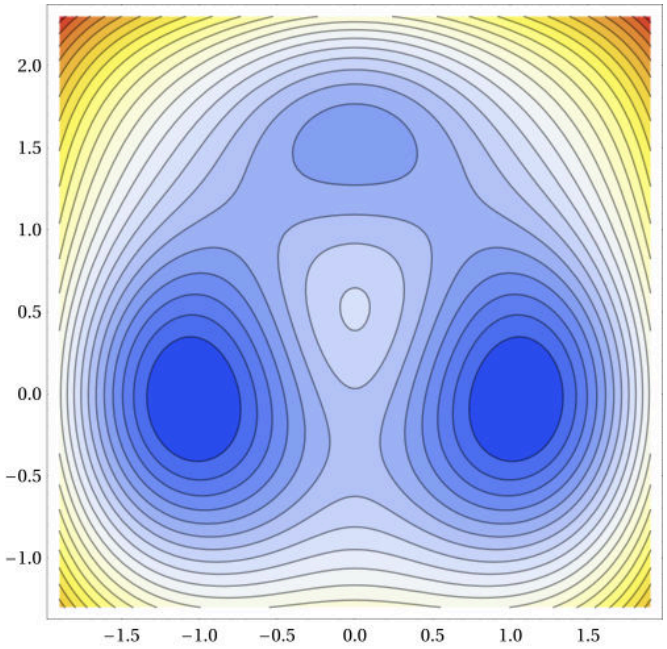

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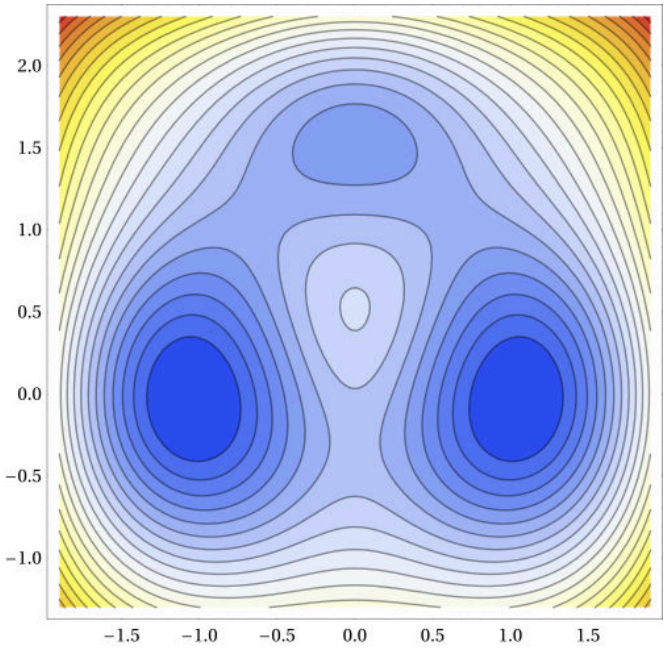

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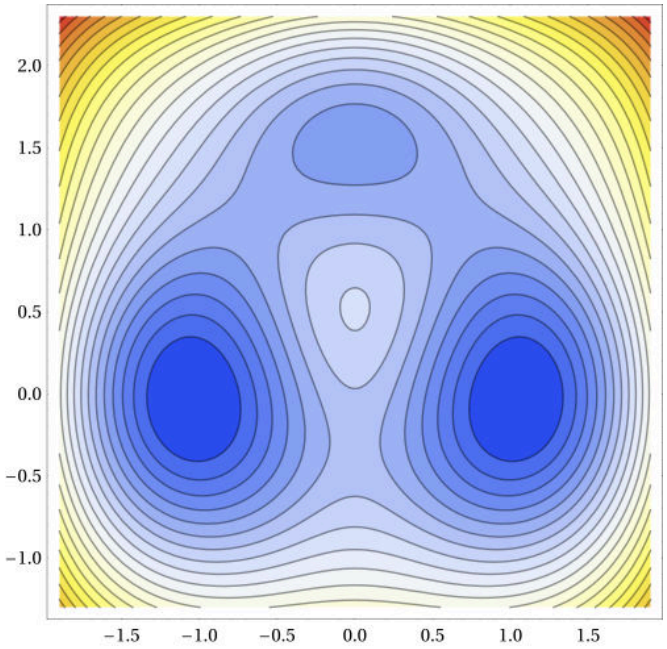

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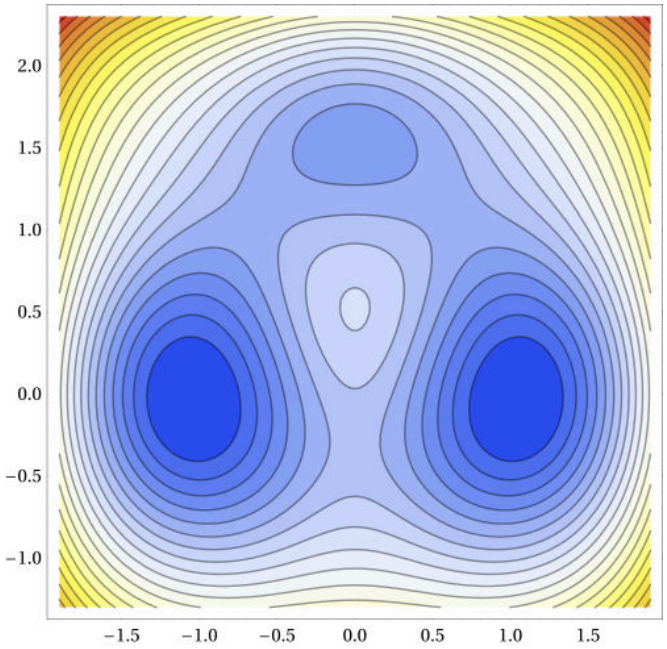

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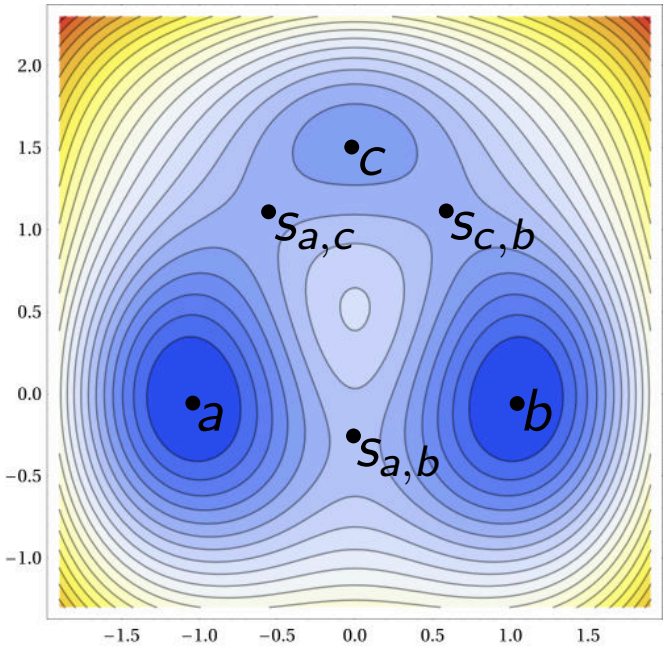

