An optimal Transport Perspective on the Schrödinger Equation

Max von Renesse

Technische Universität Berlin

August 11 2009
Univ. Toronto

Agenda

- 1^{st}-order Calculus on the Wasserstein Space and Gradient Flows
- Geometric Application: Generalized Ricci Curvature Bounds
- 2^{nd}-order Calulus on Wasserstein Space and Lagrangian Flows
- Example: The Madelung Flow and the Schrödinger equation
- The symplectic structure on $T\mathcal{P}(M)$.
- The Madelung transform as a symplectic submersion
- Concluding Remarks

The Wasserstein (metric) space

Setup

Base space M: $\mathbb{R}^d$ or Riemannian manifold
$\mathcal{P}(M)$ Space of probability measures (with $\int_M d^2(o,x)\mu(dx) < \infty$)

The Wasserstein (metric) space

Setup

Base space M: $\mathbb{R}^d$ or Riemannian manifold
$\mathcal{P}(M)$ Space of probability measures (with $\int_M d^2(o,x)\mu(dx) < \infty$)

The Wasserstein metric on $\mathcal{P}(M)$

$d_{\mathcal{W}} : \mathcal{P}(M) \times \mathcal{P}(M) \to \mathbb{R}$

$$d^2_{\mathcal{W}}(\mu,\nu) = \inf_{\substack{\Pi \in \mathcal{P}(M\times M) \\ \Pi^1_* = \mu; \Pi^2_* = \nu}} \iint_{M\times M} d^2(x,y)\Pi(dx,dy)$$

The Wasserstein (metric) space

Setup

Base space M: $\mathbb{R}^d$ or Riemannian manifold
$\mathcal{P}(M)$ Space of probability measures (with $\int_M d^2(o,x)\mu(dx) < \infty$)

The Wasserstein metric on $\mathcal{P}(M)$

$d_{\mathcal{W}} : \mathcal{P}(M) \times \mathcal{P}(M) \to \mathbb{R}$

$$d^2_{\mathcal{W}}(\mu,\nu) = \inf_{\substack{\Pi \in \mathcal{P}(M\times M)\\ \Pi^1_* = \mu; \Pi^2_* = \nu}} \iint_{M\times M} d^2(x,y)\Pi(dx,dy)$$

Properties

d_W metrizes weak topology
$(P(M), d_{\mathcal{W}})$ is a complete geodesic metric space
(M,d) is embedded via $M \ni x \to \delta_x \in \mathcal{P}(M)$

The continuity equation

- Let $X \in \Gamma(M)$ vector field inducing flow $(x,t) \to \Phi(x,t) \in M$
- Acts on $\mu \in \mathcal{P}(M)$ via push forward $\mu_t = (\Phi_t)_*(\mu)$
- Infinitesimal variation

$$\dot{\mu} = \partial_{|t=0}\mu_t = -\operatorname{div}(X \cdot \mu)$$

1^{st}-order Riem. Calculus on $P(M)$ (F. Otto, *Comm. PDE* '01)

The continuity equation

- Let $X \in \Gamma(M)$ vector field inducing flow $(x,t) \to \Phi(x,t) \in M$
- Acts on $\mu \in \mathcal{P}(M)$ via push forward $\mu_t = (\Phi_t)_*(\mu)$
- Infinitesimal variation

$$\dot{\mu} = \partial_{|t=0}\mu_t = -\operatorname{div}(X \cdot \mu)$$

Riemannian Structure of $(\mathcal{P}(M), d_W)$

Riemannian tensor (g_{ij})

$$T_\mu\mathcal{P}(M) = \{\eta = -\operatorname{div}(\mu\nabla\psi)\,|\,\psi \in C^\infty(M)\}$$
$$\|\eta\|^2_{T_\mu} = \int_M |\nabla\psi|^2 d\mu$$

1^{st}-order Riem. Calculus on $P(M)$ (F. Otto, *Comm. PDE* '01)

