Optimal transport with Coulomb cost: theory and applications to electronic structure of atoms & molecules (lecture 1)

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(Young European Probabilists)

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$$\min_{\gamma \in \mathcal{P}_{sym}(\mathbb{R}^{3N})} \underbrace{\int_{\mathbb{R}^{3N}} \sum_{1 \le i < j \le N} |x_i - x_j|^{-1} \, d\gamma(x_1, \ldots, x_N)}_{C[\gamma]}$$

s/to $\mathbb{R}^3$-marg. ρ, ie $\gamma(\mathbb{R}^{3(i-1)} \times A_i \times \mathbb{R}^{3(N-i-1)}) = \int_{A_i} \rho$
$\forall i$, $\forall$ Borel $A_i \subseteq \mathbb{R}^3$.

symmetric ; $\gamma(A_1 \times \ldots \times A_N) = \gamma(A_{\sigma(1)} \times \ldots \times A_{\sigma(N)})$ $\forall$ perm.

$\rho \in \mathcal{P}(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$

- all marg's equal (since γ symm.)
- cost decreases w/ dist. ; multi-marginal

$N=2$: $\min \int |x-y|^{-1} d\gamma(x,y)$ $\quad \gamma(A \times \mathbb{R}^3) = \gamma(\mathbb{R}^3 \times A) = \int_A \rho$

Plan

1. Motivation
2. Qualitative theory — L1
3. Exactly integrable ex's
4. Precise connection QM → OT — L2
5. Large N — L3

References (downloadable from http://www-m7.ma.tum.de)

C. Cotar, G.F., C. Klüppelberg, CPAM 2013 (arXiv 2011)

G.F., Ch. Mendl, B. Pass, C. Cotar, C. Klüppelberg, J. Chem. Phys. 139, 16409, 2013

C. Cotar, G.F., B. Pass, arXiv: 1307.6540, 2013

1. Motivation

QM for N electrons ($\rightsquigarrow$ energy levels, mol. geometries, ...)

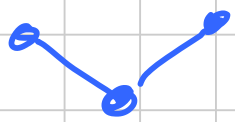
$\psi(x_1, \dots, x_N)$ $\qquad \psi : \mathbb{R}^{3N} \to \mathbb{C}$

Linear PDE for ψ (electronic Schrödinger equation)

