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An Optimal Transport View of Schrödinger's Equation

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Abstract. We show that the Schrödinger equation is a lift of Newton's third law of motion $\nabla^{\mathcal{W}}_{\dot\mu}\dot\mu = -\nabla^{\mathcal{W}}F(\mu)$ on the space of probability measures, where derivatives are taken with respect to the Wasserstein Riemannian metric. Here the potential $\mu \to F(\mu)$ is the sum of the total classical potential energy $\langle V,\mu\rangle$ of the extended system and its Fisher information $\frac{\hbar^2}{8}\int|\nabla \ln\mu|^2\,d\mu$. The precise relation is established via a well-known (Madelung) transform which is shown to be a symplectic submersion of the standard symplectic structure of complex valued functions into the canonical symplectic space over the Wasserstein space. All computations are conducted in the framework of Otto's formal Riemannian calculus for optimal transportation of probability measures.

1 Introduction and Statement Of Results

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 nicely be treated in the corresponding (Wasserstein) space of probability measures

$$\mathcal{P}_2(X) = \Big\{\mu \in \mathcal{P}(X) \;\Big|\; \int_X d^2(x,o)\mu(dx) < \infty \text{ for some } o \in X\Big\}$$

equipped with the quadratic Wasserstein metric

$$d_{\mathcal{W}}(\mu,\nu) = \inf_{\Pi\in\Gamma(\mu,\nu)}\Big\{\iint_{X^2} d^2(x,y)\Pi(dx,dy)\Big\}^{1/2},$$

where $\Gamma(\mu,\nu)$ denotes the set of probability measures $\Pi \in \mathcal{P}(X^2)$ on $X^2 = X\times X$ such that $\Pi(X\times A) = \nu(A)$ and $\Pi(A\times X) = \mu(A)$ for all Borel subsets $A \subset X$. This metric corresponds to a relaxed version of Monge's optimal transportation problem with cost function $c(x,y) = d^2(x,y)$

$$\inf\Big\{\int_X c(x,Ty)\mu(dx) \mid T\colon X \to X, T_*\mu = \nu\Big\},$$

with $T_*\mu$ denoting 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

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Benamou–Brenier [4] and McCann [13] who established, in the case when X is Euclidean, resp. smooth Riemannian, and $\mu \in \mathcal{P}_2(X)$ is smooth, that

$$d_{\mathcal{W}}^2(\mu,\nu) = \inf_{(\phi,\mu)\in\Phi(\mu,\nu)} \Big\{ \int_0^1 \int_M |\nabla\phi_t(x)|^2 \mu_t(dx)dt \Big\},$$

with

$$\Phi(\mu,\nu) = \left\{ \begin{array}{l} \phi \in C^\infty(]0,1[\times M), \mu \in C([0,1],\mathcal{P}(M)) \\ \dot\mu_t = -\operatorname{div}(\nabla\phi_t\mu_t), t\in]0,1[, \mu_0=\mu, \mu_1=\nu \end{array} \right\},$$

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

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

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

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 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

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

A major reason for the success of this framework is Otto's interpretation [15] of evolution equations of type $\partial_t u = \operatorname{div}(u_t\nabla F'(u))$, with F' being the L^2-Frechet derivative of some smooth functional F on $L^2(M,dx)$, as $d_{\mathcal{W}}$-gradient (steepest descent) flow $\dot\mu = -\nabla^{\mathcal{W}}F(\mu)$ for the measures $\mu(dx) = u(x)dx$. Properties of the flow may thus be deduced from the geometry of the funtional F with respect to $d_{\mathcal{W}}$. An important case is the Boltzmann entropy $F(u) = \int_M u\ln u\, dx$ inducing the heat flow.