The continuity equation

- Let $X \in \Gamma(M)$ vector field inducing flow $(x,t) \to \Phi(x,t) \in M$
- Acts on $\mu \in \mathcal{P}(M)$ via push forward $\mu_t = (\Phi_t)_*(\mu)$
- Infinitesimal variation

$$\dot{\mu} = \partial_{|t=0}\mu_t = -\operatorname{div}(X \cdot \mu)$$

Riemannian Structure of $(\mathcal{P}(M), d_W)$

Riemannian tensor (g_{ij})

$$T_\mu \mathcal{P}(M) = \{\eta = -\operatorname{div}(\mu \nabla \psi) \,|\, \psi \in C^\infty(M)\}$$
$$\|\eta\|^2_{T_\mu} = \int_M |\nabla \psi|^2 d\mu$$

Intrinsic metric (J. Benamou & Y. Brenier, *Numer. Math* '00)

$$d_{(g_{ij})}(\mu,\nu) = d_W(\mu,\nu)$$

The continuity equation

- Let $X \in \Gamma(M)$ vector field inducing flow $(x,t) \to \Phi(x,t) \in M$
- Acts on $\mu \in \mathcal{P}(M)$ via push forward $\mu_t = (\Phi_t)_*(\mu)$
- Infinitesimal variation

$$\dot{\mu} = \partial_{|t=0}\mu_t = -\operatorname{div}(X \cdot \mu)$$

Riemannian Structure of $(\mathcal{P}(M), d_W)$

Riemannian tensor (g_{ij})

$$T_\mu \mathcal{P}(M) = \{\eta = -\operatorname{div}(\mu \nabla \psi) \,|\, \psi \in C^\infty(M)\}$$
$$\|\eta\|^2_{T_\mu} = \int_M |\nabla \psi|^2 d\mu$$

Intrinsic metric (J. Benamou & Y. Brenier, *Numer. Math* '00)

$$d_{(g_{ij})}(\mu,\nu) = d_W(\mu,\nu)$$

Gradient flows

Gradient flows

The L^2-Parametrization/'Chart'

- Curves: $u \in L^2; \int_M u dx = 0$

$$\gamma_u(t) = \mu + t\, u$$

Gradient flows

The L^2-Parametrization/'Chart'

- Curves: $u \in L^2; \int_M u dx = 0$

$$\gamma_u(t) = \mu + t\, u$$

- Inner product

$$\langle \dot\gamma_u, \dot\gamma_v \rangle_{T_\mu \mathcal{P}} = \langle u, (-\Delta^\mu)^{-1} v \rangle_{L^2(M)}$$
$$\Delta^\mu(f) = \mathrm{div}(\mu \nabla f)$$

The L^2-Parametrization/'Chart'

- Curves: $u \in L^2$; $\int_M u dx = 0$

$$\gamma_u(t) = \mu + t\, u$$

- Inner product

$$\langle \dot\gamma_u, \dot\gamma_v \rangle_{T_\mu \mathcal{P}} = \langle u, (-\Delta^\mu)^{-1} v \rangle_{L^2(M)}$$
$$\Delta^\mu(f) = \mathrm{div}(\mu \nabla f)$$

- Riemannian metric matrix/operator

$$g_{ij}(\mu) : L^2 \to L^2; \qquad g_{ij}(\mu) = (-\Delta^\mu)^{-1}$$

Gradient flows

The L^2-Parametrization/'Chart'

- Curves: $u \in L^2; \int_M u dx = 0$
$$\gamma_u(t) = \mu + t\, u$$
- Inner product
$$\langle \dot\gamma_u, \dot\gamma_v \rangle_{T_\mu \mathcal{P}} = \langle u, (-\Delta^\mu)^{-1} v \rangle_{L^2(M)}$$
$$\Delta^\mu(f) = \mathrm{div}(\mu \nabla f)$$
- Riemannian metric matrix/operator
$$g_{ij}(\mu) : L^2 \to L^2; \qquad g_{ij}(\mu) = (-\Delta^\mu)^{-1}$$