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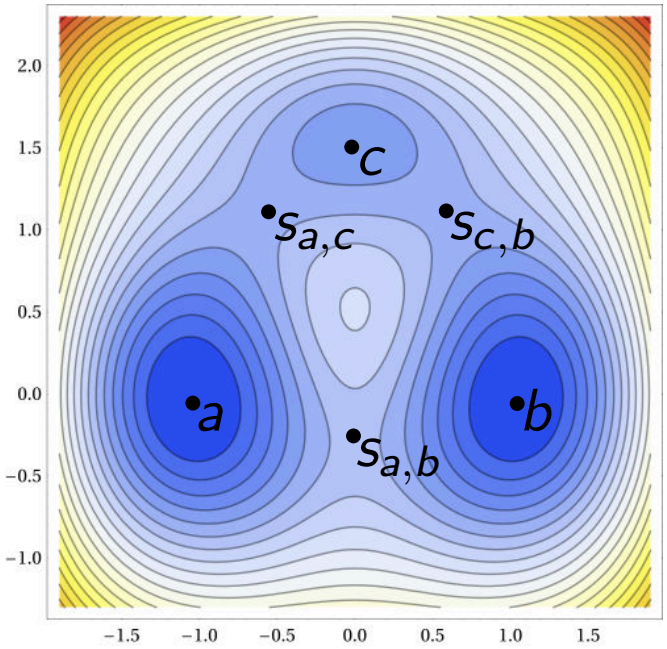

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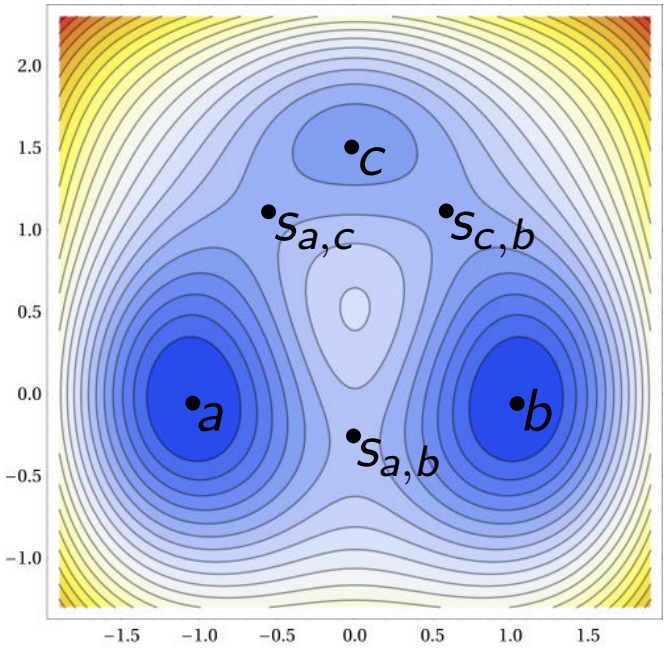


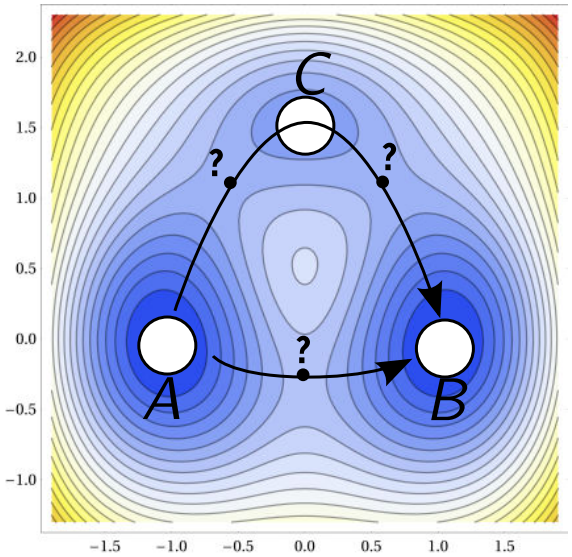
two small parameters:
ε and δ

Fluxes and reaction rates

Interpretation as chemical reactions

- $A = \{|x - a| \leq r\}$ reactant
- $B = \{|x - a| \leq r\}$ product
- $C = \{|x - a| \leq r\}$ intermediate product

What are typical reaction rates and paths?



How to define the reaction rate?

Steady state with inflow of reactants and outflow of products:

$$Lh_{A,B} = 0 \quad \text{in } (A \cup B)^c \quad \text{and} \quad h_{A,B} = \mathbb{1}_A \quad \text{in } A \cup B.$$

Definition (Reaction rate)

$$k_{A,B} := \varepsilon \int |J_{A,B}|^2 \, \mathrm{d}\mu = \varepsilon \int |\nabla h_{A,B}|^2 \, \mathrm{d}\mu.$$

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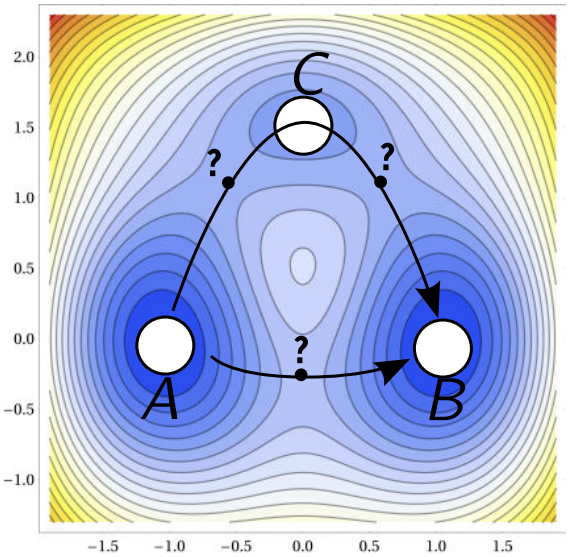

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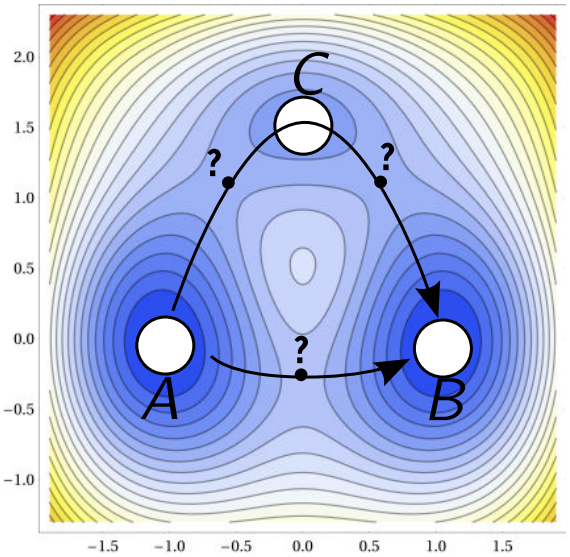