$\mathbb{R} \rightsquigarrow 10$ gridpts

$\mathbb{R}^{3N} \rightsquigarrow 10^{3N}$ –"–

H_2O $\quad N = 10 \rightsquigarrow 10^{30}$



$\rightsquigarrow$ approximate

Density functional theory (DFT) Nobel Prize W. Kohn

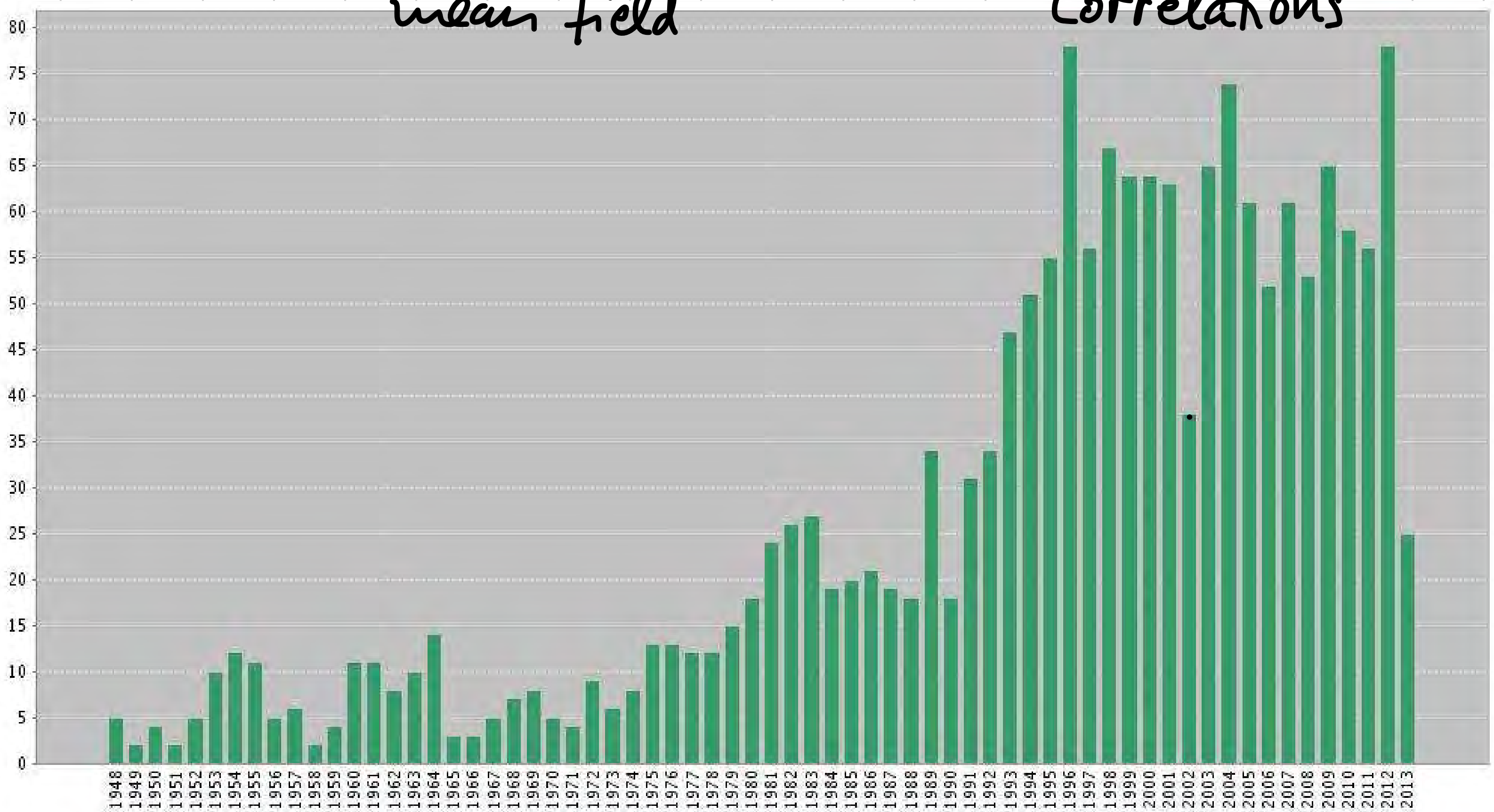
$\rho(x_1) = \int_{\mathbb{R}^{3N-3}} |\psi(x_1, \dots, x_N)|^2 \, dx_2 \dots dx_N$ one-body density

nonl. eq./var. principle for ρ ("DFT model")

Key challenge good functional $V[\rho]$ for interaction en. of el's as fctnal of marginal ρ

Historical ex. (Dirac 1930)

$$V = \underbrace{\frac{1}{2}\int\int \frac{\rho(x)\,\rho(y)}{|x-y|}\,dx\,dy}_{\text{mean field}} - \frac{4}{3}\underbrace{\left(\frac{3}{\pi}\right)^{1/3}\int \rho(x)^{4/3}}_{\text{correlations}}\,dx$$



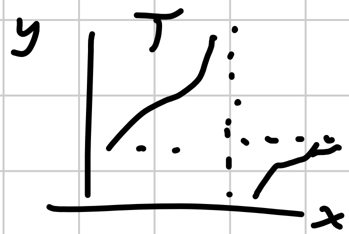
OT with Coulomb cost $\rightsquigarrow$ alternative $V[\rho]$

(incorporates correlations • non-perturbatively
• non-additively)

$$V[\rho] := \min_{\gamma \to \rho} C[\gamma]$$

3. Qualitative theory

<u>Thm</u> (N=2, Cotar/GF/Klüppelberg, arXiv 2011, CPAM 2013)



For $\rho \in \mathcal{P}(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$

- unique minimizer γ
- γ of Monge form $\gamma = (I,T)_\# \rho$ $\quad \gamma(x,y) = \rho(x)\,\delta_{T(x)}(y)$
- $T(x) = x + \dfrac{\nabla\psi(x)}{|\nabla\psi(x)|^{3/2}}$ $(x\notin M)$, ψ Kantorovich pot.

Similar statements on physical grounds: Seidl '99, Seidl, Gori-Giorgi, Savin '07
Similar rigorous results: Buttazzo, Gori-Giorgi, De Pascale, Phys. Rev. A, '12

Why (**)?