Riemannian gradient

For $F : \mathcal{P}(M) \to \mathbb{R}$
$$\nabla^{\mathcal{W}} F(\mu) = -\Delta^\mu (DF)_{|\mu}(.)) = -\,\mathrm{div}(\mu \nabla^M (DF)_{|\mu}(.))$$

(Negative) Gradient flows - Example

Boltzmann Entropy

$$F(\mu) = \begin{cases} \int_M \log\left(\frac{d\mu}{dx}\right) d\mu & \text{if } \mu \ll dx \\ \infty & \text{else} \end{cases}$$

(Negative) Gradient flows - Example

Boltzmann Entropy

$$F(\mu) = \begin{cases} \int_M \log\left(\frac{d\mu}{dx}\right) d\mu & \text{if } \mu \ll dx \\ \infty & \text{else} \end{cases}$$

Computation of Gradient field

$$DF_{|\mu} = \log'(\mu) \cdot \mu + \log(\mu) \cdot 1 = 1 + \log(\mu) \in L^2(M)$$

(Negative) Gradient flows - Example

Boltzmann Entropy

$$F(\mu) = \begin{cases} \int_M \log\left(\frac{d\mu}{dx}\right) d\mu & \text{if } \mu \ll dx \\ \infty & \text{else} \end{cases}$$

Computation of Gradient field

$$DF_{|\mu} = \log'(\mu) \cdot \mu + \log(\mu) \cdot 1 = 1 + \log(\mu) \in L^2(M)$$

$$\begin{aligned} -\nabla^{\mathcal{W}} F(\mu) &= \Delta^{\mu} DF_{|\mu} = \operatorname{div}(\mu \nabla (1 + \log(\mu))) \\ &= \operatorname{div}(\mu(0 + \frac{\nabla \mu}{\mu}) = \Delta \mu \end{aligned}$$

(Negative) Gradient flows - Example

Boltzmann Entropy

$$F(\mu) = \begin{cases} \int_M \log\left(\frac{d\mu}{dx}\right) d\mu & \text{if } \mu \ll dx \\ \infty & \text{else} \end{cases}$$

Computation of Gradient field

$$DF_{|\mu} = \log'(\mu) \cdot \mu + \log(\mu) \cdot 1 = 1 + \log(\mu) \in L^2(M)$$

$$\begin{aligned} -\nabla^{\mathcal{W}} F(\mu) &= \Delta^{\mu} DF_{|\mu} = \mathrm{div}(\mu \nabla(1 + \log(\mu))) \\ &= \mathrm{div}(\mu(0 + \frac{\nabla \mu}{\mu}) = \Delta \mu \end{aligned}$$

Gradient Flow = Heat Equation

$$\dot{\mu} = -\nabla^{\mathcal{W}} F(\mu) \Leftrightarrow \partial_t \mu = \Delta \mu$$

Application: Ricci Curvature for Metric Measure Spaces

Application: Ricci Curvature for Metric Measure Spaces

Theorem (v. R./Sturm, *Comm. Pure Appl. Math.* '05)

Let (M, g) be smooth Riem. Mf. then

$$Ricc \geq \kappa \in \mathbb{R}$$

$$\Leftrightarrow \quad d_{\mathcal{W}}(p_t\mu, p_t\nu) \leq e^{-\kappa t} d_W(\mu, \nu)$$

$$\Leftrightarrow \quad Ent(\gamma_s) \leq sEnt(\gamma_1) + (1-s)Ent(\gamma_0) - \frac{\kappa}{2} s(1-s) d_{\mathcal{W}}(\gamma_0, \gamma_1)$$

for all Wasserstein geodesics $\gamma : [0,1] \to (\mathcal{P}(M), d_{\mathcal{W}})$

Application: Ricci Curvature for Metric Measure Spaces

Theorem (v. R./Sturm, *Comm. Pure Appl. Math.* '05)