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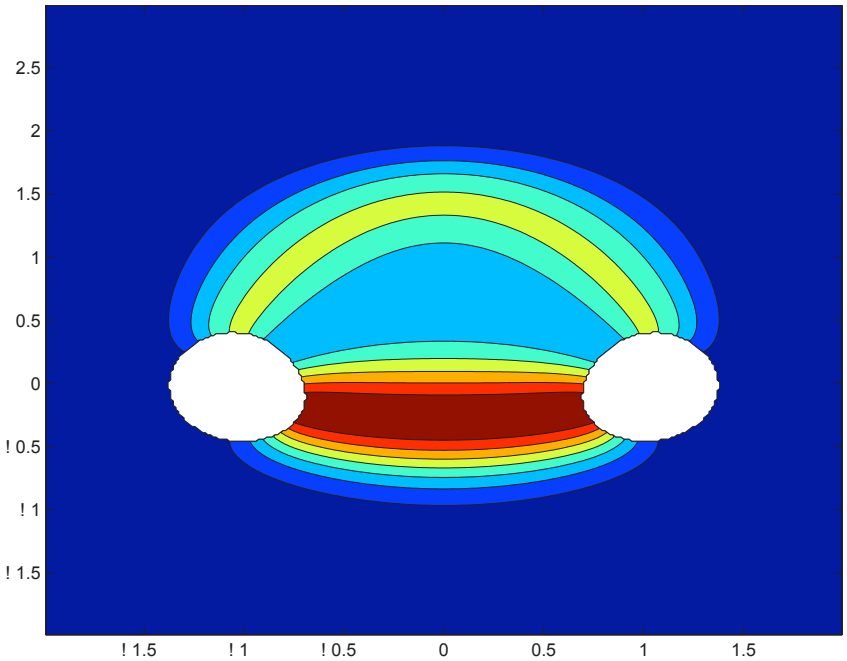
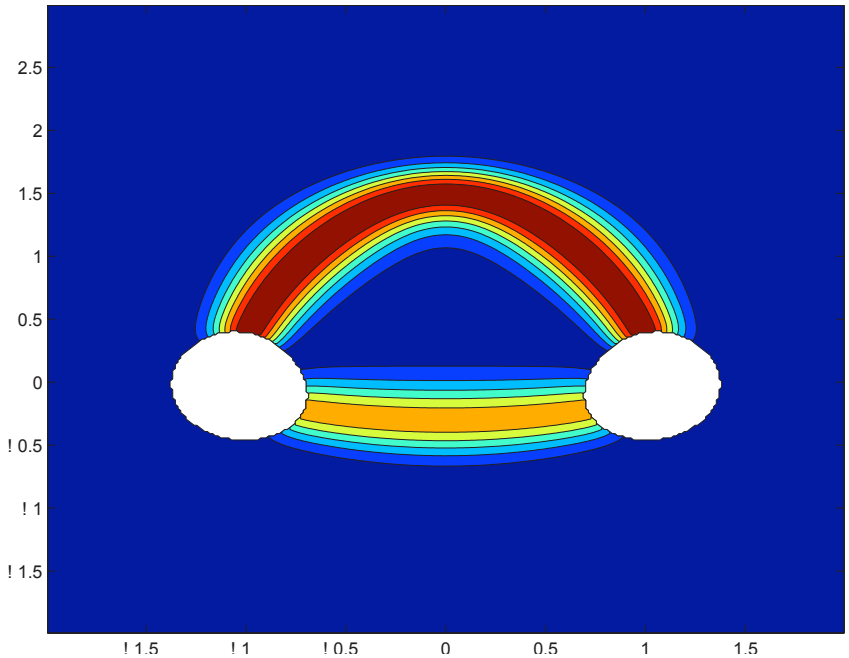
Entropic switching

Numerics: P. Metzner, C. Schütte and E. Vanden-Eijnden 2006 [MSE06]



very low temperature $\varepsilon \ll \delta$



vs. low temperature $\varepsilon \approx \delta$

Very low temperature regime analytical accessible via:

- Large deviations (Freidlin-Wentzell)
- Metastability/Potential theory (Bovier, Eckhoff, Garyard, Klein)
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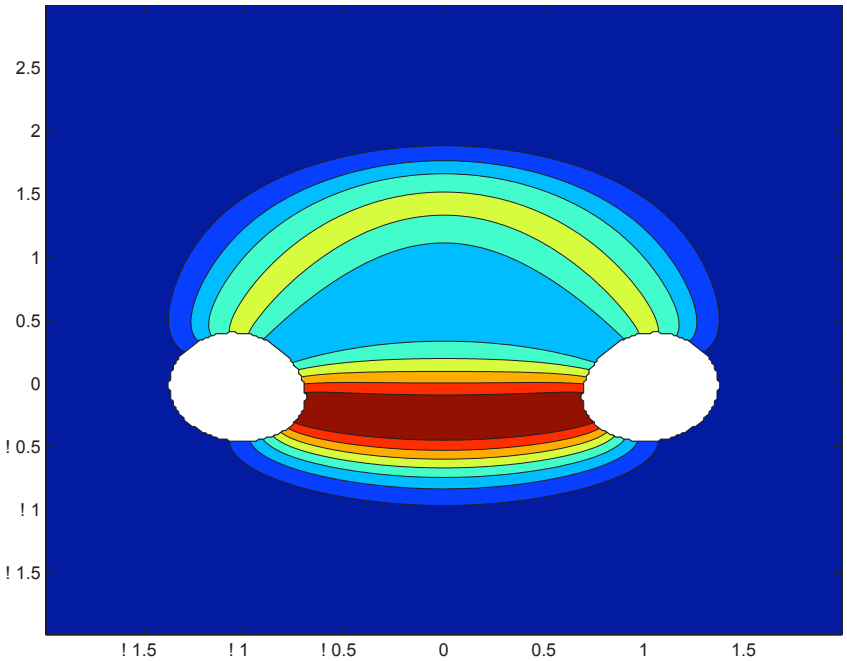