Here we propose an example of a second natural class of dynamical systems associated with the Riemannian metric on $\mathcal{P}(M)$ which can be written as

$$\nabla^{\mathcal{W}}_{\dot\mu}\dot\mu = -\nabla^{\mathcal{W}}F(\mu). \tag{1.1}$$

Equation (1.1) describes the Hamiltonian flow on $T\mathcal{P}(M)$ induced from the Lagrangian

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

with the functional $F\colon \mathcal{P}(M)\to\mathbb{R}$ now playing the role of a potential field for the system. Apart from the closely related works [2, 7], it seems that a systematic approach to such Hamiltonian flows on $\mathcal{P}(M)$ is missing in the literature. The example we want to propose is obtained by choosing

$$F(\mu) = \int_M V(x)\mu(dx) + \frac{\hbar^2}{8}I(\mu), \tag{1.2}$$

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where

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

We show that, via an appropriate transform, the flow (1.1) solves the Schrödinger equation

$$i\hbar\partial_t \Psi = -\hbar^2/2\Delta\Psi + \Psi V. \tag{1.3}$$

The functional I is also known as Fisher information. Physically, $I(\mu)$ is the energy dissipation of the unperturbed heat flow at state μ. The prominent role of I for quantum behaviour was noticed long ago, *e.g.,* in a classical paper by Bohm [5], using the following well-known system of generalized Hamilton–Jacobi and transport equations:

$$\begin{aligned} \partial_t S + \frac{1}{2}|\nabla S|^2 + V + \frac{\hbar^2}{8}\Big(|\nabla \ln \mu|^2 - \frac{2}{\mu}\Delta\mu\Big) &= 0 \\ \partial_t \mu + \operatorname{div}(\mu \nabla S) &= 0. \end{aligned} \tag{1.4}$$

This system was proposed very early by Madelung [12] as an equivalent description of the wave function $\Psi = \sqrt{\mu} e^{\frac{i}{\hbar}S}$ under the Schrödinger equation. In the sequel it will be referred to as Madelung flow. Various attempts to derive it from first order principles can be found in the physics literature, *e.g.,* most recently in [9].

In fact, using Lott's recently proposed second order calculus on Wasserstein space, (see [11]) we show that equations (1.4) and (1.1) are essentially the same (Theorem 2.1). A virtue of formula (1.1) is its very intuitive physical interpretation as Newton's law for the motion of an extended system with inertia (we have put mass density equal to one). Acceleration comes from a gradient field of a potential F which is the total mechanical potential of the extended system plus its 'dissipative potential' with respect to the heat flow. (Note that the case of a classical Hamiltonian particle moving in a potential field ∇F is embedded naturally in (1.1) if one puts $\hbar = 0$ and $\mu = \delta_x$.)

Secondly we show that the two equations (1.1) and (1.3) are, modulo constant phase shifts, symplectically equivalent. More precisely, we compute the canonical symplectic form on the tangent bundle $T\mathcal{P}(M)$ induced from the Levi–Civita connection of the Wasserstein metric on $\mathcal{P}(M)$ (Proposition 3.2) and show that the map $\Psi = |\Psi| e^{\frac{i}{\hbar}S} \mapsto -\operatorname{div}(|\Psi|^2 \nabla S)$, which we shall call Madelung transform, is a symplectic submersion of the standard Hamiltonian structure of the Schrödinger equation on the space of complex valued functions into the Hamiltonian structure associated with (1.1) on the tangent bundle $T\mathcal{P}(M)$ (Theorem 4.3).

Except for its curiosity in Wasserstein geometry this result seems to support the point of view of some authors that the familiar complex valued form (1.3) of the Schrödinger equation is the consequence of a smart choice of coordinates in which the intuitive, but unhandy, dynamical system (1.1), resp. (1.4), can be solved very efficiently.

Much of what is presented below is well known in the literature, in particular in Nelson's theory of stochastic mechanics [14] and its follow-ups, *e.g.,* most notably by

Lafferty [10]. However, the aim here is to demonstrate that the Riemannian formalism of optimal transport yields a simple and compelling picture of the Schrödinger equation as a lift of Hamiltonian mechanics from point to diffuse systems.

2 Schrödinger Equation and Newton's Third Law on $(\mathcal{P}(M), d_{\mathcal{W}})$

The computations below are conducted on the formal Riemannian manifold of fully supported smooth probability measures equipped with the Wasserstein metric tensor, as initiated in [15,16] and extended in [11], ignoring full mathematical generality or rigor. (The basic background material taken from [11, 15] can be found in the appendix; see also [17].) In the sequel we shall often identify $\mu \in \mathcal{P}^\infty(M)$ with its density $\mu \triangleq d\mu/dx$.