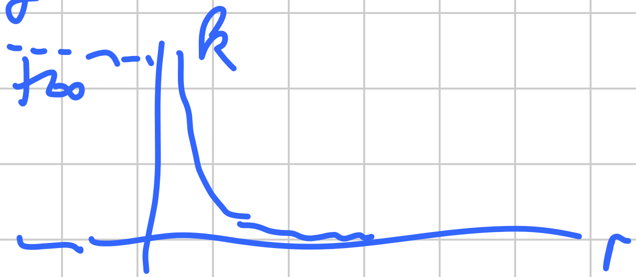
OT: $|x-y|^{-1} \rightsquigarrow c(x,y) = \ell(x-y) = k(|x-y|)$

ℓ^* generalized Legendre trf

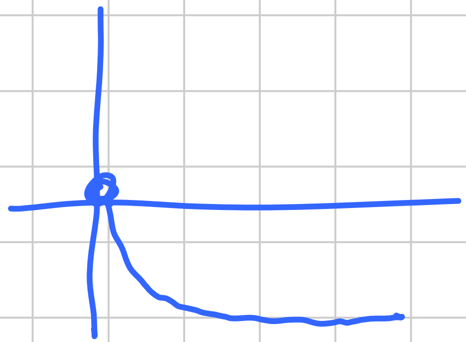
$\Big[$ extend $k(r) = +\infty \ (r<0)$

$k^*(p) := \sup_r \big(p\cdot r - k(r)\big)$

$\ell^*(z) = k^*(-|z|)$ $\Big]$



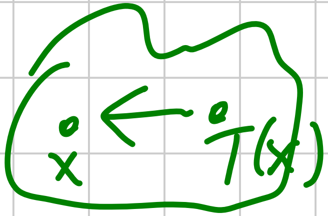
$$\ell(z) = \frac{1}{|z|} \rightsquigarrow \ell^*(z) = -2\sqrt{|z|}$$



Gangbo-McCann formula:

$$T(x) = x - \nabla \ell^*(\nabla\psi(x))$$

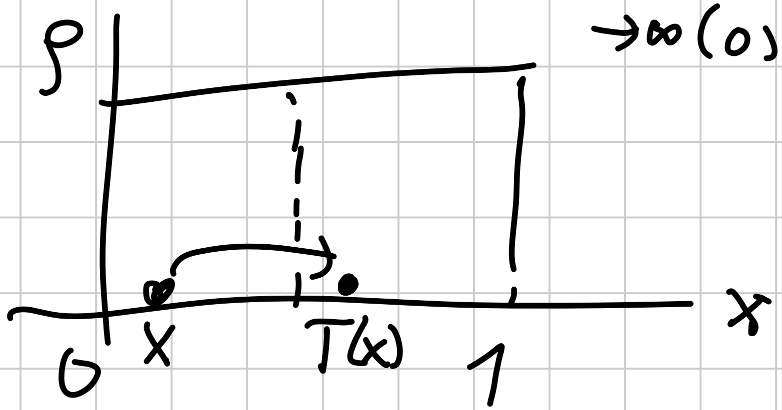
Physics (Seidl '1999)