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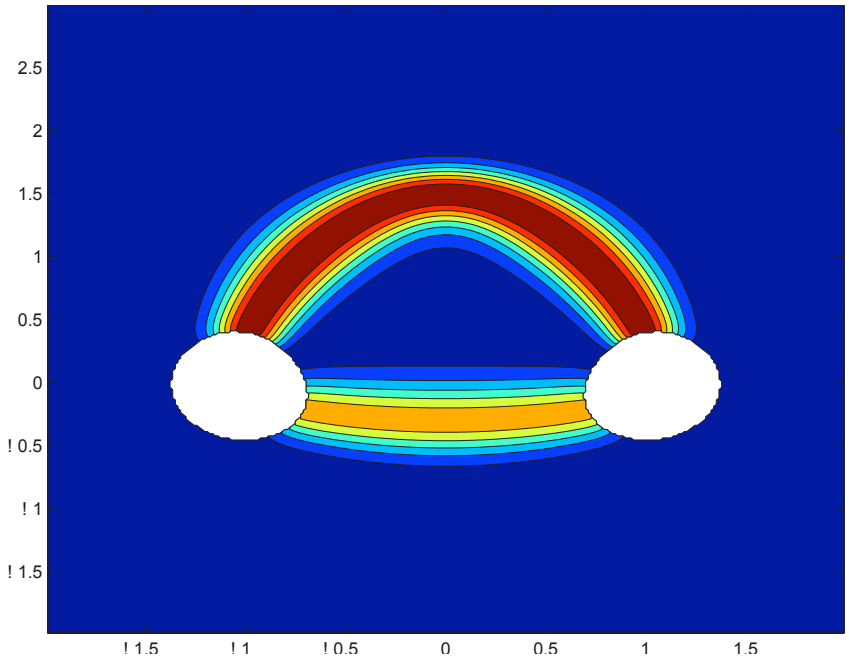

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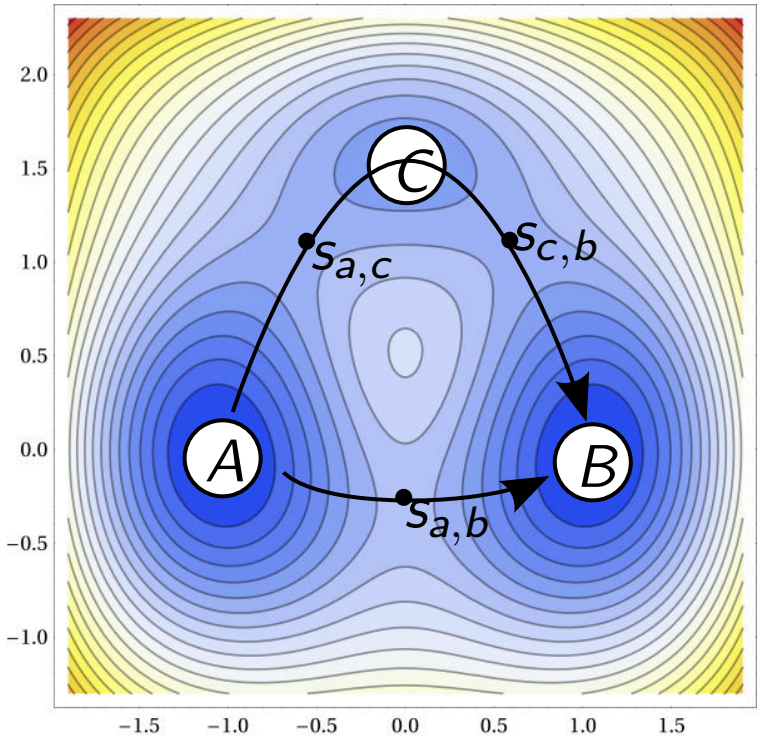
Connection to electrical networks

series and parallel law



$\Rightarrow$

- minima become nodes
- saddles become resistors
- boundary condition becomes voltage source

series and parallel law

The total resistance R between A and B of the network satisfies

$$\frac{1}{R} = \frac{1}{R_{AB}} + \frac{1}{R_{AC} + R_{CB}} \quad .$$

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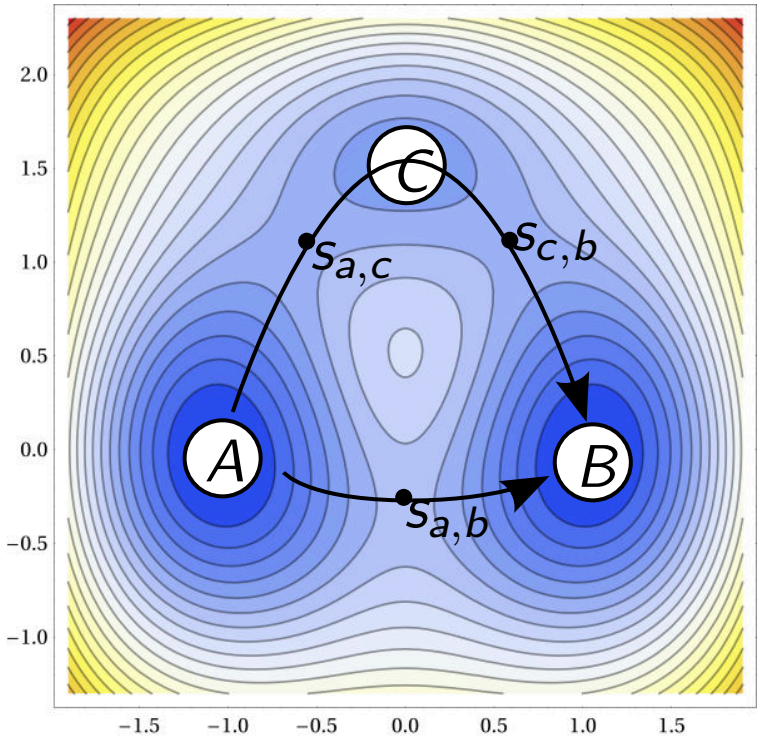

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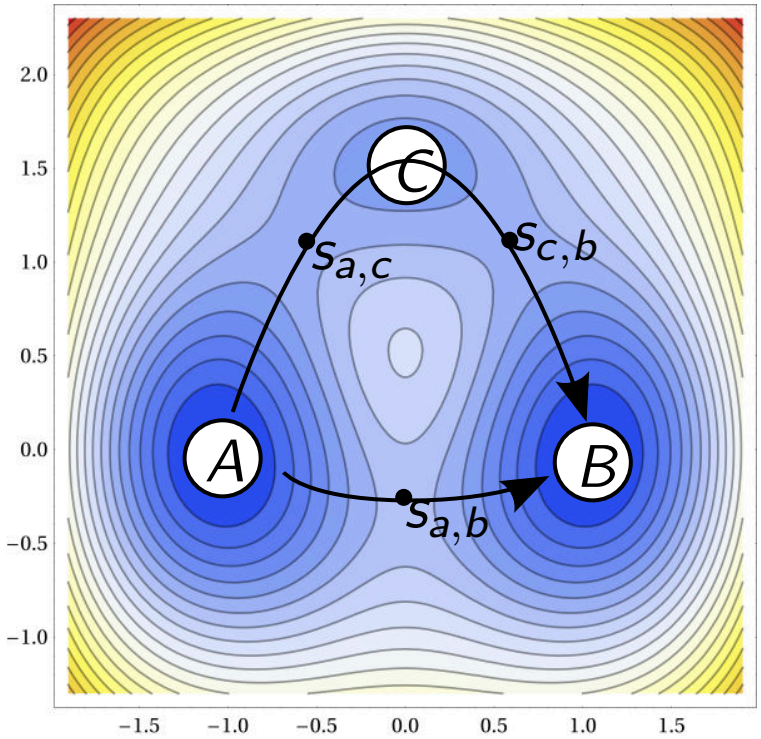