Let (M, g) be smooth Riem. Mf. then

$$Ricc \geq \kappa \in \mathbb{R}$$

$$\Leftrightarrow \quad d_{\mathcal{W}}(p_t\mu, p_t\nu) \leq e^{-\kappa t} d_W(\mu, \nu)$$

$$\Leftrightarrow \quad Ent(\gamma_s) \leq sEnt(\gamma_1) + (1-s)Ent(\gamma_0) - \frac{\kappa}{2} s(1-s) d_{\mathcal{W}}(\gamma_0, \gamma_1)$$

for all Wasserstein geodesics $\gamma : [0, 1] \to (\mathcal{P}(M), d_{\mathcal{W}})$

Definition

Let (X, d, m) be a geodesic metric measure space. Then

$$Ricc(X, d, m) \geq \kappa :\Longleftrightarrow Ent(\cdot|m) \text{ is } \kappa\text{-konvex in } \mathcal{P}(M, d_{\mathcal{W}}).$$

Application: Ricci Curvature for Metric Measure Spaces

Theorem (v. R./Sturm, *Comm. Pure Appl. Math.* '05)

Let (M, g) be smooth Riem. Mf. then

$$Ricc \geq \kappa \in \mathbb{R}$$

$$\Leftrightarrow \; d_{\mathcal{W}}(p_t\mu, p_t\nu) \leq e^{-\kappa t} d_W(\mu, \nu)$$

$$\Leftrightarrow \; Ent(\gamma_s) \leq sEnt(\gamma_1) + (1-s)Ent(\gamma_0) - \frac{\kappa}{2}s(1-s)d_{\mathcal{W}}(\gamma_0, \gamma_1)$$

for all Wasserstein geodesics $\gamma : [0,1] \to (\mathcal{P}(M), d_{\mathcal{W}})$

Definition

Let (X, d, m) be a geodesic metric measure space. Then

$$Ricc(X, d, m) \geq \kappa :\Longleftrightarrow Ent(\cdot|m) \text{ is } \kappa\text{-konvex in } \mathcal{P}(M, d_{\mathcal{W}}).$$

Remark

Ricci-Analogue of Cartan-Toponogov-Alexandrov curvature bound for CAT(κ) spaces.

(Generalized) Ricci Curvature and Optimal Transport

(Generalized) Ricci Curvature and Optimal Transport

Ricci Curvature for Metric Measure Spaces

- K.-T. Sturm, 'On the geometry of metric measure spaces', *Acta Math.* '06
- C. Villani & J. Lott, 'Ricci curvature for metric-measure spaces via optimal transport', *Ann. of Math.* '09
- Y. Ollivier 'Ricci curvature of Markov chains on metric spaces', *J. Funct. Anal.* '09

(Generalized) Ricci Curvature and Optimal Transport

Ricci Curvature for Metric Measure Spaces

- K.-T. Sturm, 'On the geometry of metric measure spaces', *Acta Math.* '06
- C. Villani & J. Lott, 'Ricci curvature for metric-measure spaces via optimal transport', *Ann. of Math.* '09
- Y. Ollivier 'Ricci curvature of Markov chains on metric spaces', *J. Funct. Anal.* '09

Ricci Flow and Optimal Transport (R. McCann & P. Topping, *Amer. J. Math.*, to appear)

Theorem *The $t \to g_t$ is a supersolution to the backward Ricci flow iff for all $\mu_t^{(1)}, \mu_t^{(2)}$ with $\partial_t \mu_t^{(i)} = \Delta_{g_t} \mu^{(i)}$, $i \in \{1, 2\}$*

$$s \to d_{\mathcal{W}_{g_s}}(\mu_s^{(1)}, \mu_s^{(2)}) \text{ is non-increasing.}$$

2^{nd}-order Riem. Calculus on $\mathcal{P}(M)$ (J. Lott, *CMP* '07)

2^{nd}-order Riem. Calculus on $\mathcal{P}(M)$ (J. Lott, *CMP* '07)