$$-\nabla\psi(x) = \text{force} = \frac{x - T(x)}{|x-T(x)|^3}$$

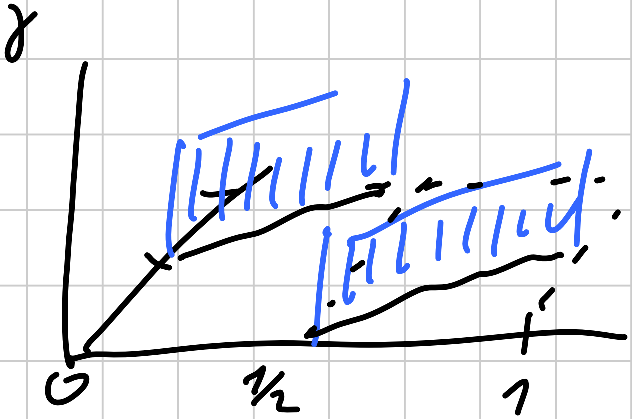
3. Exactly soluble ex's

$c(|x-y|)$ decr., cvx, $\to\infty\ (0)$

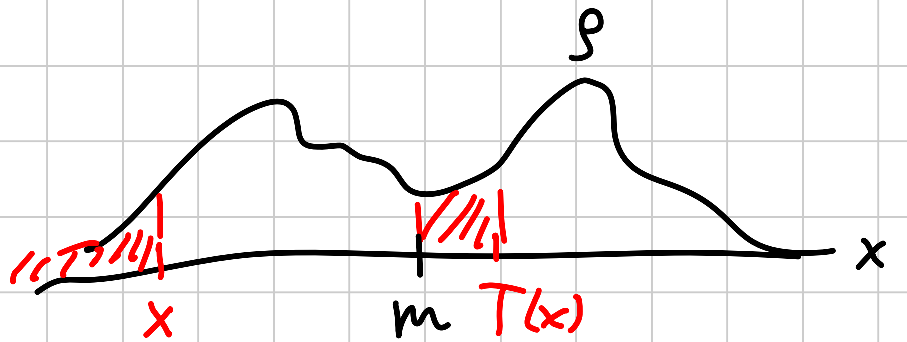


1) $N=2$, ρ = uniform on $[0,1]$

$$T(x) = \begin{cases} x + \frac{1}{2} & x < \frac{1}{2} \\ x - \frac{1}{2} & x > \frac{1}{2} \end{cases}$$



2) $N=2$, ρ non uniform on $\mathbb{R}$

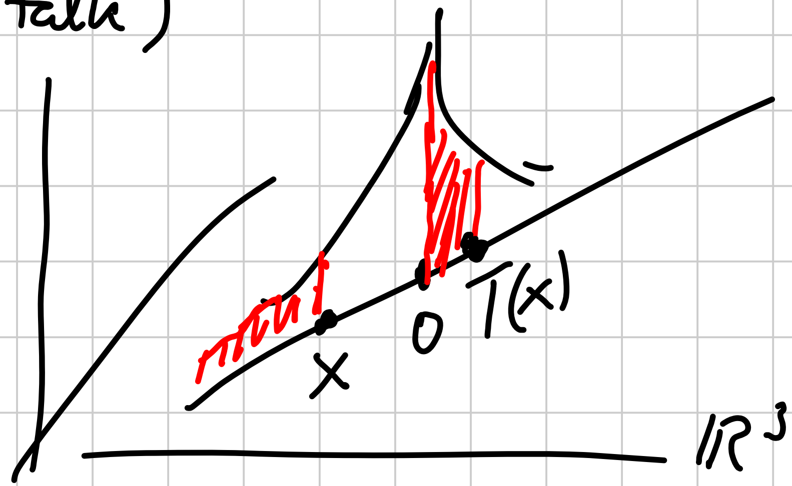


$\leadsto$ median

$x<m$: $\displaystyle\int_{-\infty}^{x}\rho \overset{!}{=} \int_{m}^{T(x)}\rho$ mass balancing

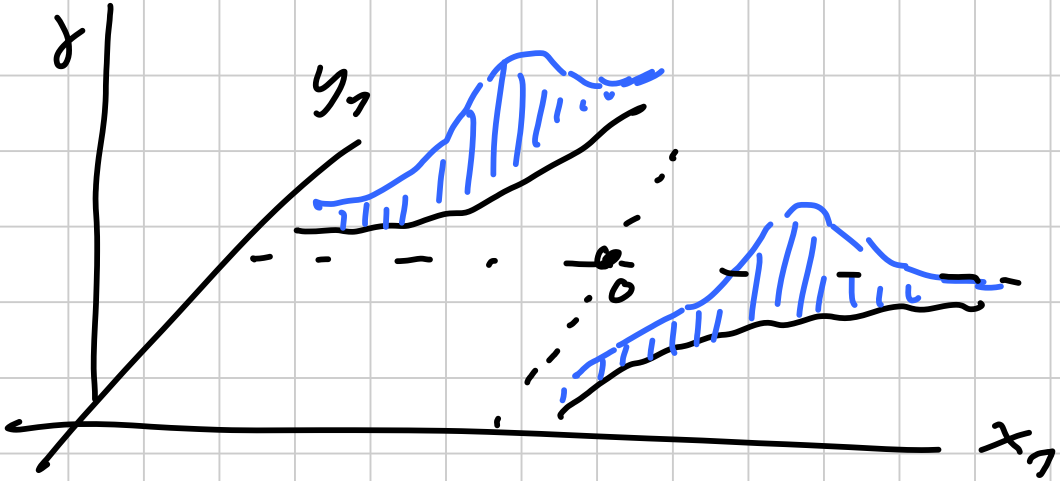
($N>2$; Simone Di Marino's talk)

3) 2 particles, ρ radial, $\mathbb{R}^3$



$\dfrac{T(x)}{|T(x)|} = -\dfrac{x}{|x|}$ (same line, opposite direction)

$4\pi\displaystyle\int_{|x|}^{\infty} r^2\rho(r)\,dr \overset{!}{=} 4\pi\int_0^{|T(x)|} r^2\rho(r)\,dr$



γ
y_1
x_1