Theorem 2.1 *For $V \in C^\infty(M)$ let $F\colon \mathcal{P}^\infty(M) \to \mathbb{R}$ defined as in* (1.2). *Then any smooth local solution $t \to \mu(t) \in \mathcal{P}(M)$ of* (1.1) *yields a local solution $(\mu_t, \overline{S}_t)$ of the Madelung flow* (1.4)*, 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 $\int_M S\, d\mu = 0$ and $\dot{\mu}_t = -\operatorname{div}(\nabla S_t \mu)$. Conversely, let (μ_t, S_t) be a smooth local solution of* (1.4). *Then $t \to \mu_t \in \mathcal{P}(M)$ solves* (1.1).

Proof Let μ solve (1.1) where $\nabla^{\mathcal{W}}$ is the Wasserstein gradient and $\nabla^{\mathcal{W}}_{\dot{\mu}}\dot{\mu}$ is the covariant derivative associated with the Levi–Civita connection on $T\mathcal{P}(M)$. Let $(x,t) \to S(x,t)$ denote the velocity potential of $\dot{\mu}$ (see §5); then according to [11, Lemmas 3 and 4] the left-hand side of (1.1) is computed as

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

where the right-hand side of (1.1) equals (see §A)

$$\operatorname{div}\Big(\mu\nabla\Big(V + \frac{\hbar^2}{8}\Big(|\nabla \ln \mu|^2 - \frac{2}{\mu}\Delta\mu\Big)\Big)\Big).$$

Since μ_t is fully supported on M, this implies

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

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 $\bar{S}(x,t) = S(x,t) + \int_0^t L_F(S_\sigma, \mu_\sigma) d\sigma$ solves (1.4). The converse statement is now also obvious. ∎

Corollary 2.2 *For $V \in C^\infty(M)$ let $F\colon \mathcal{P}^\infty(M) \to \mathbb{R}$ defined as in* (1.2). *Then any smooth local solution $t \to \mu(t) \in \mathcal{P}(M)$ of $\nabla^{\mathcal{W}}_{\mu}\dot{\mu} = -\nabla^{\mathcal{W}} F(\mu)$ yields a local solution of the Schrödinger equation* (1.3) *via*

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

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 $\int_M S d\mu = 0$ and $\dot{\mu}_t = -\operatorname{div}(\nabla S_t \mu)$.*

Remark 2.3 The passage from S to $\overline{S} = S + \text{const}$ does not bear any physical relevance, since two wave functions $\Psi, \tilde{\Psi}$ with $\tilde{\Psi} = e^{i\kappa}\Psi$ for some $\kappa \in \mathbb{R}$ parameterize the same physical system.

Remark 2.4 The $d_{\mathcal{W}}$-gradient flow on $\mathcal{P}(M)$ for F as in (1.2) corresponding to the overdamped limit of (1.1) gives a nonlinear fourth-order equation which is sometimes called the Derrida–Lebowitz–Speer–Spohn or quantum-drift-diffusion equation. A rigorous treatment of it can be found in [8].

The usual argument for the derivation of Euler–Lagrange equations yields the following statement.

Corollary 2.5 *For $V \in C^\infty(M)$ let $F\colon \mathcal{P}^\infty(M) \to \mathbb{R}$ defined as in* (1.2)*. Then any smooth local Lagrangian flow $[0,\epsilon] \ni t \to \dot{\mu}_t \in T\mathcal{P}^\infty(M)$ associated with L_F yields a local solution of the Schrödinger equation $i\hbar\partial_t\Psi = -\hbar^2/2\Delta\Psi + \Psi V$ via*

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

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 $\int_M S d\mu = 0$ and $\dot{\mu}_t = -\operatorname{div}(\nabla S_t \mu)$.*

