AN OPTIMAL TRANSPORT VIEW ON SCHRÖDINGER'S EQUATION

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Abstract

Rephrasing results by HALL and REGINATTO [9] in the language of Wasserstein geometry leads to a representation of the Schrödinger flow as a Lagrangian system on the space of probability measures $\mathcal{P}(M)$ of physical space M where the potential field $\mu \to \langle \phi, \mu \rangle$ is augmented by the Fisher information functional $\mu \to \frac{\hbar^2}{8} \int |\nabla \ln \mu|^2 d\mu$.

1 INTRODUCTION

Recent applications of optimal transport theory have demonstrated that certain analytical and geometric problems on finite dimensional Riemannian manifolds (M, g) or more general metric measure spaces (X, d, m) can effectively be treated in the corresponding ('Wasserstein') space of probability measures $\mathcal{P}_2(X) = \{\mu \in \mathcal{P}(X) \mid \int_X d^2(x, o)\mu(dx) < \infty\}$ equipped with the Wasserstein metric

$$d_w(\mu, \nu) = \inf \left\{ \iint_{X^2} d^2(x, y)\Pi(dx, dy) \;\middle|\; \Pi \in \mathcal{P}(X^2), \Pi(X \times A) = \nu, \Pi(A \times X) = \mu(A), A \in \mathcal{B}(X) \right\}^{1/2},$$

which defines a relaxed version of Monge's optimal transportation problem on X with $c(x, y) = d^2(x, y)$

$$\inf \left\{ \int_X c(x, Ty)\mu(dx) \mid T : X \to X, T_*\mu = \nu \right\}.$$

Here $T_*\mu$ denotes the image (push forward) measure of $\mu \in \mathcal{P}(X)$ under the map T.
The physical relevance of the Wasserstein distance was highlighted by the works of e.g. BRENIER [4] and OTTO who established in [15] for the smooth Riemannian case $X = M$ and smooth initial distribution μ

$$d_w^2(\mu, \nu) = \inf \left\{ \int_0^1 \int_M |\nabla \phi_t(x)|^2 \mu_t(dx)dt \;\middle|\; \begin{array}{c} \phi \in C^\infty(]0, 1[\times M), t \to \mu_t \in C([0, 1], \mathcal{P}(M)) \\ \dot{\mu}_t = -\operatorname{div}(\nabla \phi_t \mu_t), t \in]0, 1[, \mu_0 = \mu, \mu_1 = \nu \end{array} \right\},$$

showing that d_w is associated to a formal Riemannian structure on $\mathcal{P}(M)$ given by

$$T_\mu \mathcal{P}(M) = \{\psi : M \to \mathbb{R}, \int_M \psi(x)dx = 0\}$$

$$\|\psi\|_\mu^2 = \int_M |\nabla \phi|^2 d\mu, \text{ where } \psi = -\operatorname{div}(\mu \nabla \phi).$$

In view of the continuity equation

$$\dot{\mu}_t = -\operatorname{div}(\dot{\Phi}_t \mu_t)$$

for a smooth flow $(t, x) \to \Phi_t(x)$ on M, acting on a measures μ through push forward $\mu_t = (\Phi_t)_*\mu_0$, this identifies the Riemannian energy of a curve $t \to \mu_t \in \mathcal{P}(M)$ with the minimal required kinetic energy

$$E_{0,t}(\mu) = \int_0^t \|\dot{\mu}_s\|^2_{T_{\mu_s}\mathcal{P}(M)} ds = \int_0^t \int_M |\dot{\Phi}(x, s)|^2 \mu_s(dx)ds.$$

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A crucial implication of this perspective on $\mathcal{P}(M)$ is the d_w-gradient flow ('steepest descent') interpretation of evolution equations of the form

$$\partial_t u = \operatorname{div}(u_t \nabla F'(u)),$$

where F' is the Frechet derivative of some smooth functional F on $L^2(M, dx)$, showing that the evolution is completely determined by the geometric properties of F with respect to d_w. A particularly important example is the Boltzmann entropy $F(u) = \int_M u \ln u \, dx$ inducing the heat equation as gradient flow, which initiated substantial progress in a synthetic theory of generalized Ricci curvature bounds [5, 12, 18, 22].

