BONN INTERNATIONAL GRADUATE SCHOOL OF MATHEMATICS

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Heat Flow with Dirichlet Boundary Condition on Metric Measure Spaces

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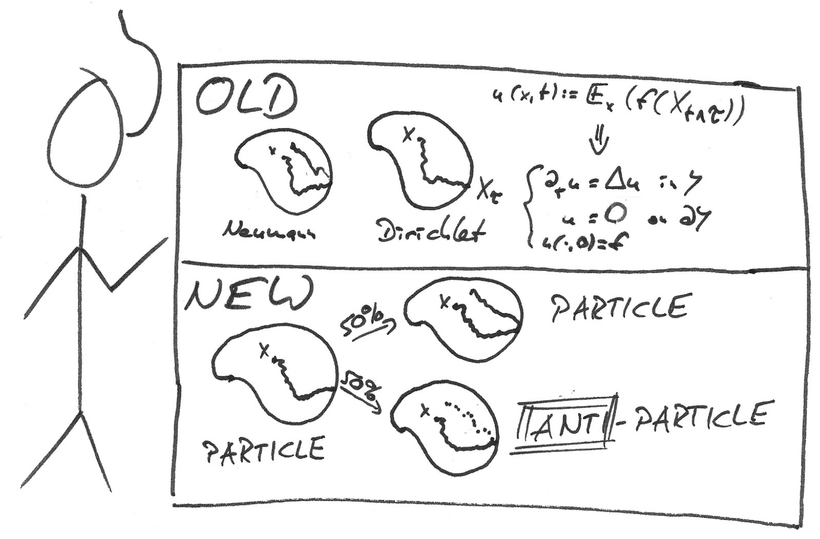
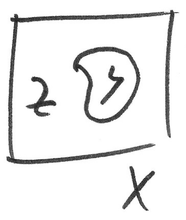
It is known since "ancient times" that reflected Brownian motion is connected to the heat equation with Neumann boundary conditions whereas killed Brownian motion is connected to Dirichlet boundary conditions (keyword "Feynman-Kac formula"). While there are many ways to interpret the equation with Neumann conditions as a gradient flow, this is not the case for Dirichlet conditions so far. We propose a new particle interpretation which makes it possible to view the heat equation with Dirichlet boundary conditions as a gradient flow in some "appropriate" geometry. For this, the main novelty is to introduce **anti-particles**. A particle changes its "charge" with a 50% chance when it hits the boundary. Looking at the densities σ_t^+ of particles and σ_t^- of anti-particles over time, the "effective" density $\mathring{\sigma}_t := \sigma_t^+ - \sigma_t^-$ will turn out to be the heat flow with Dirichlet boundary conditions.





Let $(X, d, \mathfrak{m})$ be a complete, separable metric measure space, $Y \subset X$ open, and denote by $Z := X \setminus Y$ the "boundary". We will be working with pairs of sub-probability measures which represent the particle densities of particles and anti-particles, called *charged measures*:
$\tilde{\mathcal{P}}(Y|X) := \{(\sigma^+, \sigma^-) \,|\, \sigma^\pm \in \mathcal{P}^{\leq 1}(X), (\sigma^+ + \sigma^-)(X) = 1, \sigma^+|_Z = \sigma^-|_Z\}$.