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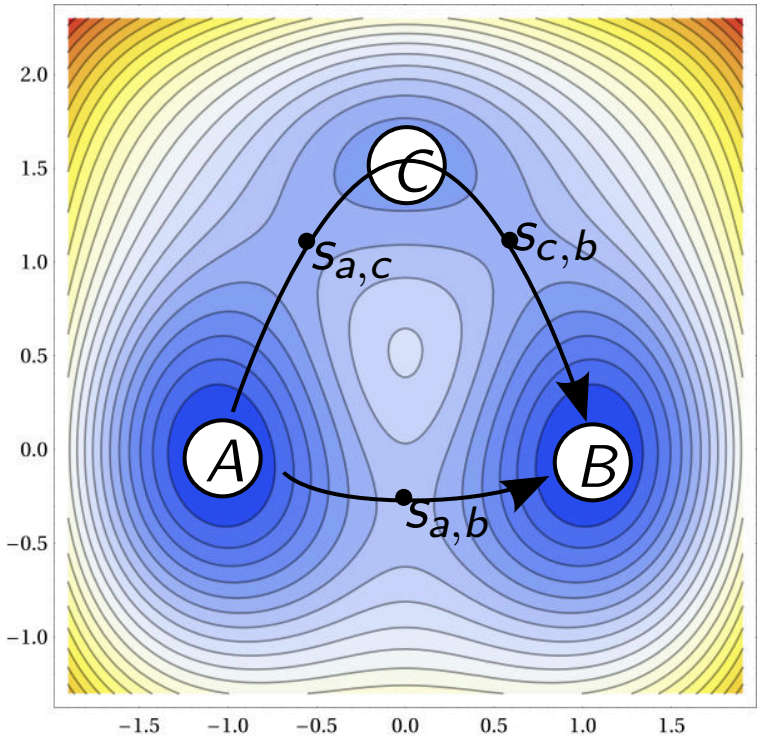

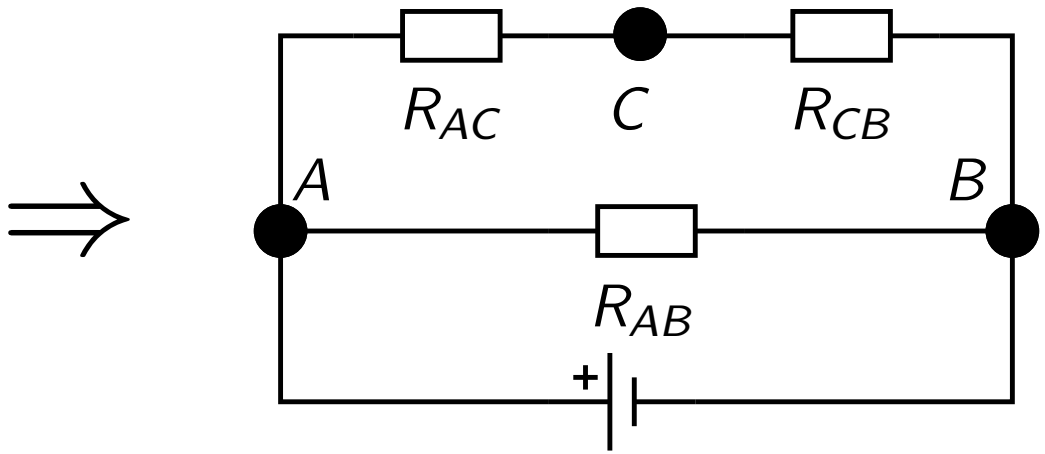

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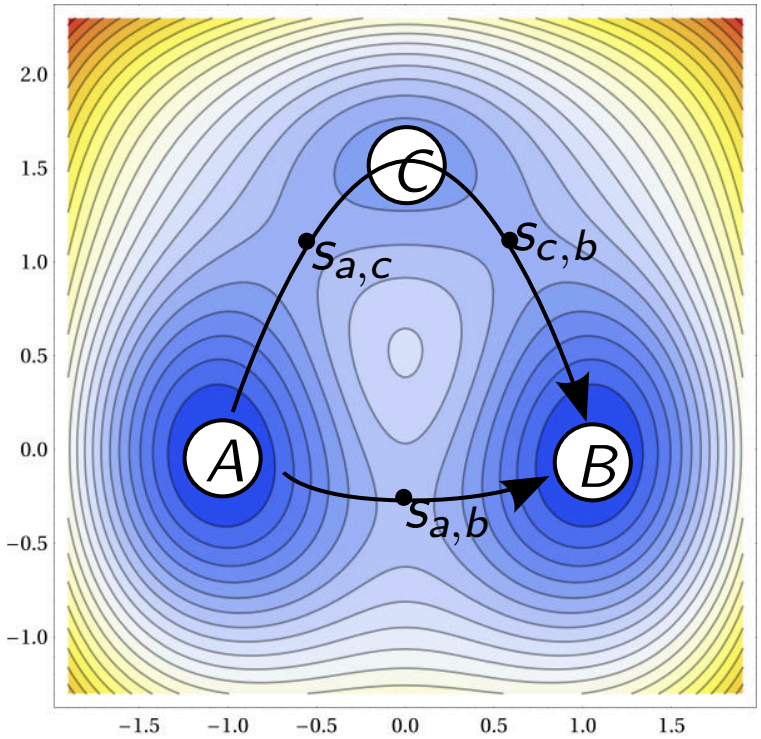