Remark 2.6 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 $t \geq 0$

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

3 Hamiltonian Structure of the Madelung Flow on $T\mathcal{P}(M)$

In this section we show that the Madelung flow (1.4) has a Hamiltonian structure with respect to the canonical symplectic form induced from the Wasserstein metric tensor on the tangent bundle $T\mathcal{P}(M)$. To this aim we use the representation

$$T\mathcal{P}(M) = \{-\operatorname{div}(\nabla f \mu) \mid f \in C^\infty(M), \mu \in \mathcal{P}(M)\}.$$

Definition 3.1 (Standard Vector Fields on $T\mathcal{P}(M)$) Each pair $(\psi, \phi) \in C^\infty(M) \times C^\infty(M)$ induces a vector field $V_{\phi,\psi}$ on $T\mathcal{P}(M)$ via

$$V_{\psi,\phi}(-\operatorname{div}(\nabla f\mu)) = \dot{\gamma}$$

where $t \to \gamma^{\psi,\phi}(t) = \gamma(t) \in T\mathcal{P}(M)$ is the curve satisfying

$$\gamma(t) = -\operatorname{div}(\mu(t)\nabla(f + t\phi))$$
$$\mu_t = \exp(t\nabla\psi)_*\mu$$

Recall that the standard symplectic form on the tangent bundle of a Riemannian manifold is given by $\omega = d\Theta$, where the canonical 1-form Θ is defined as

$$\Theta(X) = \langle \xi, \pi_*(X)\rangle_{T_{\pi\xi}}, \quad X \in T_\xi(TM),$$

and where π denotes the projection map $\pi\colon TM \to M$.

Proposition 3.2 *Let $\omega_{\mathcal{W}} \in \Lambda^2(T\mathcal{P}(M))$ be the standard symplectic form associated with the Wasserstein Riemannian structure on $\mathcal{P}(M)$. Then*

$$\omega_{\mathcal{W}}(V_{\psi,\phi}, V_{\tilde{\psi},\tilde{\phi}})(-\operatorname{div}(\nabla f\mu)) = \langle \nabla\psi, \nabla\tilde{\phi}\rangle_\mu - \langle \nabla\tilde{\psi}, \nabla\phi\rangle_\mu. \tag{3.1}$$

Proof We use the formula

$$\omega_{\mathcal{W}}(V_{\psi,\phi}, V_{\tilde{\psi},\tilde{\phi}}) = V_{\psi,\phi}\Theta(V_{\tilde{\psi},\tilde{\phi}}) - V_{\tilde{\psi},\tilde{\phi}}\Theta(V_{\psi,\phi}) - \Theta([V_{\psi,\phi}, V_{\tilde{\psi},\tilde{\phi}}]), \tag{3.2}$$

where $[V_{\psi,\phi}, V_{\tilde{\psi},\tilde{\phi}}]$ denotes the Lie-bracket of the vector fields $V_{\psi,\phi}$ and $V_{\tilde{\psi},\tilde{\phi}}$. From the definition of Θ we obtain $\Theta(V_{\tilde{\psi},\tilde{\phi}})(-\operatorname{div}(\nabla f\mu)) = \langle \nabla f, \nabla\tilde{\psi}\rangle_\mu$. Hence

$$\begin{aligned} V_{\psi,\phi}(\Theta(V_{\tilde{\psi},\tilde{\phi}})) &= \frac{d}{dt}_{|t=0}\Theta(V_{\tilde{\psi},\tilde{\phi}})(\gamma^{\psi,\phi}(t)) = \frac{d}{dt}_{|t=0}\langle \nabla(f + t\phi), \nabla\tilde{\psi}\rangle_{\mu(t)} \\ &= \langle \nabla\phi, \nabla\tilde{\psi}\rangle_\mu - \int_M \nabla f\cdot\nabla\tilde{\psi}(-\operatorname{div}\nabla\psi\mu)\,dx \\ &= \langle \nabla\phi, \nabla\tilde{\psi}\rangle_\mu + \int_M \nabla(\nabla f\cdot\nabla\tilde{\psi})\nabla\psi\,d\mu. \end{aligned} \tag{3.3}$$

Next, since Θ measures tangential variations only, one gets that

$$\Theta([V_{\psi,\phi}, V_{\tilde{\psi},\tilde{\phi}}])(-\operatorname{div}(\nabla f\mu)) = \langle \nabla f, [\nabla\psi, \nabla\tilde{\psi}]\rangle_\mu. \tag{3.4}$$