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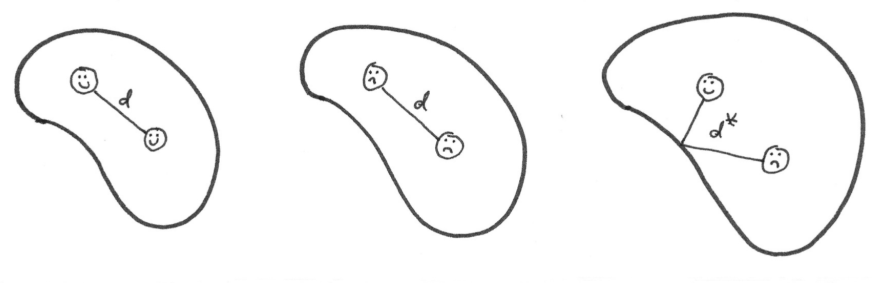
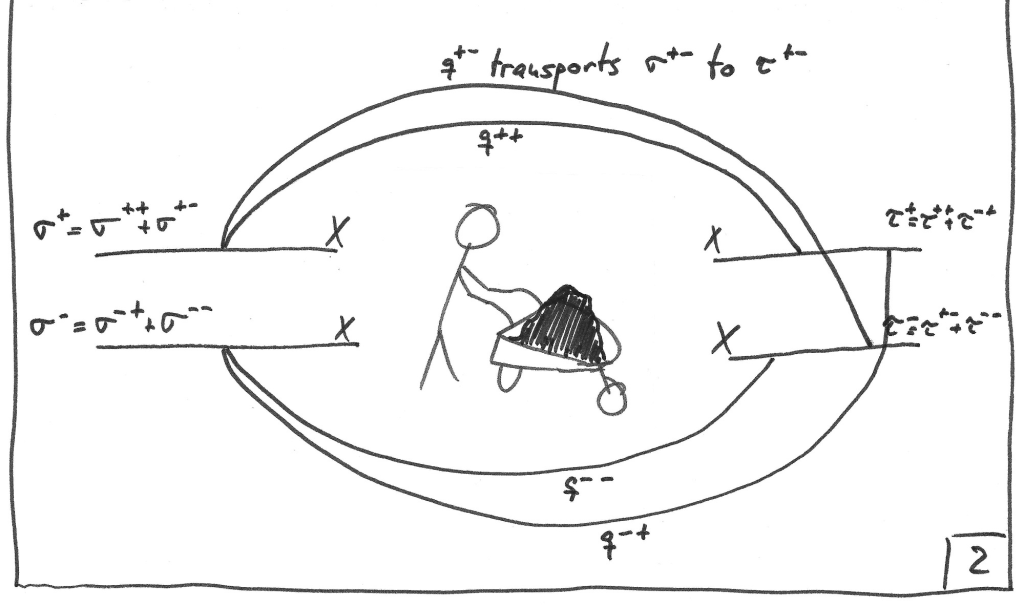
The distance between a particle x and an anti-particle y is defined as

$$d^*(x,y) := \inf_{z \in Z} [d(x,z) + d(z,y)]$$



We want a kind of "Wasserstein metric" to measure the distance between sub-probabilities. But to define it, we first need a metric for pairs of measures $\sigma = (\sigma^+, \sigma^-), \tau = (\tau^+, \tau^-) \in \tilde{\mathcal{P}}(Y|X)$. For a coupling $q \in \mathrm{Cpl}(\sigma^+ + \sigma^-, \tau^+ + \tau^-)$, there are decompositions $\sigma^i = \sigma^{i+} + \sigma^{i-}$ and $\tau^j = \tau^{+j} + \tau^{-j}$, $i, j \in \{+,-\}$, and couplings $q^{ij} \in \mathrm{Cpl}(\sigma^{ij}, \tau^{ij})$ such that $q = q^{++} + q^{+-} + q^{-+} + q^{--}$.



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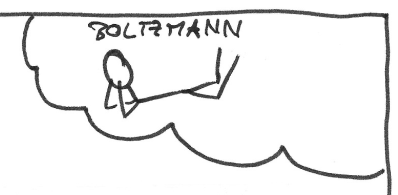
With this coupling, we can define the cost of it by

$$C(q) := \int_{X \times X} d^2(x,y)\, \mathrm{d}q^{++} + \int_{X \times X} (d^*)^2(x,y)\, \mathrm{d}q^{+-} + \int_{X \times X} (d^*)^2(x,y)\, \mathrm{d}q^{-+} + \int_{X \times X} d^2(x,y)\, \mathrm{d}q^{--}$$

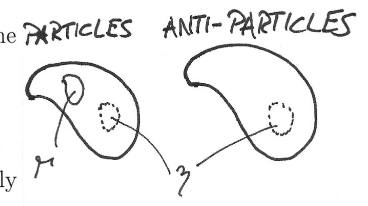
and subsequently the Wasserstein metric in $\tilde{\mathcal{P}}(Y|X)$ as $\tilde{W}_2^2(\sigma,\tau) := \inf_q C(q)$, where the infimum is over all couplings as above. Then $(\tilde{\mathcal{P}}_2(Y|X), \tilde{W}_2)$ is a complete, separable metric space.



Given sub-probabilities $\mu, \nu \in P^{\leq 1}(X)$, we finally can define

$$\begin{aligned} \mathring{W}_2(\mu,\nu) &:= \inf\{\tilde{W}_2(\sigma,\tau) \,|\, \sigma,\tau \in \tilde{\mathcal{P}}(Y|X), \mathring{\sigma} = \mu, \mathring{\tau} = \nu\} \\ &= \inf\{\tilde{W}_2((\mu+\eta,\eta),(\nu+\zeta,\zeta)) \,|\, \eta,\zeta \in \mathcal{P}^{\leq 1}(X), (\mu+2\eta)(X) = 1 = (\nu+2\zeta)(X)\} \end{aligned}$$

This is actually *not* a metric since it doesn't necessarily satisfy the triangle inequality.