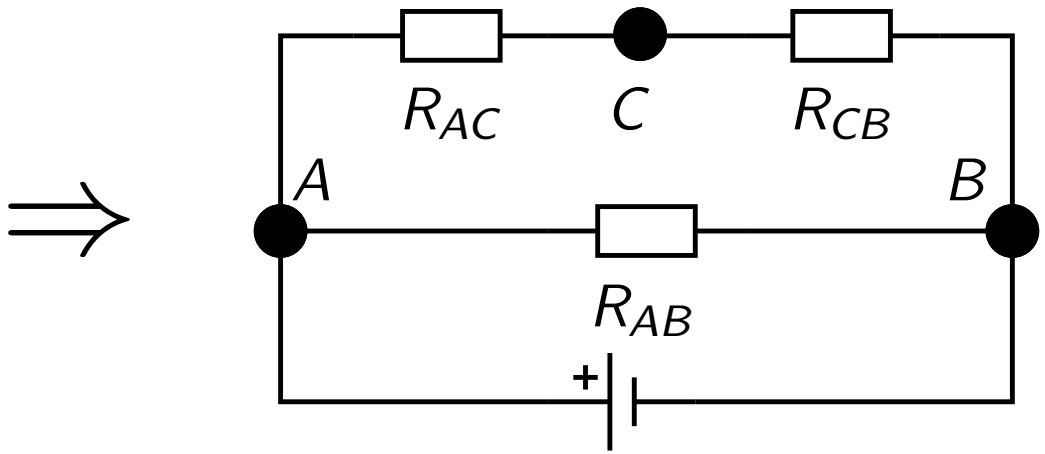

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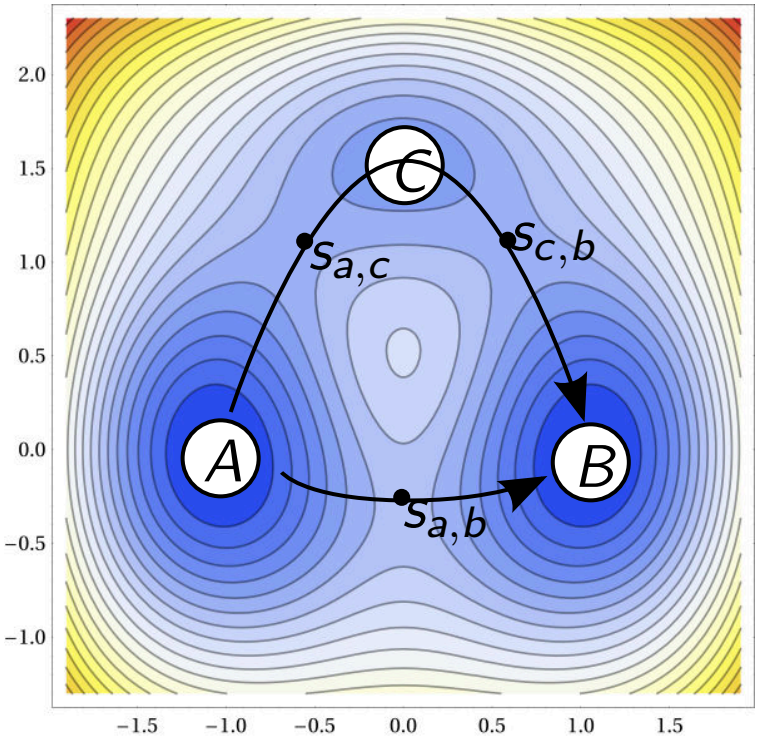

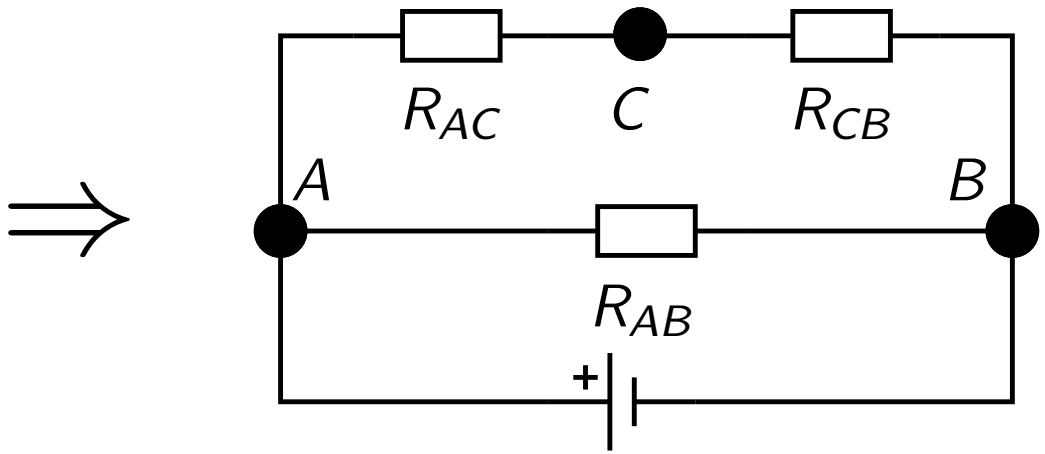

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Result

An analytical formula for the reaction rate

Theorem

The reaction rate $k_{A,B}$ (conductance) is given by

$$k_{A,B} = \varepsilon \left(\frac{1}{R_{A,B}} + \frac{1}{R_{A,C} + R_{C,B}} \right) (1 + o(1)),$$

where

$$R_{A,B} = Z_\mu \frac{\sqrt{|\det \nabla^2 H(s_{a,b})|}}{|\lambda^-(\nabla^2 H(s_{a,b}))|} e^{\varepsilon^{-1} H(s_{a,b})}$$

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Comparison with numerics

Analytical expansion of Z_μ

$$Z_\mu = 2\left(\frac{2\pi\varepsilon}{\sqrt{\det \nabla^2 H(a)}} + O(\varepsilon^{\frac{3}{2}})\right) e^{-\varepsilon^{-1}H(a)} + O\left(e^{-\varepsilon^{-1}(H(c))-H(a))}\right)$$

	$\varepsilon^{-1} = 6.67$	$\varepsilon^{-1} = 1.67$
[MSE06] TPT, flux	9.47×10^{-8}	1.912×10^{-2}
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[MSE06] finite difference		$(1.918 \pm 0.052) \times 10^{-2}$
Theorem, analytical Z_μ	9.63×10^{-8}	2.373×10^{-2}
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Upto numerical integration, the Theorem provides exact analytical results.

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Comparison with numerics

Analytical expansion of Z_μ

$$Z_\mu = 2\left(\frac{2\pi\varepsilon}{\sqrt{\det \nabla^2 H(a)}} + O(\varepsilon^{\frac{3}{2}})\right) e^{-\varepsilon^{-1}H(a)} + O\left(e^{-\varepsilon^{-1}(H(c))-H(a))}\right)$$

	$\varepsilon^{-1} = 6.67$	$\varepsilon^{-1} = 1.67$
[MSE06] TPT, flux	9.47×10^{-8}	1.912×10^{-2}
[MSE06] TPT, commitor	9.22×10^{-8}	1.924×10^{-2}
[MSE06] finite difference		$(1.918 \pm 0.052) \times 10^{-2}$
Theorem, analytical Z_μ	9.63×10^{-8}	2.373×10^{-2}
Theorem, numerical Z_μ	9.33×10^{-8}	1.926×10^{-2}

Upto numerical integration, the Theorem provides exact analytical results.