Finally, it is easy to check that

$$\int_M \nabla(\nabla f\cdot\nabla\tilde{\psi})\nabla\psi\,d\mu - \int_M \nabla(\nabla f\cdot\nabla\psi)\nabla\tilde{\psi}\,d\mu - \langle \nabla f, [\nabla\psi, \nabla\tilde{\psi}]\rangle_\mu = 0,$$

which together with (3.2), (3.3), and (3.4) establishes the claim. ■

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Remark 3.3 Proposition 3.2 should be compared to [11, §6], where the lift of the Poisson bracket from a closed symplectic manifold M to $\mathcal{P}(M)$ is studied.

Using the the Riemannian inner product in each fiber of $T\mathcal{P}(M)$, the Hamiltonian associated with L_F is

$$H_F\colon T\mathcal{P}(M)\to\mathbb{R};\quad H_F(-\operatorname{div}(\nabla f\mu))=\frac{1}{2}\int_M|\nabla f|^2\,d\mu+F(\mu).$$

Proposition 3.4 *Let X_F denote the Hamiltonian vector field X_F induced on $T\mathcal{P}(M)$ from H_F and $\omega_{\mathcal{W}}$. Then*

$$X_F(-\operatorname{div}(\nabla f\mu))=V_{f,-(\frac{1}{2}|\nabla f|^2+V+\frac{\hbar^2}{8}(|\nabla\ln\mu|^2-2\frac{\Delta\mu}{\mu}))}(-\operatorname{div}(\nabla f\mu)).$$

Proof Fix $\psi,\phi\in C^\infty(M)$ and let $V_{\psi,\phi}(.)$ denote the corresponding standard vector field. Let $t\to\gamma(t)=-\operatorname{div}((\nabla f+t\phi)\mu_t)$, where $\mu_t=\exp(t\nabla\psi)_*\mu$, denote the corresponding curve on $T\mathcal{P}(M)$. Then

$$\begin{aligned}V_{\psi,\phi}(H_F)(-\operatorname{div}(\nabla f\mu))&=\partial_{t|t=0}H_F(\gamma(t))\\&=\partial_{t|t=0}\Big(\frac{1}{2}\int_M|\nabla(f+t\phi)|^2d\mu_t+\langle V,\mu_t\rangle+\frac{\hbar^2}{8}I(\mu_t)\Big)\\&=\mathrm{I}+\mathrm{II}+\mathrm{III},\end{aligned}$$

where

$$\begin{aligned}\mathrm{I}&=\int_M\nabla f\nabla\phi d\mu+\frac{1}{2}\int_M|\nabla f|^2(-\operatorname{div}(\nabla\psi\mu))\\&=\langle\nabla f,\nabla\phi\rangle_\mu+\Big\langle\nabla\psi,\nabla\Big(\frac{1}{2}|\nabla f|^2\Big)\Big\rangle,\\\mathrm{II}&=\int_M V(-\operatorname{div}(\nabla\psi\mu))=\langle\nabla V,\nabla\psi\rangle_\mu,\\\mathrm{III}&=\frac{\hbar^2}{8}\int_M 2\nabla\ln\mu_t\nabla\Big(\frac{-\operatorname{div}(\nabla\psi\mu)}{\mu}\Big)\,d\mu+\frac{\hbar^2}{8}\int_M|\nabla\ln\mu|^2(-\operatorname{div}(\nabla\psi\mu))\\&=\frac{\hbar^2}{8}\Big(\Big\langle\nabla\psi,\nabla\Big(-\frac{2\Delta\mu}{\mu}\Big)\Big\rangle_\mu+\langle\nabla\psi,\nabla|\nabla\ln\mu|^2\rangle_\mu\Big).\end{aligned}$$