Next, we define a Boltzmann entropy for pairs of measures. The gradient flow of this functional in the space $\tilde{\mathcal{P}}(Y|X)$ will give us the evolution $\sigma_t = (\sigma_t^+, \sigma_t^-)$, which will yield a description of the Neumann and Dirichlet heat flows. For $\sigma \in \tilde{\mathcal{P}}_2(Y|X)$ set $\widetilde{\mathrm{Ent}}(\sigma) := \mathrm{Ent}(\sigma^+) + \mathrm{Ent}(\sigma^-)$.

Assumption: The entropy is K-convex in $(\tilde{\mathcal{P}}(Y|X), \tilde{W}_2)$.

Let $(\sigma_t)_{t>0}$ be the EVI_K-gradient flow of $\widetilde{\mathrm{Ent}}$ in $\tilde{\mathcal{P}}_2(Y|X)$, i.e. for every $\rho \in \tilde{\mathcal{P}}_2(Y|X)$ and almost every $t > 0$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}\tilde{W}_2^2(\sigma_t,\rho) + \frac{K}{2}\tilde{W}_2^2(\sigma_t,\rho) + \widetilde{\mathrm{Ent}}(\sigma_t) \leq \widetilde{\mathrm{Ent}}(\rho).$$

Consider the time-dependent measures

$$\begin{aligned} \mu_t &:= \sigma^+ - \sigma^- \\ \nu_t &:= \sigma^+ + \sigma^-. \end{aligned}$$

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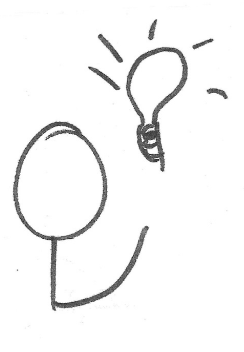
RESULTS



Theorem. *Let Y be an open, bounded, convex subset of a complete Riemannian manifold M with Ricci curvature uniformly bounded from below by $K \in \mathbb{R}$. Put $X = \overline{Y}$, let d be the Riemannian distance, and let $\mathfrak{m}$ be the Riemannian volume restricted to Y. Then the entropy $\widetilde{\mathrm{Ent}}$ is K-convex.*

Proposition.
i) *For each $\sigma \in \tilde{\mathcal{P}}(Y|X)$, there exists a unique EVI_K-gradient flow $(\sigma_t)_{t>0}$ for the Boltzmann entropy $\widetilde{\mathrm{Ent}}$ in $(\tilde{\mathcal{P}}(Y|X), \tilde{W}_2)$.*
ii) *Given $\mu \in \mathcal{P}^{\leq 1}(X)$, let $\sigma \in \tilde{\mathcal{P}}(Y|X)$ with $\mu = \sigma^+ - \sigma^-$. Then $\mu_t := \sigma_t^+ - \sigma_t^-$ is the heat flow with Dirichlet boundary condition starting in μ.*
iii) *Given $\nu \in \mathcal{P}(X)$, let $\sigma \in \tilde{\mathcal{P}}(Y|X)$ with $\mu = \sigma^+ + \sigma^-$. Then $\nu_t := \sigma_t^+ + \sigma_t^-$ is the heat flow with Neumann boundary condition starting in ν.*

Proposition. *For all $\sigma, \tau \in \tilde{\mathcal{P}}(Y|X)$ and all $t > 0$*

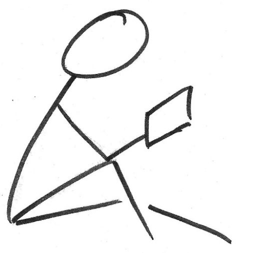
$$\tilde{W}_2(\sigma_t, \tau_t) \leq e^{-Kt} \cdot \tilde{W}_2(\sigma, \tau),$$

where $(\sigma_t)_{t>0}$ and $(\tau_t)_{t>0}$ are the EVI_K-flows starting in σ, τ.

Theorem. *For all $\mu, \nu \in \mathcal{P}^{\leq 1}(Y)$, and all $t > 0$*

$$\mathring{W}_p(\mu_t, \nu_t) \leq e^{-Kt} \cdot \mathring{W}_p(\mu, \nu),$$

where $(\mu_t)_{t>0}$ and $(\nu_t)_{t>0}$ denote the heat flows on Y with Dirichlet boundary conditions starting in μ and ν, resp.