Standard Vector fields on $\mathcal{P}(M)$

$$\mu \to V_\phi(\mu) = -\operatorname{div}(\mu \nabla \phi)$$
$$[V_{\phi_1}, V_{\phi_2}](\mu) = -\operatorname{div}(\mu(\nabla^2\phi_2 \cdot \nabla\phi_1 - \nabla^2\phi_1 \cdot \nabla\phi_2))$$
$$V_{\phi_1}\langle V_{\phi_2}, V_{\phi_3}\rangle = \int_M \langle \nabla\phi_1, \nabla^2\phi_2 \cdot \nabla\phi_3 + \nabla^2\phi_3 \cdot \nabla\phi_2 \rangle d\mu$$

2^{nd}-order Riem. Calculus on $\mathcal{P}(M)$ (J. Lott, *CMP* '07)

Standard Vector fields on $\mathcal{P}(M)$

$$\mu \to V_\phi(\mu) = -\operatorname{div}(\mu \nabla \phi)$$
$$[V_{\phi_1}, V_{\phi_2}](\mu) = -\operatorname{div}(\mu(\nabla^2 \phi_2 \cdot \nabla \phi_1 - \nabla^2 \phi_1 \cdot \nabla \phi_2))$$
$$V_{\phi_1} \langle V_{\phi_2}, V_{\phi_3} \rangle = \int_M \langle \nabla \phi_1, \nabla^2 \phi_2 \cdot \nabla \phi_3 + \nabla^2 \phi_3 \cdot \nabla \phi_2 \rangle d\mu$$

Levi-Civita-Connection (Koszul Identity)

$$\langle \nabla_{V_1} V_2, V_3 \rangle = \frac{1}{2}(V_1 \langle V_2, V_3 \rangle + V_2 \langle V_3, V_1 \rangle - V_3 \langle V_1, V_2 \rangle + \langle V_3, [V_1, V_2] \rangle - \langle V_2, [V_1, V_3] \rangle - \langle V_1, [V_2, V_3] \rangle)$$

2^{nd}-order Riem. Calculus on $\mathcal{P}(M)$ (J. Lott, *CMP* '07)

Standard Vector fields on $\mathcal{P}(M)$

$$\mu \to V_\phi(\mu) = -\operatorname{div}(\mu \nabla \phi)$$
$$[V_{\phi_1}, V_{\phi_2}](\mu) = -\operatorname{div}(\mu(\nabla^2\phi_2 \cdot \nabla\phi_1 - \nabla^2\phi_1 \cdot \nabla\phi_2))$$
$$V_{\phi_1}\langle V_{\phi_2}, V_{\phi_3}\rangle = \int_M \langle \nabla\phi_1, \nabla^2\phi_2 \cdot \nabla\phi_3 + \nabla^2\phi_3 \cdot \nabla\phi_2\rangle d\mu$$

Levi-Civita-Connection (Koszul Identity)

$$\langle \nabla_{V_1} V_2, V_3\rangle = \frac{1}{2}(V_1\langle V_2, V_3\rangle + V_2\langle V_3, V_1\rangle - V_3\langle V_1, V_2\rangle + \langle V_3, [V_1, V_2]\rangle - \langle V_2, [V_1, V_3]\rangle - \langle V_1, [V_2, V_3]\rangle)$$

Lemma (Lott)

For $t \to \mu(t)$, $\dot\mu(t) = -\operatorname{div}(\mu(t)\nabla\psi(t))$ and $V(t) = V_{\eta(t)}$

$$\nabla_{\dot\mu} V_\eta = -\operatorname{div}(\mu(\nabla\dot\eta + \nabla^2\eta \cdot \nabla\psi))$$

Remark on the Geodesic Equation

Corollary

For $t \to \mu(t)$ with $\text{supp}(\mu) = M$ then

$$t \to \mu(t) \text{ geodesic } \Leftrightarrow \dot{\psi} + \frac{1}{2}|\nabla \psi|^2 = c = c(t).$$

Remark on the Geodesic Equation

Corollary

For $t \to \mu(t)$ with $\text{supp}(\mu) = M$ then

$$t \to \mu(t) \text{ geodesic } \Leftrightarrow \dot{\psi} + \frac{1}{2}|\nabla\psi|^2 = c = c(t).$$

Proof.