Hence, collecting terms,

$$\begin{aligned}V_{\psi,\phi}(H_F)(-\operatorname{div}(\nabla f\mu))&=\langle\nabla f,\nabla\phi\rangle_\mu\\&\quad-\Big\langle\nabla\Big(-\Big(\frac{1}{2}|\nabla f|^2+V+\frac{\hbar^2}{8}\Big(|\nabla\ln\mu|^2-2\frac{\Delta\mu}{\mu}\Big)\Big)\Big),\nabla\psi\Big\rangle_\mu.\end{aligned}$$

From this and formula (3.1) the claim follows. ■

Corollary 3.5 *The pair $t\to(S_t,\mu_t)\in C^\infty(M)\times\mathcal{P}(M)$ solves the Madelung flow equation* (1.4) *if and only if $t\to-\operatorname{div}(\nabla S_t\mu_t)\in T\mathcal{P}(M)$ is an integral curve for X_F.*

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4 The Madelung Transform as a Symplectic Submersion

In this section we prove that the two equations, (1.1) and (1.3), are related via a symplectic submersion.

Definition 4.1 A smooth map $s\colon (M,\omega) \to (N,\eta)$ between two symplectic manifolds is called a *symplectic submersion* if its differential $s_*\colon TM \to TN$ is surjective and satisfies $\eta(s_*X, s_*Y) = \omega(X,Y)$ for all $X, Y \in TM$.

Note that this definition implies in particular that the map s itself is surjective. The following proposition is easily verified. Its meaning is that in order to solve a Hamiltonian system on N we may look for solutions for the lifted Hamiltonian $g \circ s$ on the larger state space M and project them via s back again to N.

Proposition 4.2 *Let $s\colon (M,\omega) \to (N,\eta)$ be a symplectic submersion and let $f \in C^\infty(M)$ and $g \in C^\infty(N)$ with $g \circ s = f$. Then s maps Hamiltonian flows associated with f on (M,ω) to Hamiltonian flows associated with g on (N,η).*

Now let $\mathcal{C}(M) = C^\infty(M;\mathbb{C})$ denote the linear space of smooth complex valued functions on M. Identifying as usual the tangent space over an element $\Psi \in \mathcal{C}$ with $\mathcal{C}$, $T\mathcal{C}$ is naturally equipped with the symplectic form

$$\omega_{\mathcal{C}}(F,G) = -2\int_M \operatorname{Im}(F \cdot \overline{G})(x)\,dx.$$

It is a well-known fact that the Schrödinger equation (1.3) is the Hamiltonian flow induced from the symplectic form $\hbar \cdot \omega_C$ and the Hamiltonian function on $\mathcal{C}$

$$H_S(\Psi) = \frac{\hbar^2}{2}\int_M |\nabla\Psi|^2\,dx + \int_M |\Psi(x)|^2 V(x)\,dx.$$

Let $\mathcal{C}_*(M)$ denote the subset of nowhere vanishing functions from $\mathcal{C}$ such that $\int_M |\Psi(x)|^2\,dx = 1$ and note that $\mathcal{C}_*(M)$ is invariant under the Schrödinger flow.

Assuming simple connectedness of M implies (via a standard lifting theorem of algebraic topology) that each function $\Psi \in \mathcal{C}_*$ admits a decomposition $\Psi = |\Psi|e^{\frac{i}{\hbar}S}$, where the smooth field $S\colon M \to \mathbb{R}$ is uniquely defined up to an additive constant $\hbar 2\pi k$, $k \in \mathbb{N}$. Hence we may define the *Madelung transform*

$$\sigma\colon \mathcal{C}_*(M) \to TP(M), \quad \sigma(\Psi) = -\operatorname{div}(|\Psi|^2\nabla S).$$

For the next theorem recall that in our definition of $T\mathcal{P}(M)$ we assume that the supporting measures are smooth and strictly positive on M.

Theorem 4.3 *Let M be simply connected. Then the Madelung transform*

$$\sigma\colon \mathcal{C}_*(M) \to T\mathcal{P}(M), \quad \sigma(|\Psi|e^{\frac{i}{\hbar}S}) = -\operatorname{div}(|\Psi|^2\nabla S)$$

defines a symplectic submersion from $(\mathcal{C}_*(M), \hbar\cdot\omega_{\mathcal{C}})$ to $(T\mathcal{P}(M), \omega_{\mathcal{W}})$ that preserves the Hamiltonian, i.e., $H_S = H_F \circ \sigma$.