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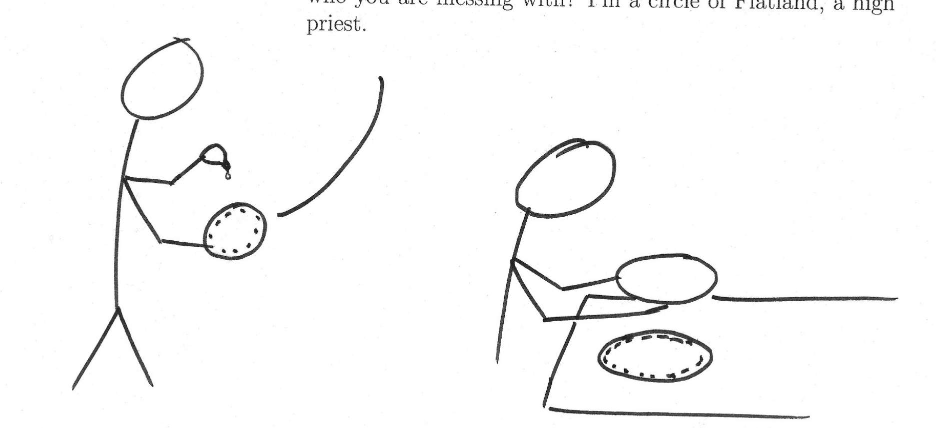
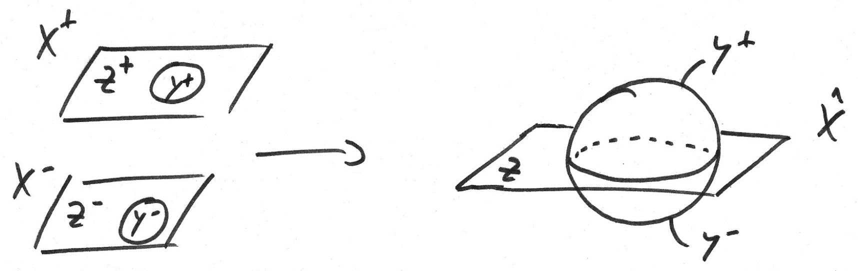
BEHIND THE SCENES



Take two copies $(X^+, d^+, \mathfrak{m}^+)$, $(X^-, d^-, \mathfrak{m}^-)$ of the same space, and the "same" subset $Y^+ \subset X^+$, $Y^- \subset X^-$ which we want to glue together along the "boundary" $Z^\pm := X^\pm \setminus Y^\pm$. We glue them together by identifying Z^+ and Z^-:

$$\begin{aligned} \hat{X} &:= (X^+ \sqcup X^-)/\sim_Z \\ \hat{\mathfrak{m}} &:= \frac{1}{2}\mathfrak{m}^+ + \frac{1}{2}\mathfrak{m}^- \\ \hat{d}(x,y) &:= \begin{cases} d^*(x,y), & \text{if } x \in X^i, y \in X^j, i \neq j \\ d(x,y), & \text{otherwise} \end{cases} \end{aligned}$$



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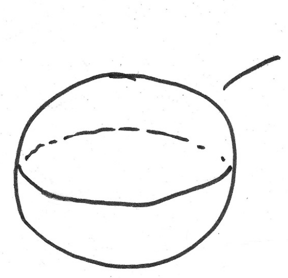

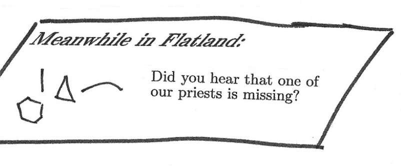

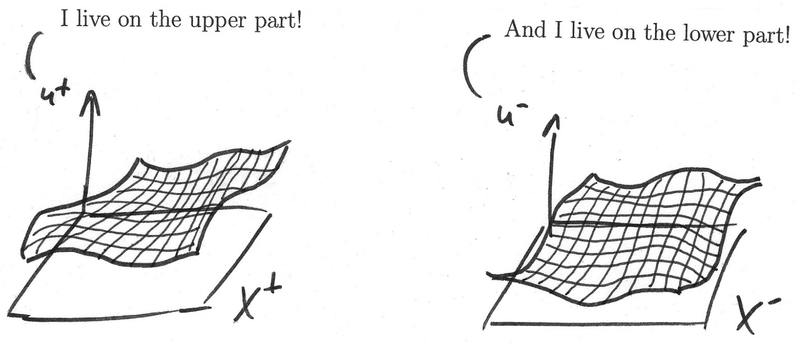

We coincide on Z. Together, we live on $\hat{X}$ under the name $\hat{u}$.
We have kids living on X (or on the X^i when needed):

$$\overline{u} := \frac{1}{2}u^+ + \frac{1}{2}u^-, \quad \mathring{u}^i := u^i - \overline{u}$$