In this note we propose a second class of dynamical systems associated with the formal Riemannian structure on $\mathcal{P}(M)$ which is given by Lagrangian flows on $T\mathcal{P}(M)$ associated to Lagrangians of the form

$$L_F : T\mathcal{P}(M) \to \mathbb{R}; \quad L_F(V) = \frac{1}{2} \|\psi\|^2_{T_\mu \mathcal{P}} - F(\mu) \quad \text{for } V = (\psi, \mu) \in T_\mu \mathcal{P}(M)$$

where the functional $F : \mathcal{P}(M) \to \mathbb{R}$ now plays the role of a potential field for the infinite dimensional system. We do not aim to develop a full theory here but give an interesting example instead which leads to a Lagrangian representation of the Schrödinger flow by putting

$$F(\mu) = \int_M \phi(x)\mu(dx) + \frac{\hbar^2}{8} I(\mu), \tag{1}$$

where

$$I(\mu) = \int_M |\nabla \ln \mu|^2 d\mu$$

is known today as Fisher information functional. - In this form I appears already in the Hamiltonian of BOHM's famous 1952 paper [3, eq. (9)] as a consequence of the choice of polar coordinates $\Psi = Re^{\frac{i}{\hbar}S}$ but is not further analysed as such. The first detailed discussion of the meaning of I in the Schrödinger context seems to be given in [17], using information-theoretic concepts. This was later complemented by a simplified physical approach in [9].

Mathematically the connection between Wasserstein geometry and the Schrödinger flow is based on the representation of the latter via a system of a generalized Hamilton-Jacobi and transport equations (4) which is known since long [13]. (In fact this representation is the nucleus of the de Broglie-Bohm 'causal' interpretation of the laws of quantum mechanics [6, 3], cf. eg. [7, 10].) The Riemannian Wasserstein formalism now allows to write this system as a geometric Euler-Lagrange equation (3) induced from L_F. Hence our example (theorem 2.1 below) is interesting in two ways. Physically it shows how the Wasserstein formalism can provide a unifying framework in which both classical and quantum behaviour of a particle can be described in a seemingly classical fashion, cf. remark 2.2 ii). Mathematically it directs towards an important class of dynamics on $T\mathcal{P}(M)$ which is worth systematic study.

2 RESULT - SCHRÖDINGER EQUATION FROM A LAGRANGIAN FLOW ON $\mathcal{P}(M)$

The observation below is based on formal Riemannian calculations on the d_w-dense subset $P^\infty(M) \subset \mathcal{P}_2(M)$ of fully supported smooth probability measures as conducted in [15, 16] and extended by LOTT in [11], ignoring the question of full mathematical generality. (The relevant results from [11, 15] are summarized in section 3.) In the sequel we shall often identify $\mu \in \mathcal{P}^\infty(M)$ with its density $\mu \overset{\triangle}{=} d\mu/dx$.

Theorem 2.1. *For $\phi \in C^\infty(M)$ let $F : \mathcal{P}^\infty(M) \to \mathbb{R}$ defined as in (1). Then any smooth local Lagrangian flow $[0,\epsilon] \ni t \to \dot\mu_t \in T\mathcal{P}^\infty(M)$ associated to L_F yields a local solution of the Schrödinger equation*

$$i\hbar\partial_t\Psi = -\hbar^2/2\Delta\Psi + \Psi\,\phi \tag{2}$$

via the Madelung transform

$$\Psi(t,x) = \sqrt{\mu(t,x)}e^{\frac{i}{\hbar}\bar{S}(x,t)}$$

where

$$\bar{S}(x,t) = S(x,t) + \int_0^t L_F(S_\sigma,\mu_\sigma)d\sigma$$

and $S(x,t)$ is the velocity potential of the flow μ, i.e. satisfying $\int_M Sd\mu = 0$ and $\dot\mu_t = -\operatorname{div}(\nabla S_t\mu)$.

Proof . The Lagrangian flow $(\mu_t)_{t\geq 0}$ is a local critical point of the action functional

$$S_{a,b}(\gamma) = \int_a^b \left[\frac{1}{2}\|\dot\gamma\|^2_{T_\mu} - F(\gamma(t))\right]dt,$$

defined on the set of smooth curves $t \to \gamma_t \in \mathcal{P}(M)$, i.e μ solves the Euler-Lagrange equations

$$\nabla^w_{\dot\mu}\dot\mu = -\nabla^w F(\mu), \tag{3}$$

where ∇^w is the Wasserstein gradient and $\nabla^w_{\dot\mu}\dot\mu$ is the (pulled back on $\Gamma(\mu^*T\mathcal{P}(M))$) covariant derivative associated to the Levi-Civita connection on $T\mathcal{P}(M)$. Let $(x,t) \to S(x,t)$ denote the velocity potential of $\dot\mu$ (cf. section 3), then according to [11, proposition 4.24] the left hand side above is computed as

$$-\operatorname{div}\left(\mu\nabla\left(\partial_t S + \frac{1}{2}|\nabla S|^2\right)\right),$$

where the right hand side equals (cf. section 3)

$$\operatorname{div}\left(\mu\nabla\left(\phi + \frac{\hbar^2}{8}\big(|\nabla\ln\mu|^2 - \frac{2}{\mu}\Delta\mu\big)\right)\right).$$