Geodesic equation $\nabla_{\dot{\mu}}\dot{\mu} = 0$. Using Lott's lemma with $\eta = \psi$

$$\begin{aligned} \nabla_{\dot{\mu}}\dot{\mu} &= -\text{div}(\mu(\nabla\dot{\psi} + \nabla^2\psi \cdot \nabla\psi)) \\ &= -\text{div}(\mu\nabla(\dot{\psi} + \frac{1}{2}|\nabla\psi|^2)) = 0 \end{aligned}$$

Corollary

For $t \to \mu(t)$ with $\text{supp}(\mu) = M$ then

$$t \to \mu(t) \text{ geodesic } \Leftrightarrow \dot{\psi} + \frac{1}{2}|\nabla\psi|^2 = c = c(t).$$

Proof.

Geodesic equation $\nabla_{\dot{\mu}}\dot{\mu} = 0$. Using Lott's lemma with $\eta = \psi$

$$\begin{aligned}\nabla_{\dot{\mu}}\dot{\mu} &= -\,\text{div}(\mu(\nabla\dot{\psi} + \nabla^2\psi \cdot \nabla\psi)) \\ &= -\,\text{div}(\mu\nabla(\dot{\psi} + \frac{1}{2}|\nabla\psi|^2)) = 0\end{aligned}$$

Test with $(\dot{\psi} + \frac{1}{2}|\nabla\psi|^2)$ yields $\int_M |\nabla(\dot{\psi} + \frac{1}{2}|\nabla\psi|^2)|^2 d\mu = 0$. □

Lagrangian flows on $T\mathcal{P}(M)$

State space

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

Action Functional on curves $s \to \eta(s) = -\operatorname{div}(\mu_s \nabla f_s) \in T\mathcal{P}(M)$

$$A(\eta) = \int_0^T L_F(\eta(s))ds, \quad L_F((-\operatorname{div}(\mu\nabla f)) = \int_M |\nabla f|^2 d\mu - F(\mu)$$

Lagrangian flows on $T\mathcal{P}(M)$

State space

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

Action Functional on curves $s \to \eta(s) = -\operatorname{div}(\mu_s \nabla f_s) \in T\mathcal{P}(M)$

$$A(\eta) = \int_0^T L_F(\eta(s))ds, \quad L_F((-\operatorname{div}(\mu\nabla f)) = \int_M |\nabla f|^2 d\mu - F(\mu)$$

'Theorem'

The flow $\eta : s \to -\operatorname{div}(\mu_s \nabla f_s) \in T\mathcal{P}(M)$ is critical for A

$$\Leftrightarrow \nabla^W_{\dot\mu} \dot\mu = -\nabla^{\mathcal{W}} F(\mu)$$

$$\Leftrightarrow \begin{cases} \partial_t f + \frac{1}{2}|\nabla f|^2 - DF(\mu) = c(t) \\ \partial_t \mu = -\operatorname{div}(\mu\nabla f) \end{cases}$$

Example - The Madelung flow

Augmented Mechanical Potential

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

where $V \in C^\infty(M)$, $I(\mu) = \int_M |\nabla \ln \mu|^2 d\mu$ (Fisher information).

Example - The Madelung flow

Augmented Mechanical Potential

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

where $V \in C^\infty(M)$, $I(\mu) = \int_M |\nabla \ln \mu|^2 d\mu$ (Fisher information).

Corollary

Let $s \to \mu_s \in \mathcal{P}(M)$ solve $\nabla^{\mathcal{W}}_{\dot\mu} \dot\mu = -\nabla^{\mathcal{W}} F(\mu)$, then

$$\partial_t \overline{S} + \frac{1}{2}|\nabla \overline{S}|^2 + V + \frac{\hbar^2}{8}\left(|\nabla \ln \mu|^2 - \frac{2}{\mu}\Delta\mu\right) = 0$$
$$\partial_t \mu + \operatorname{div}(\mu \nabla \overline{S}) = 0.$$

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, i.e. $\int_M S d\mu = 0$ and $\dot\mu_t = -\operatorname{div}(\nabla S_t \mu)$.