THE END

Now I wanna sniff some glue

If you want to know something about the slope of functions on the glued space, you can look on the separate parts:

$$\hat{\mathcal{E}}(\hat{u}) = \int_{\hat{X}} |\nabla \hat{u}|^2 \,\mathrm{d}\hat{\mathfrak{m}} = \frac{1}{2}\int_{X^+} |\nabla u^+|^2 \,\mathrm{d}\mathfrak{m}^+ + \frac{1}{2}\int_{X^-} |\nabla u^-|^2 \,\mathrm{d}\mathfrak{m}^- = \frac{1}{2}\mathcal{E}(u^+) + \frac{1}{2}\mathcal{E}(u^-).$$

The glued heat flow is not so easy to describe – we will need to introduce one more object on X. Besides the Dirichlet form $(\mathcal{E}, D(\mathcal{E}))$ which corresponds to the heat flow with Neumann boundary values on X, there is also the Dirichlet form $(\mathcal{E}^0, D(\mathcal{E}^0))$ for the Dirichlet boundary values defined by

$$\begin{cases} D(\mathcal{E}^0) := \{f \in D(\mathcal{E}) \,|\, f = 0 \text{ on } Z\} \\ \mathcal{E}^0(f) := \mathcal{E}(f) \text{ for } f \in D(\mathcal{E}^0). \end{cases}$$

The associated heat semigroups P_t and P_t^0 make it possible to get an expression for the glued semigroup.

Theorem. *The heat semigroup corresponding to the Dirichlet form $(\hat{\mathcal{E}}, D(\hat{\mathcal{E}}))$ is given by*

$$\hat{P}_t\hat{u} = \begin{cases} P_t\overline{u} + P_t^0\mathring{u}^+, & \text{on } X^+ \\ P_t\overline{u} + P_t^0\mathring{u}^-, & \text{on } X^-, \end{cases} \tag{1}$$

for a function $\hat{u} \in L^2(\hat{X}, \hat{\mathfrak{m}})$.

This formula expresses the fact that particles hitting the boundary set Z are reflected with probability 1/2 or change to the other copy of the space (i.e. change their "charge") with probability 1/2.
To prove this you first show that the right-hand side of (1) is indeed a strongly continuous contraction semigroup on $L^2(\hat{X}, \hat{\mathfrak{m}})$. Then you identify the associated Dirichlet form with the one given by the Cheeger energy by using the *approximate* Dirichlet forms like $\mathcal{E}_t(u,v) := -\frac{1}{t}\int_X v(P_t u - u)\,\mathrm{d}\mathfrak{m}$ defined on all of $L^2(X,\mathfrak{m})$, and analogously for the other semigroups.
The other results follow by identifying the first setting (the two densities σ^+, σ^- on X) with the second one (the glued space with probability measures on it) and using the **Assumption**.

Break on through (to the other side)

Theorem. *The spaces $(\tilde{\mathcal{P}}(Y|X), \tilde{W}_2)$ and $(\mathcal{P}(\hat{X}), \hat{W}_2)$ are isometric. Here, $\hat{W}_2$ is the L^2-Wasserstein metric to the metric measure space $(\hat{X}, \hat{d}, \hat{\mathfrak{m}})$.*

Also, the entropy $\widetilde{\mathrm{Ent}}$ and the "usual" entropy on $\hat{X}$ coincide up to a constant under this isometry, so that the **Assumption** translates to the $\mathrm{RCD}^*(K,\infty)$ condition for $\hat{X}$. The result on manifolds now follows by a theorem of [Schlichting] on gluing Riemannian manifolds, whereas the other results follow directly by the properties of $\mathrm{RCD}^*(K,\infty)$-spaces. Additionally, the gradient estimate for $\hat{X}$ gives a mixed gradient estimate for the heat flow with Dirichlet boundary values on X:

Theorem. *For all $t > 0$ and all $u \in D(\mathcal{E}^0)$*

$$|\nabla P_t^0 u|^2 \leq e^{-2Kt} P_t |\nabla u|^2.$$

To prove this, you insert the function $\hat{u} = u$ on X^+, $\hat{u} = -u$ on X^- into the gradient estimate on $\hat{X}$. There is an equivalent mixed Bochner inequality attached to it, namely

$$\frac{1}{2}\Delta|\nabla u|^2 - \nabla u \cdot \nabla \Delta^0 u \geq K|\nabla u|^2.$$

References

- Profeta, Sturm – Heat Flow with Dirichlet Boundary Conditions via Optimal Transport and Gluing of Metric Measure Spaces, in progress
- Schlichting – Smoothing singularities of Riemannian metrics while preserving lower curvature bounds, PhD thesis, Magdeburg, 2013

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