Since μ_t is fully supported on M this implies

$$\partial_t S + \frac{1}{2}|\nabla S|^2 + \phi + \frac{\hbar^2}{8}\big(|\nabla\ln\mu|^2 - \frac{2}{\mu}\Delta\mu\big) = c(t)$$

for some function $c(t)$. To compute $c(t)$ note that due to the normalization $\langle S_t,\mu_t\rangle = 0$

$$\begin{aligned}
0 &= \partial_t\langle S_t,\mu_t\rangle \\
&= c(t) - \frac{1}{2}\langle|\nabla S|^2, d\mu\rangle - F(\mu) + \langle S,\dot\mu\rangle \\
&= c(t) - \frac{1}{2}\langle|\nabla S|^2, d\mu\rangle - F(\mu) + \langle|\nabla S|^2,\mu\rangle = c(t) + L_F(S_t,\mu_t).
\end{aligned}$$

Hence the pair $t \to (\overline{S}_t,\mu_t)$ with $\bar{S}(x,t) = S(x,t) + \int_0^t L_F(S_\sigma,\mu_\sigma)d\sigma$ satisfies

$$\begin{gathered}
\partial_t\bar{S} + \frac{1}{2}|\nabla\overline{S}|^2 + \phi + \frac{\hbar^2}{8}\big(|\nabla\ln\mu|^2 - \frac{2}{\mu}\Delta\mu\big) = 0 \\
\partial_t\mu + \operatorname{div}(\mu\nabla\overline{S}) = 0,
\end{gathered} \tag{4}$$

which is computed to provide a solution to Schrödinger's equation via $\Psi(x,t) = \sqrt{\mu}(x,t)e^{\frac{i}{\hbar}\bar{S}(x,t)}$. □

Remarks 2.2. i) An equivalent version of theorem 2.1 puts $\Psi = \sqrt{\mu}(x,t)e^{\frac{i}{\hbar}S(x,t)}$ where $t \to (-\operatorname{div}(\nabla S_t \mu_t), \mu_t)$ is a Lagrangian flow for L_F and S is chosen to satisfy for all $t \geq 0$

$$\langle S_t, \mu_t \rangle - \langle S_0, \mu_0 \rangle = \int_0^t L_F(\dot{\mu}_s) ds.$$

ii) The case of a classicle particle moving in a potential field $\phi : M \to \mathbb{R}$ is embedded in the Lagrangian formalism on $T\mathcal{P}(M)$ by choosing $\hbar = 0$ for initial condition $\mu_0 = \delta_{x_0}$ and $\psi_0 = -\operatorname{div}(\dot{x}_0 \delta_{x_0})$. The case of $\hbar = 0$ and an extended initial field $p(0,x) \in \mathcal{P}^\infty(M)$ is delicate because of collisions of classical Hamiltonian trajectories, i.e. after finite time $\dot{\mu}_t$ will assume values outside $T\mathcal{P}(M)$ where the formalism no longer applies.

iii) In [9] the authors argue that the Madelung transform is part of a unique canonical i.e. symplectic transformation for the Hamiltonian structure associated with L_F under which the new coordinates decouple. From such a perspective the familiar complex valued form (2) of the Schrödinger equation would appear to result from an ingenious choice of coordinates.

iv) The d_w-gradient flow of F_V gives the nonlinear 4th order 'Derrida-Lebowitz-Speer-Spohn' or 'quantum drift-diffusion' equation, which is thoroughly analysed in [8].

v) Based on NELSON's stochastic mechanics [14] the paper [20] aims to present a very different approach to a potential link between (in this case 'stochastic') optimal transport theory and the Schrödinger equation.

3 APPENDIX - FORMAL RIEMANNIAN CALCULUS ON $\mathcal{P}(M)$

Let $\mathcal{P}_2(M)$ denote the set of Borel probability measures μ on a smooth closed finite dimensional Riemannian manifold (M,g) having finite second moment $\int_M d^2(o,x)\mu(dx) < \infty$. As argued in [11] the subsequent calculations make strict mathematical sense on the d_w-dense subset of smooth fully supported probabilities $\mathcal{P}^\infty(M) \subset \mathcal{P}_2(M)$ which shall often be identified with the corresponding density $\mu \overset{\triangle}{=} d\mu/dx$.