Mapping to the Schrödinger equation

Lemma (Madelung '27)

Let $t \to (\mu_t, S_t)$ satisfy

$$\partial_t S + \frac{1}{2}|\nabla S|^2 + V + \frac{\hbar^2}{8}\left(|\nabla \ln \mu|^2 - \frac{2}{\mu}\Delta\mu\right) = 0$$
$$\partial_t \mu + \operatorname{div}(\mu \nabla S) = 0.$$

then $t \to \sqrt{\mu_t} e^{\frac{i}{\hbar} S_t} =: \Psi_t$ solves the Schrödinger equation

$$i\hbar\partial_t \Psi = -\hbar^2/2\Delta\Psi + \Psi V.$$

Mapping to the Schrödinger equation

Lemma (Madelung '27)

Let $t \to (\mu_t, S_t)$ satisfy

$$\partial_t S + \frac{1}{2}|\nabla S|^2 + V + \frac{\hbar^2}{8}\big(|\nabla \ln \mu|^2 - \frac{2}{\mu}\Delta\mu\big) = 0$$

$$\partial_t \mu + \operatorname{div}(\mu \nabla S) = 0.$$

then $t \to \sqrt{\mu_t} e^{\frac{i}{\hbar} S_t} =: \Psi_t$ solves the Schrödinger equation

$$i\hbar\partial_t \Psi = -\hbar^2/2\Delta\Psi + \Psi V.$$

Corollary

Any flow $t \to \mu_t \in \mathcal{P}(M)$ with $\nabla^{\mathcal{W}}_{\dot\mu} \dot\mu = -\nabla^{\mathcal{W}} F(\mu)$ solves the Schrödinger equation via $\Psi = \sqrt{\mu} e^{\frac{i}{\hbar}\overline{S}}$.

Comparison of Hamiltonian Structures

Aim

Identify/compute the symplectic structure on $T\mathcal{P}(M)$ and relate the Hamiltonian structure of $\nabla^{\mathcal{W}}_{\dot{\mu}}\dot{\mu} = -\nabla^{\mathcal{W}} F(\mu)$ to that of the Schrödinger equation.

Comparison of Hamiltonian Structures

Aim

Identify/compute the symplectic structure on $T\mathcal{P}(M)$ and relate the Hamiltonian structure of $\nabla^{\mathcal{W}}_{\dot\mu}\dot\mu = -\nabla^{\mathcal{W}}F(\mu)$ to that of the Schrödinger equation.

Reminder: Symplectic form associated to Riem. metric

Standard symplectic form on the tangent bundle of a Riemannian manifold:

$$\omega = d\Theta,$$

with canonical 1-form Θ

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

and where $\pi : TM \to M$ projection map.

The Symplectic Form on $T\mathcal{P}(M)$

Definition (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

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

The Symplectic Form on $T\mathcal{P}(M)$

Definition (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

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

Lemma

Let $\omega_{\mathcal{W}} \in \Lambda^2(T\mathcal{P}(M))$ be the standard symplectic form associated to the Wasserstein Riemannian structure on $\mathcal{P}(M)$, then

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

Proof

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

Proof

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

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

Proof

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

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

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

Proof

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

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

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

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

Proof

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

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

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

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

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

Proof

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

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

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

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

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

Putting formulas together yields the claim.

Hamiltonian Structure for Newton's Law on $\mathcal{P}(M), d_{\mathcal{W}})$

Corollary

The curve $t \to \mu_t \in \mathcal{P}(M)$ solves the equation $\nabla^{\mathcal{W}}_{\dot\mu}\dot\mu = -\nabla^{\mathcal{W}} F$ iff if it is an integral curve for the Hamiltonian vector field on X_F induced from $\omega_{\mathcal{W}}$ and the energy function $H_F : T\mathcal{P}(M) \to \mathbb{R}$,

$$H_F((-\operatorname{div}(\mu\nabla f)) = \frac{1}{2}\int_M |\nabla f|^2 d\mu + F(\mu).$$

Definition of 'Madelung Transform'

Definition

$$\mathcal{C}_*(M) = \{\Psi \in C^\infty(M;\mathbb{C}) \,\big|\, |\Psi(.)| > 0\}$$

M simply connected $\Rightarrow \Psi = |\Psi| e^{\frac{i}{\hbar}S}$ with S unique up to a constant.