Variational formulation of reaction rates

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Theorem

The reaction rate $k_{A,B}$ has the following variational representation

$$k_{A,B} = \varepsilon \sup_{\varrho_A \in \mathcal{P}_\mu(A), \varrho_B \in \mathcal{P}_\mu(B)} \frac{1}{\|\varrho_A - \varrho_B\|^2_{\dot{H}^{-1}(\mu)}}.$$

Hereby $\mathcal{P}_\mu(S)$ are probability measures on $S \subset \mathbb{R}^n$, i.e.

$$\mathcal{P}_\mu(S) := \left\{ \varrho \in \dot{H}^{-1}(S;\mu) : \varrho \geq 0, \int_S \varrho \, \mathrm{d}\mu = 1 \right\}.$$

$\dot{H}^{-1}(\mu)$ is dual of $\dot{H}^1(\mu)$, i.e. for ϱ with $\int \varrho \, \mathrm{d}\mu = 0$ holds

$$\|\varrho\|_{\dot{H}^{-1}(\mu)} := \sup_{f \in \dot{H}^1(\mu)} \left\{ \frac{|\langle f, \varrho \rangle_\mu|^2}{\|f\|^2_{\dot{H}^1(\mu)}} \right\}, \quad \text{where} \quad \|f\|^2_{\dot{H}^1(\mu)} = \int |\nabla f|^2 \, \mathrm{d}\mu.$$

Negative Sobolev norm as transportation cost

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Lemma

Assume $\varrho_A, \varrho_B \ll \mu$, *then it holds*

$$\|\varrho_A - \varrho_B\|_{\dot{H}^{-1}(\mu)} = \mathcal{T}_\mu(\varrho_A \mu, \varrho_B \mu).$$

For two probability measures ν_A *and* ν_B, $\mathcal{T}_\mu(\nu_A, \nu_B)$ *is defined by*

$$\mathcal{T}_\mu^2(\nu_A, \nu_B) = \inf_{\Phi \in \Pi(\nu_A, \nu_B)} \int \left| \int_0^1 \dot{\Phi}_s \circ \Phi_s^{-1} \, \frac{\mathrm{d}\nu_s}{\mathrm{d}\mu} \, \mathrm{d}s \right|^2 \mathrm{d}\mu,$$

where ν_s *is the push-forward of* ν_A *under* Φ_s *denoted by* $\Phi_s \sharp \nu_A = \nu_s$. *The infimum is taken over*

$$\Pi(\nu_A, \nu_B) := \{\Phi \in \mathrm{AC}([0,1], \mathrm{Diff}(\mathbb{R}^n, \mathbb{R}^n)) : \Phi_0 = \mathrm{Id}, \Phi_1 \sharp \nu_A = \nu_B\}.$$

Circuit laws for transport

Series and parallel law for transport cost

$$\frac{1}{\mathcal{T}_\mu^2(\nu_A,\nu_B)} = \left(\frac{1}{T_{A,B}^2} + \frac{1}{T_{A,C}^2 + T_{B,C}^2}\right)(1+o(1)).$$

$T_{A,B}$, $T_{A,C}$, $T_{C,B}$ are support restricted transport costs.

Support restricted transport costs:

- Level set $\{H(x) \le H(s^*)\}$
  $\Rightarrow$ 3 connected components: $\Omega_a, \Omega_b, \Omega_c$
- $B_{a,b}, B_{a,c}, B_{c,b}$ $\sqrt{\delta}$-balls around saddles
- transport interpolations of $T_{A,B}$
  supported on $\Omega_a \cup B_{a,b} \cup \Omega_b$
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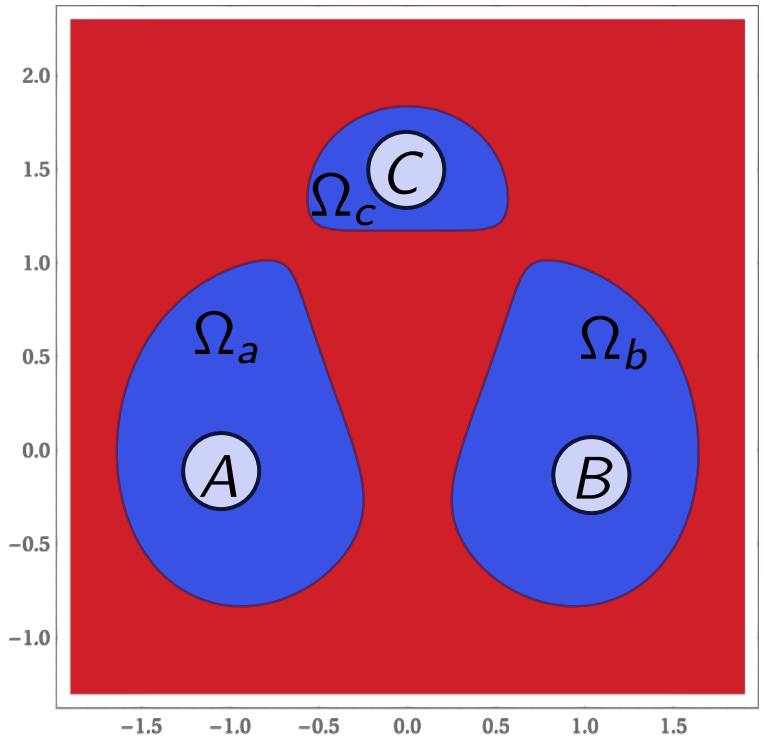

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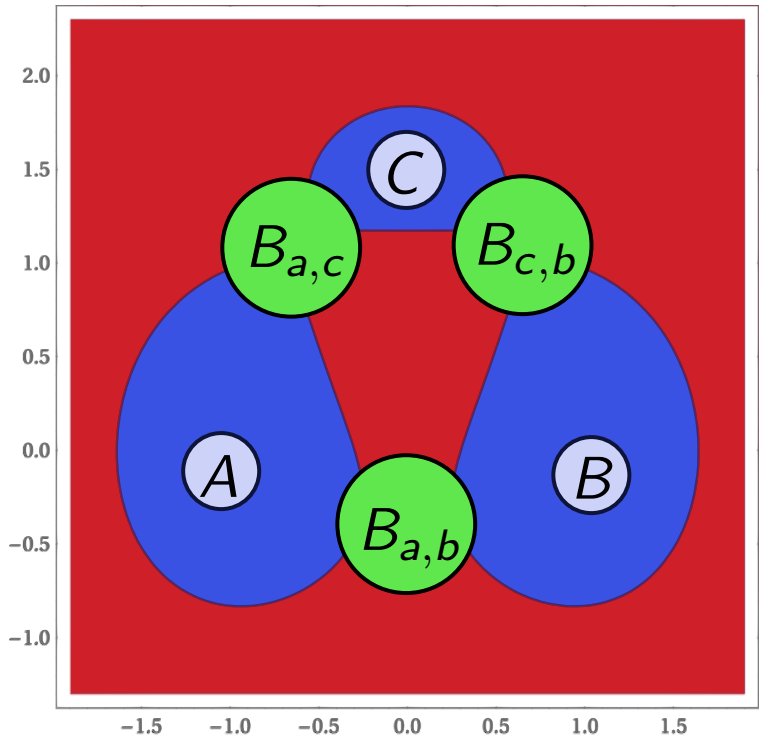