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Remark 4.4 Together with Proposition 4.2 this result presents the Schrödinger equation (1.3) as a symplectic lifting of Newton's law on Wasserstein space (1.1) to the larger space $\mathcal{C}_*(M)$, and which can be solved much more easily because it is linear. Projecting the solution down to $T\mathcal{P}(M)$ via σ yields the desired solution to (1.1). Going in inverse direction from (1.1) to (1.3) requires a scalar correction term in the phase field (see Remark 2.3).

Proof of Theorem 4.3 Clearly, $\sigma(C_*(M)) = T\mathcal{P}(M)$. To see that $\sigma\colon C_*(M) \to T\mathcal{P}(M)$ is a submersion, fix a reference point $0 \in M$. Then for each $r \in [0, 2\pi\hbar[$ the map $\tau = \tau^{(r)}$

$$\tau\colon T\mathcal{P}(M) \to C_*(M), \quad -\operatorname{div}(\nabla S\mu) \to \sqrt{\mu}e^{\frac{i}{\hbar}(S-(S(0)-r))},$$

is a bijection from $T\mathcal{P}(M)$ to the subset $\{\Psi \in C_*, \frac{\Psi}{|\Psi|}(0) = e^{\frac{i}{\hbar}r}\}$ which satisfies $\sigma \circ \tau = \mathrm{Id}_{T\mathcal{P}(M)}$. This proves that the differential s_* of s is surjective.

To prove that σ is symplectic, let $\Psi = \sqrt{\mu}e^{\frac{i}{\hbar}f} \in \mathcal{C}_*$ with $f(0) = r \in [0, 2\pi\hbar[$ and let $\eta = -\operatorname{div}(\mu\nabla f) = \sigma(\Psi) \in T\mathcal{P}(M)$. Again due to the identity $\sigma \circ \tau = \mathrm{Id}_{T\mathcal{P}(M)}$, it suffices to prove that $\tau^*\omega_{\mathcal{C}} = 1/\hbar \cdot \omega_{\mathcal{W}}$ on $T_\eta(T\mathcal{P}(M))$. Since the set $\{V_{\psi,\phi}(-\operatorname{div}(\mu\nabla f)) \mid \psi, \phi \in C^\infty(M)\}$ spans the full tangent space $T_\eta(T\mathcal{P}(M))$, it remains to verify $\mu_t := \exp(t\nabla\psi)_*(\mu)$ and $c(t) := f(0) + t\phi(0) - r$

$$\omega_{\mathcal{C}}(\tau_* V_{\psi,\phi}, \tau_* V_{\tilde\psi,\tilde\phi}) = \frac{1}{\hbar}\omega_{\mathcal{W}}(V_{\psi,\phi}, V_{\psi,\phi})$$

for all $\psi, \phi, \tilde\psi, \tilde\phi \in C^\infty(M)$. By definition of $V_{\psi,\phi}$ and $\tau = \tau^{(r)}$, setting $\mu_t := \exp(t\nabla\psi)_*(\mu)$ and $c(t) := f(0) + t\phi(0) - r$,

$$\tau_* V_{\psi,\phi} = \partial_{t|t=0}\sqrt{\mu_t}e^{\frac{i}{\hbar}(f+t\phi-c(t))} = e^{\frac{i}{\hbar}f}\Big(\frac{1}{2\sqrt{\mu}}(-\operatorname{div}(\nabla\psi\mu)) + \sqrt{\mu}\frac{i}{\hbar}(\phi - \dot c)\Big).$$

Hence,

$$\begin{aligned}
\omega_{\mathcal{C}}(\tau_* V_{\psi,\phi}, \tau_* V_{\tilde\psi,\tilde\phi}) = -2\int_M \Big(&\frac{1}{2\sqrt{\mu}}(-\operatorname{div}(\nabla\psi\mu)) \cdot \Big(-\sqrt{\mu}\frac{1}{\hbar}(\tilde\phi + \dot{\tilde c})\Big) \\
&+ \sqrt{\mu}\frac{1}{\hbar}(\phi + \dot c) \cdot \frac{1}{2\sqrt{\mu}}(-\operatorname{div}(\nabla\tilde\psi\mu))\Big)\,dx \\
= \frac{1}{\hbar}\big(\langle\nabla\psi, \nabla\tilde\phi\rangle_\mu &- \langle\nabla\phi, \nabla\tilde\psi_\mu\rangle\big) = \frac{1}{\hbar}\omega_{\mathcal{W}}(V_{\psi,\phi}, V_{\tilde\psi,\tilde\phi}).
\end{aligned}$$

Finally, for $\Psi = \tau(-(\operatorname{div}\nabla f\mu))$, $\nabla\Psi = \sqrt{\mu}e^{\frac{i}{\hbar}f}(\frac{1}{2}\nabla\ln\mu + \frac{i}{\hbar}\nabla f)$ such that

$$\frac{\hbar^2}{2}\int_M |\nabla\Psi|^2 = \frac{1}{2}\int_M |\nabla f|^2 d\mu + \frac{\hbar^2}{8}I(\mu)$$

and $\int |\Psi(x)|^2 V(x)\,dx = \langle V, \mu\rangle$ which establishes the third claim $H_S = H_F \circ \sigma$ of the theorem. ■

A 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 $d_{\mathcal{W}}$-dense subset of smooth fully supported probabilities $\mathcal{P}^\infty(M) \subset \mathcal{P}_2(M)$ that shall often be identified with their corresponding density $\mu \stackrel{\triangle}{=} d\mu/dx$.

A.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 diffeormorphisms on M induced from the vector field $\nabla\phi \in \Gamma(M)$ starting from $\Phi_0 = \mathrm{Id_M}$. 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 $F\colon \mathcal{P}(M) \to \mathbb{R}$ 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 $\Delta^\mu\colon \phi \to -\operatorname{div}(\mu\nabla\phi)$ on

$$L_0^2(M, dx) = L_0^2(M, dx) \cap \{\langle f, dx\rangle = 0\}.$$

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

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

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

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A.2 Riemannian Gradient on $\mathcal{P}(M)$.

The Riemannian gradient of a smooth functional $F\colon \operatorname{Dom}(F) \subset \mathcal{P}(M) \to \mathbb{R}$ is computed to be $\nabla^{\mathcal{W}} F|_\mu = -\Delta^\mu (DF|_\mu)$, 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.

$$\begin{aligned}
F(\mu) &= \int_M \phi(x)\mu(dx), &\quad \nabla^{\mathcal{W}} F|_\mu &= V_\phi(\mu) = -\operatorname{div}(\nabla\phi\mu)\\
F(\mu) &= \int_M \mu \log\mu dx, &\quad \nabla^{\mathcal{W}} F|_\mu &= -\operatorname{div}(\mu\nabla\log\mu) = -\Delta\mu\\
F(\mu) &= \int_M |\nabla \ln\mu|^2 d\mu, &\quad \nabla^{\mathcal{W}} F|_\mu &= -\operatorname{div}\Big(\mu\nabla\Big(|\nabla\ln\mu|^2 - \frac{2}{\mu}\Delta\mu\Big)\Big).
\end{aligned}$$

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.*,

$$\big\|\nabla^{\mathcal{W}}\operatorname{Ent}|_\mu\big\|^2_{T_\mu\mathcal{P}} = \|-\operatorname{div}(\mu\nabla\log\mu)\|^2_{T_\mu\mathcal{P}} = \int_M |\nabla\log\mu|^2\,d\mu = I(\mu).$$

A.3 Covariant Derivative.

The Koszul identity for the Levi–Civita connection and a straightforward computation of commutators show ([11]) for the covariant derivative $\nabla^{\mathcal{W}}$ associated with $d_{\mathcal{W}}$ that

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

For a smooth curve $t \to \mu(t)$ with $\dot\mu_t = V_{\phi_t}$, this yields $\nabla^{\mathcal{W}}_{\dot\mu}\dot\mu = V_{\partial_t\phi + \frac{1}{2}|\nabla\phi|^2}$.

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