3.1 *Vector Fields on $\mathcal{P}(M)$ and Velocity Potentials*

A function $\phi \in \mathcal{C}_c^\infty(M)$ induces a flow on $\mathcal{P}(M)$ via push forward

$$t \to \mu_t = (\Phi_t^{\nabla\phi})_* \mu_0,$$

where $t \to \Phi_t$ is the local flow of difformorphisms on M induced from the vector field $\nabla\phi \in \Gamma(M)$ starting from $\Phi_0 = \mathrm{Id_M}$. The the continuity equation yields the infinitesimal variation of $\mu \in \mathcal{P}(M)$ as

$$\dot{\mu} = \partial_{t|t=0}\mu_t = -\operatorname{div}(\nabla\phi\mu) \in T_\mu(\mathcal{P}).$$

Hence the function ϕ induces a vector field $V_\phi \in \Gamma(\mathcal{P}(M))$ by

$$V_\phi(\mu) = -\operatorname{div}(\nabla\phi\mu),$$

acting on smooth functionals $F : \mathcal{P}(M) \to \mathbb{R}$ via

$$V_\phi(F)(\mu) = \partial_{\epsilon|\epsilon=0} F(\mu - \epsilon \operatorname{div}(\nabla\phi\mu)) = \partial_{t|t=0} F((\Phi_t^{\nabla\phi})_*\mu)$$

with Riemannian norm

$$\|V_\phi(\mu)\|^2_{T_\mu\mathcal{P}} = \int_M |\nabla\phi|^2(x)\mu(dx).$$

Conversely, each smooth variation $\psi \in T_\mu(\mathcal{P})$ can be identified with

$$\psi = -V_\phi(\mu) \quad \text{with } \phi = G_\mu\psi,$$

where G_μ is the Green operator for $\Delta^\mu : \phi \to -\operatorname{div}(\mu\nabla\phi)$ on $L^2_0(M, dx) = L^2_0(M, dx) \cap \{\langle f, dx\rangle = 0\}$. Hence, for each $\psi \in T_\mu\mathcal{P}$ there exists a unique $\phi \in \mathcal{C}^\infty \cap L^2(M, dx)$ such that

$$\psi = -\operatorname{div}(\mu\nabla\phi) \text{ and } \langle\phi, \mu\rangle = 0,$$

which we call velocity potential for $\psi \in T_\mu\mathcal{P}(M)$.

3.2 *Riemannian Gradient on $\mathcal{P}(M)$*

The Riemannian gradient of a smooth functional $F : \mathrm{Dom}(F) \subset \mathcal{P}(M) \to \mathbb{R}$ is computed to be

$$\nabla^w F_{|\mu} = -\Delta^\mu(DF_{|\mu}),$$

where $x \to DF_{|\mu}(x)$ is the $L^2(M, dx)$-Frechet-derivative of F in μ, which is defined through the relation

$$\partial_{\epsilon|\epsilon=0}F(\mu + \epsilon\xi) = \int_M DF_\mu(x)\xi(x)dx,$$

for all ξ chosen from a suitable dense set of test functions in $L^2(M, dx)$. The following examples are easily obtained.

Linear case:	$F(\mu) = \int_M \phi(x)\mu(dx)$	$\nabla^w F_{\|\mu} = V_\phi(\mu) = -\operatorname{div}(\nabla\phi\mu)$
Boltzmann entropy:	$F(\mu) = \int_M \mu\log\mu dx$	$\nabla^w F_{\|\mu} = -\operatorname{div}(\mu\nabla\log\mu) = -\Delta\mu$
Renyi entropy:	$F(\mu) = \int_M \mu^p dx$	$\nabla^w F_{\|\mu} = -p(p-1)\operatorname{div}(\mu^{p-1}\nabla\mu)$
Fisher information:	$F(\mu) = \int_M \|\nabla\ln\mu\|^2 d\mu$	$\nabla^w F_{\|\mu} = -\operatorname{div}(\mu\nabla(\|\nabla\ln\mu\|^2 - \frac{2}{\mu}\Delta\mu))$.

Here Δ denotes the Laplace-Beltrami operator on (M, g). As a consequence, the Boltzmann entropy induces the heat equation as gradient flow on $\mathcal{P}(M)$, and the information functional is the norm-square of its gradient, i.e.

$$\left\|\nabla^w \mathrm{Ent}_{|\mu}\right\|^2_{T_\mu\mathcal{P}} = \|-\operatorname{div}(\mu\nabla\log\mu)\|^2_{T_\mu\mathcal{P}} = \int_M |\nabla\log\mu|^2 d\mu = I(\mu).$$

3.3 *Covariant Derivative*

The Koszul identity for the Levi-Civita connection and a straightforward computation of commutators show [11] for the covariant derivative ∇^w associtated to d_w that

$$\langle\nabla^w_{V_{\phi_1}} V_{\phi_2}, V_{\phi_3}\rangle_{T_\mu} = \int_M \operatorname{Hess}\phi_2(\nabla\phi_1, \nabla\phi_2)d\mu.$$

For a smooth curve $t \to \mu(t)$ with $\dot\mu_t = V_{\phi_t}$ this yields

$$\nabla^w_{\dot\mu}\dot\mu = V_{\partial_t\phi + \frac{1}{2}|\nabla\phi|^2}.$$

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