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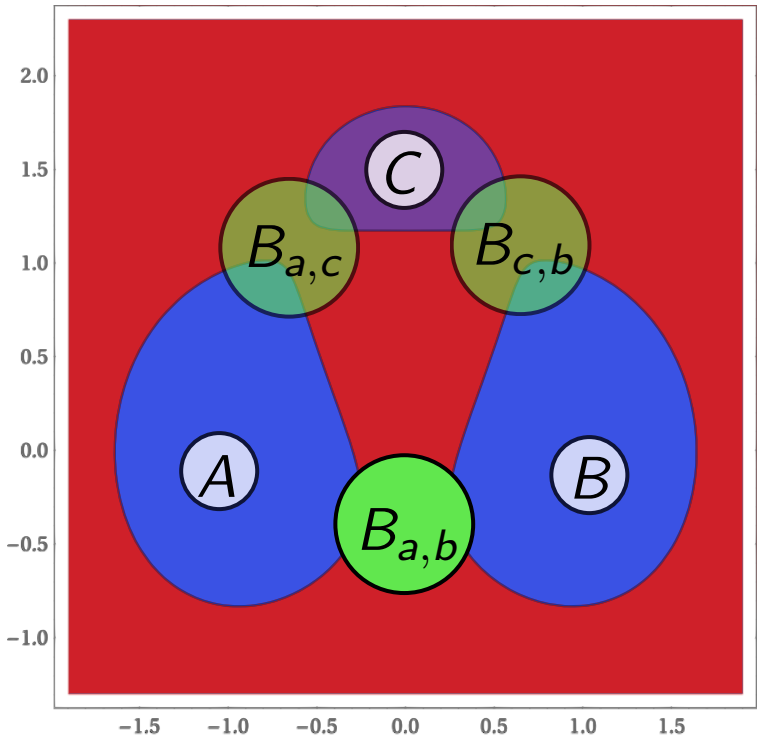

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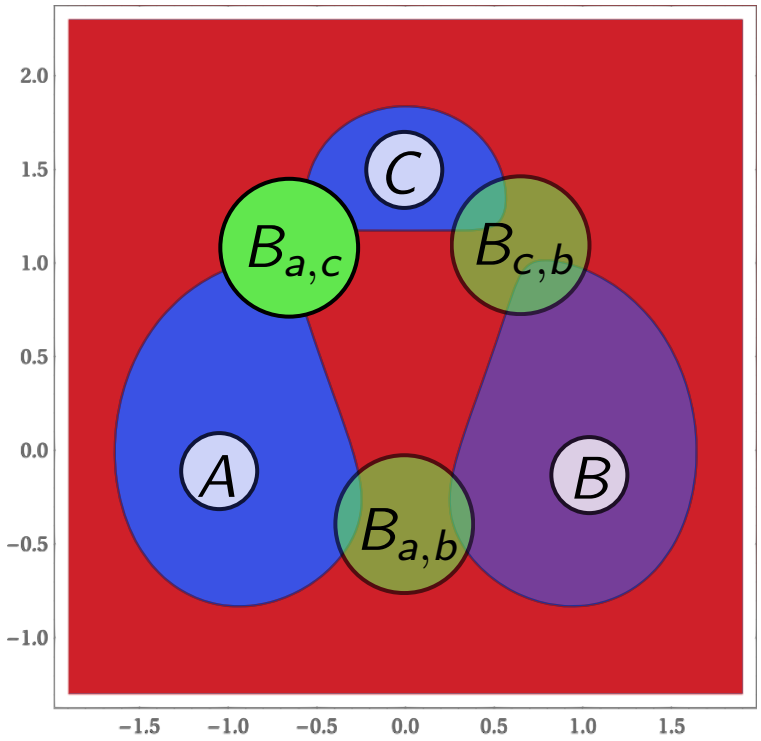

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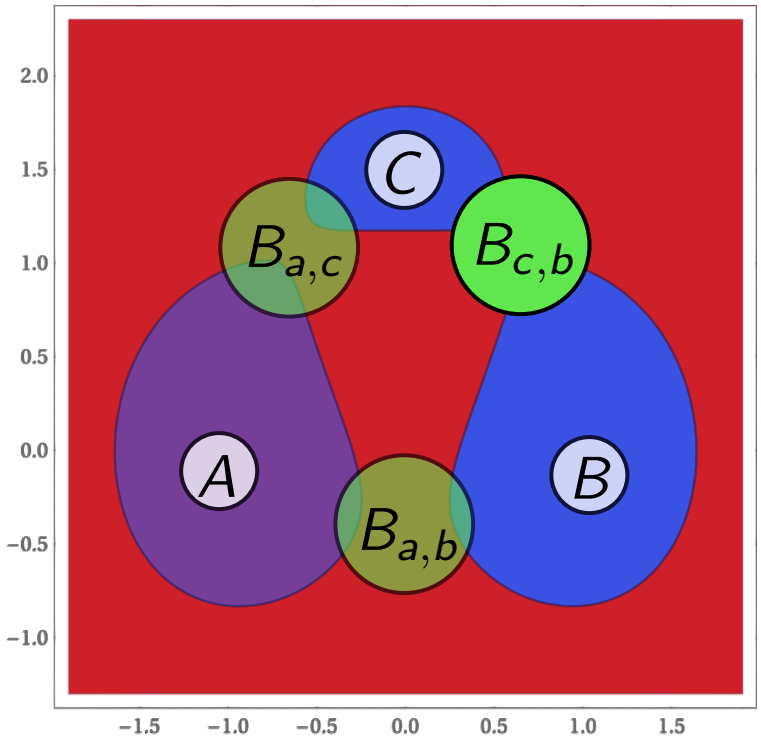

Evaluation of transport costs

Single transport costs are equal to resistances

$$T^2_{A,B}(1+o(1)) = R_{A,B} = Z_\mu \frac{\sqrt{|\det \nabla^2 H(s_{a,b})|}}{|\lambda^-(\nabla^2 H(s_{a,b}))|} e^{\varepsilon^{-1} H(s_{a,b})}$$

$$T^2_{A,C}(1+o(1)) = R_{A,C} = Z_\mu \frac{\sqrt{|\det \nabla^2 H(s_{a,c})|}}{|\lambda^-(\nabla^2 H(s_{a,c}))|} e^{\varepsilon^{-1} H(s_{a,c})}$$

$$T^2_{B,C}(1+o(1)) = R_{C,B} = Z_\mu \frac{\sqrt{|\det \nabla^2 H(s_{c,b})|}}{|\lambda^-(\nabla^2 H(s_{c,b}))|} e^{\varepsilon^{-1} H(s_{c,b})}.$$