Define **Madelung transform** by

$$\sigma : C_*(M) \to T\mathcal{P}(M); \qquad \sigma(\Psi) = -\operatorname{div}(|\Psi|^2 \nabla S)$$

Definition of 'Madelung Transform'

Definition

$$\mathcal{C}_*(M) = \{\Psi \in C^\infty(M;\mathbb{C}) \,\big|\, |\Psi(.)| > 0\}$$

M simply connected $\Rightarrow \Psi = |\Psi| e^{\frac{i}{\hbar}S}$ with S unique up to a constant.

Define **Madelung transform** by

$$\sigma : C_*(M) \to T\mathcal{P}(M); \qquad \sigma(\Psi) = -\operatorname{div}(|\Psi|^2 \nabla S)$$

Reminder: Hamiltonian Structure of Schrödinger equation

Schrödinger = flow on $\mathcal{C}_*$ induced from $\hbar \cdot \omega_{\mathcal{C}}$

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

and Hamiltonian function

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

Symplectic Submersion

Definition

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

Symplectic Submersion

Definition

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

Proposition

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

Symplectic Submersion

Definition

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

Proposition

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

Practical Purpose

If the system looks bad on N, solve it on a bigger space and then project back to N.

Precise Hamiltonian Relation

Theorem

Let M be simply connected. Then the Madelung transform

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

defines symplectic submersion from $(\mathcal{C}_*(M), \hbar \cdot \omega_{\mathcal{C}})$ to $(T\mathcal{P}(M), \omega_{\mathcal{W}})$ which preserves the Hamiltonian, i.e.

$$H_S = H_F \circ \sigma.$$

Concluding Remarks

- The last theorem represents the Schrödinger equation as a 'symplectic lift' of Newton's law on the Wasserstein space. (Indeed, the the wave function has a free unphysical parameter, the constant phase shift).

Concluding Remarks

- The last theorem represents the Schrödinger equation as a 'symplectic lift' of Newton's law on the Wasserstein space. (Indeed, the the wave function has a free unphysical parameter, the constant phase shift).
- None of the computations above are proved yet rigorously.

Concluding Remarks

- The last theorem represents the Schrödinger equation as a 'symplectic lift' of Newton's law on the Wasserstein space. (Indeed, the the wave function has a free unphysical parameter, the constant phase shift).
- None of the computations above are proved yet rigorously.
- Some names (not complete) for the first part of the talk: Ambrosio, Brenier, Cordero-Erausquin, Gigli, McCann, Otto, Savare, Sturm, Villani

Concluding Remarks

- The last theorem represents the Schrödinger equation as a 'symplectic lift' of Newton's law on the Wasserstein space. (Indeed, the the wave function has a free unphysical parameter, the constant phase shift).
- None of the computations above are proved yet rigorously.
- Some names (not complete) for the first part of the talk: Ambrosio, Brenier, Cordero-Erausquin, Gigli, McCann, Otto, Savare, Sturm, Villani
- For the second part of the talk compare also theory of 'Stochastic Mechanics' by Nelson

Concluding Remarks

- The last theorem represents the Schrödinger equation as a 'symplectic lift' of Newton's law on the Wasserstein space. (Indeed, the the wave function has a free unphysical parameter, the constant phase shift).
- None of the computations above are proved yet rigorously.
- Some names (not complete) for the first part of the talk: Ambrosio, Brenier, Cordero-Erausquin, Gigli, McCann, Otto, Savare, Sturm, Villani
- For the second part of the talk compare also theory of 'Stochastic Mechanics' by Nelson and to the old controversy about de Broglie-Bohm ('pilot wave') theory: