Grand Canonical Optimal Transport

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joint work with S. Di Marino and M. Lewin

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(LMO) Université Paris-Saclay

Overview

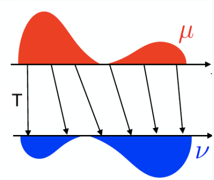
Classical Optimal Transport

Let $\mu, \nu \in \mathcal{P}(\Omega)$, $\Omega \subseteq \mathbb{R}^d$, and c a l.s.c. and bounded from below cost function, the Optimal Transport (OT) problem is defined as follows

$$\mathcal{E}(\mu, \nu) = \inf \left\{ \int_{\Omega^2} c(x, y) \mathrm{d}\mathbb{P}(x, y) \mid \mathbb{P} \in \Pi(\mu, \nu) \right\} \tag{1}$$

where $\Pi(\mu, \nu)$denotes the set of couplings $\mathbb{P}(x, y) \in \mathcal{P}(\Omega^2)$ having μ and ν as marginals.

- Solution à la Monge the transport plan $\mathbb{P}$ is deterministic (or à la Monge) if $\mathbb{P} = (\mathrm{Id}, S)_\sharp \mu$ where $S_\sharp \mu = \nu$.



Classical Optimal Transportation Theory

Let $\mu, \nu \in \mathcal{P}(\Omega)$, $\Omega \subseteq \mathbb{R}^d$, and c a l.s.c. and bounded from below cost function, the Optimal Transport (OT) problem is defined as follows

$$\mathcal{E}(\mu,\nu) = \inf\left\{\int_{\Omega^2} c(x,y)\mathrm{d}\mathbb{P}(x,y) \mid \mathbb{P} \in \Pi(\mu,\nu)\right\} \quad (1)$$

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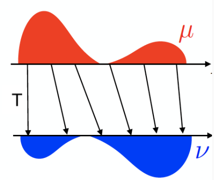

- Entropic OT (or Schrödinger) problem:

$$\inf_{\mathbb{P}\in\Pi(\mu,\nu)} \int_{\Omega^2} c(x,y)\mathrm{d}\mathbb{P}(x,y) + T\mathcal{H}(\mathbb{P},\mu\otimes\nu),$$

where $\mathcal{H}(\pi,\rho)$ between two probability measures π and ρ is defined as

$$\mathcal{H}(\rho,\pi) = \begin{cases} \int_{\Omega^2}\left(\log\left(\frac{\mathrm{d}\rho}{\mathrm{d}\pi}\right)-1\right)\mathrm{d}\rho, & \text{if } \rho \ll \pi \\ +\infty, & \text{otherwise.}\end{cases}$$

The Multi-Marginal Optimal Transportation

Take N probability measures $\mu_i \in \mathcal{P}(\Omega)$ and $c : \Omega^N \to [0, +\infty]$ a l.s.c. cost function. Then the multi-marginal OT problem reads as:

$$\mathcal{E}_c^N(\mu_1, \cdots, \mu_N) = \inf_{\mathbb{P} \in \Pi_N(\mu_1, \cdots, \mu_N)} \int_{\Omega^N} c(x_1, \cdots, x_N) \mathrm{d}\mathbb{P}(x_1, \cdots, x_N) \qquad (2)$$

where $\Pi_N(\mu_1, \cdots, \mu_N)$ denotes the set of couplings $\mathbb{P}(x_1, \cdots, x_N)$ having μ_i as marginals.

- Solution à la Monge: $\mathbb{P} = (\mathrm{Id}, S_2, \ldots, S_N)_\sharp \mu_1$ where $S_{i\sharp}\mu_1 = \mu_i$.
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- Entropic OT (or Schrödinger) problem: as in the two marginals case.
- Duality: Both 2 and N marginal OT problems admit a useful dual formulation

$$\sup \left\{ \mathcal{J}(\phi_1, \cdots, \phi_N) \mid (\phi_1, \cdots, \phi_N) \in \mathcal{K} \right\}. \quad (3)$$

where

$$\mathcal{J}(\phi_1, \cdots, \phi_N) := \sum_{i=1}^N \int_\Omega \phi_i \mathrm{d}\mu_i$$

and $\mathcal{K}$ is the set of bounded and continuous functions $(\phi_1, \cdots, \phi_N)$ such that $\sum_{i=1}^N \phi_i(x_i) \leq c(x_1, \cdots, x_N)$.

Some applications

- The Wasserstein barycenter problem can be rewritten as a MMOT problem (see **(Agueh and G. Carlier 2011)**): statistics, machine learning, image processing;
- Matching for teams problem (see **(Guillaume Carlier and Ekeland 2010)**): economics. The transport plan $\mathbb{P}$ matches individuals from each team μ_i minimizing a given cost;
- In Density Functional Theory: the electron-electron repulsion (see **(Buttazzo, De Pascale, and Gori-Giorgi 2012; Cotar, Friesecke, and Klüppelberg 2013)**). The plan $\mathbb{P}(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N)$ returns the probability of finding electrons at position $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N$;
- Incompressible Euler Equations **(Brenier 1989)** : $\mathbb{P}(\omega)$ gives "the mass of fluid" which follows a path ω.
- Mean Field Games **(Benamou, G. Carlier, S. Di Marino, and L. Nenna 2018)**;
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The electron-electron repulsion (and repulsive OT)

MMOT arises naturally in Density Functional Theory in order to study the electron-electron repulsion (ρ **represents now the electron density!**)

$$\inf \left\{ \int_{\mathbb{R}^{3N}} \sum_{i<j} \frac{1}{|x_i - x_j|} \mathrm{d}\mathbb{P}(x_1, \cdots, x_N) \mid \mathbb{P} \in \Pi_N(\rho) \right\}.$$

Some other example of repulsive costs :

- Coulomb cost;
- Repulsive harmonic $c(x_1, \cdots, x_N) = -\sum_{i<j} |x_i - x_j|^2$;
- The determinant cost $c(x_1, \cdots, x_N) = -\det(x_1, \cdots, x_N)$ with $x_i \in \mathbb{R}^N$;
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Why is it a difficult problem to treat?
Example: $N = 3$, $d = 1$, $\mu_i = \mathcal{L}_{[0,1]}$ $\forall i$ and $c(x_1, x_2, x_3) = |x_1 + x_2 + x_3|^2$.

- Uniqueness fails **(Simone Di Marino, Gerolin, and Luca Nenna 2017)**;
- $\exists$ S_i optimal, are not differentiable at any point and they are fractal maps **ibid., Thm 4.6**

Fractal solution for the repulsive harmonic cost

Assume that ρ has finite second moment, then $\forall \mathbb{P} \in \Pi_N(\rho)$

$$\mathbb{P}(c_{RH}) := \int -\sum_{i<j} |x_i - x_j|^2 \mathrm{d}\mathbb{P} = \int |\sum_i x_i|^2 \mathrm{d}\mathbb{P} - N \sum_i \int x_i^2 \mathrm{d}\mathbb{P}$$

$$= \mathbb{P}(h) - \underbrace{N^2 \int x^2 \mathrm{d}\rho}_{const.}.$$

Proposition: Take $c(x_1, \cdots, x_N) = h(\sum_{i=1}^N x_i)$ then $\mathbb{P} \in \Pi_N(\rho)$ is optimal $\Leftrightarrow$ $\mathrm{supp}(\mathbb{P}) \subset \{\sum x_i = k\}$ where $k = N \int x \mathrm{d}\rho$.

Consequences for the repulsive harmonic: Uniqueness may fail and fractal solutions exists.

Grand Canonical Optimal Transport

Subsystems are Grand Canonical

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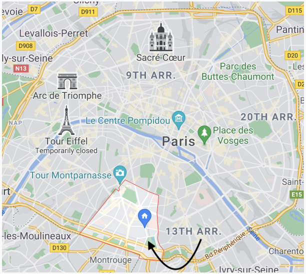

for any $B_n \subset A^n$ we have

$$\begin{cases} \mathbb{P}_0 = \mathcal{P}((\Omega \setminus A)^N) & n = 0, \\ \mathbb{P}_n(B_n) = \binom{N}{n} \mathcal{P}(B_n \times (\Omega \setminus A)^{N-n}) & 1 \leq n \leq N-1, \\ \mathbb{P}_N(B_N) = \mathcal{P}(B_N) & n = N, \\ 0 & n \geq N+1. \end{cases}$$

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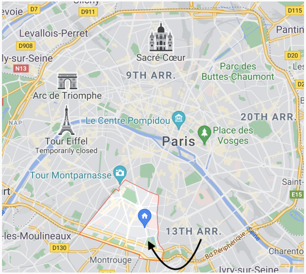

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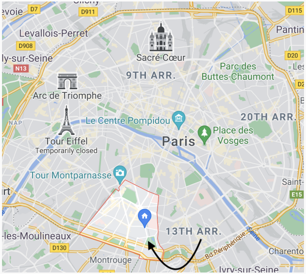

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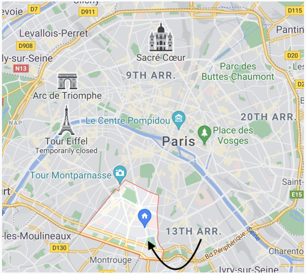

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- The average number of bicycles in A is $\sum_{n=1}^{N} n\mathbb{P}_n(A^n) \in [0, N]$.
- The density in A is $\rho_{\mathbb{P}}(B) = \mathbb{P}_1(B) + \sum_{n=2}^{N} \mathbb{P}_n(B \times A^{n-1})$.

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Definition (Grand canonical probability measure)

We say that $\mathbb{P} = (\mathbb{P}_n)_{n \geq 0}$ *is a Grand Canonical probability measure if* $\mathbb{P}_n \in \mathcal{M}_+^{sym}(\Omega^n)$ $\forall n \geq 1$, $\mathbb{P}_0 \in \mathbb{R}_+$ *and*

$$\sum_{n \geq 0} \mathbb{P}_n(\Omega^n) = 1.$$

Then, the marginal density is given by

$$\rho_{\mathbb{P}}(B) = \mathbb{P}_1(B) + \sum_{n>1} n \underbrace{\mathbb{P}_n(B \times \Omega^{n-1})}_{=\rho_{\mathbb{P}_n}}, \ \forall B \subset \Omega$$

Grand Canonical Optimal Transport

The (grand canonical) Optimal Transport problem now reads

$$\mathcal{E}_{GC}(\rho) = \inf \left\{ \sum_{n>1} \int_{\Omega^n} c_n(x_1, \cdots, x_n) \mathrm{d}\mathbb{P}_n \mid \mathbb{P} \in \Pi_{GC}(\rho) \right\}, \tag{4}$$

where $\Pi_{GC}(\rho)$ denotes the set of Grand Canonical probability measures having ρ as average marginal.

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Definition (Super-stability)

We say that the family of costs $(c_n)_{n\geq 0}$ is *super-stable* if $c_n \geq -A - Bn$ for some constants $A, B \geq 0$ and if for any compact set $K \subset \mathbb{R}^d$, there exists $\varepsilon_K > 0$ and $n_K \in \mathbb{N}$ such that

$$c_n(x_1, ..., x_n) \geq -\frac{n}{\varepsilon_K} + \varepsilon_K \left(\sum_{j=1}^{n} \mathbb{1}_{\Omega \cap K}(x_j) \right)^2 \quad \text{on } \Omega^n \text{ for all } n \geq n_K.$$

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Theorem (existence and l.s.c.)

Let $(c_n)_{n\geq 0}$ *a family of costs super stable and l.s.c then* (4) *admits a minimiser* $\mathbb{P}^\star$*. Moreover,* $\rho \mapsto \mathcal{E}_{GC}(\rho)$ *is l.s.c. for the tight convergence of measures.*

Some remarks

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$$c_0 = c_1 = 0, \ c_n = \sum_{i<j}^{n} w(x_i, x_j) \text{ for } n \geq 3.$$

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- A truncated version has been proposed by **(De Pascale, Bouchitté, Buttazzo, and Champion 2021)** : a maximum number of marginals $\mathcal{N}$ is fixed. Denote by $\mathcal{E}_{GC}^{\leqslant \mathcal{N}}$ the truncated G, then for a family of super-stable costs we have that $\mathcal{E}_{GC}^{\leqslant \mathcal{N}} \to \mathcal{E}_{GC}$ as $\mathcal{N} \to \infty$ (in the sense of $\Gamma-$convergence);

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- Given $\rho(\Omega) = n \in \mathbb{N}$, the n-marginal problem can be written in the form

$$\mathcal{E}^n(\rho) = \inf_{(0,\ldots,0,\mathbb{P}_n,0,\ldots)\in\Pi_{GC}(\rho)} \int_{\Omega^n} c_n \, \mathrm{d}\mathbb{P}_n$$

It follows from existence,

Corollary (Convex hull)

Let ρ be a positive measure with $\rho(\Omega) < \infty$ such that $\mathcal{E}_{GC}(\rho) < \infty$. Then, under the same assumptions as in the existence theorem we have

$$\mathcal{E}_{GC}(\rho) = \min_{\substack{\rho = \sum_{n\geq 1} \alpha_n \rho_n \\ \rho_n(\Omega) = n \\ \sum_{n\geq 0} \alpha_n = 1}} \sum_{n\geq 0} \alpha_n \, \mathcal{E}^n(\rho_n).$$

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Moreover, in the case of coulomb potential the following result holds

Theorem (Weak lower semi-continuous envelope)

Take $\Omega = \mathbb{R}^d$. Let ρ be any finite measure so that $\mathcal{E}_{GC}(\rho) < \infty$. Then there exists a sequence ρ^k such that $N_k := \rho^k(\mathbb{R}^d) \in \mathbb{N}$,

$$\rho^k \rightharpoonup \rho \quad \textit{locally and} \qquad \lim_{k\to\infty} \mathcal{E}^{N_k}(\rho^k) = \mathcal{E}_{GC}(\rho).$$

Compact support for Coulomb potentials

Compact support: We say that a Grand Canonical measure $\mathbb{P}$ has **compact support in** $[\![N_{min}, N_{max}]\!]$, with $N_{min} \leq \langle N \rangle \leq N_{max}$, that is

$$\mathbb{P}_n(\Omega^n) = 0 \quad \text{if } n \notin [\![N_{min}, N_{max}]\!]$$

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Theorem (Compact support for the Coulomb potential in $d = 1$)

Let $w(x_i, x_j) = \frac{1}{|x_i - x_j|}$ and $k < \bar{N} < k + 1$, with $k \in \mathbb{N}$, then the optimal solution $\mathbb{P}^\star$ has a compact support in $[\![k, k+1]\!]$.

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Theorem (Compact support for the Coulomb potential in $d \geq 2$)

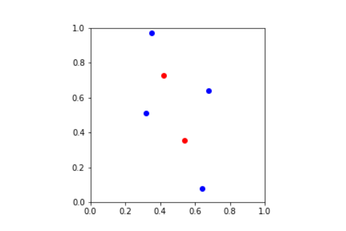
Let $w(x_i, x_j) = \frac{1}{|x_i - x_j|}$ then the optimal solution $\mathbb{P}^\star$ has a compact support in $[\![N_{min}, N_{max}]\!]$ where $N_{min} = \lfloor \bar{N} \rfloor + \frac{3}{2} - \frac{1}{2}\sqrt{9 + 8\lfloor \bar{N} \rfloor}$ and $N_{max} = \lceil \bar{N} \rceil + \frac{1}{2}\sqrt{8\lceil \bar{N} \rceil - 7} - \frac{1}{2}$

Remarks:

- The length of the support depends on $\langle N \rangle$!
- If $\bar{N} = 2$, then the Grand Canonical is always Canonical.

Gran canonical state with Coulomb in $d = 2$ and length of the support

Let $\Omega = [0,1]^2$ and the average marginal given by $\rho = \frac{1}{2} \sum_{i=1}^{6} \delta_{x_i}$.



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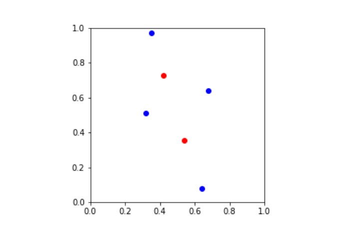

Length of the support: take $\Omega = \mathbb{R}^d$ and the point $x_1, \cdots, x_6$ front the left . Then we can inductively construct a sequence $(y_j^{(k)})_{j=1}^{6^k}$ such that

$$\rho^{(k)} = \frac{1}{2}\sum_{j=1}^{6^k}\delta_{y_j^{(k)}}, \quad \rho^{(k)}(\mathbb{R}^d) = \frac{6^k}{2},$$

the grand-canonical problem admits a unique minimiser $\mathbb{P}^{(k)}$ which satisfies

$$\mathrm{supp}(\mathbb{P}^{(k)}) = \left\{\frac{6^k - 2^k}{2}, \frac{6^k + 2^k}{2}\right\}.$$

The length of the support is of order $\rho(\mathbb{R}^d)^\alpha$ where $\alpha \sim 0.38$

Deriving the dual

Proceeding as usual we get the following dual problem

$$\sup \left\{ \int_{\Omega} \phi(x) d\rho(x) + \beta \mid (\phi, \beta) \in \mathcal{D} \right\}, \tag{5}$$

where

$$\mathcal{D} := \{\phi \in \mathcal{C}_b \mid \beta \leq c_0, \ \beta + \sum_{i=1}^{n} \phi(x_i) \leq c_n(x_1, \cdots, x_n), \ \forall n \geq 1\}.$$

Remark 1: β is the Lagrange multiplier associated to the constraint that the Grand Canonical $\mathbb{P}$ is a probability $\mathbb{P}_0 + \sum_{n\geq 1} \mathbb{P}_n(\Omega^n) = 1$;
Remark 2: Assuming that c_n is a family of super stable l.s.c. costs then strong duality holds;
Remark 3: Existence is delicate to treat: via a relaxed problem, namely $\phi \in L^{\infty}$.

Repulsive harmonic Grand Canonical

Let's compute the energy for $\mathbb{P} \in \Pi_{GC}(\rho)$

$$\mathbb{P}(c_{RH}) := \sum_{n>1} \int_{\Omega^n} -\sum_{i<j}^{n} |x_i - x_j|^2 \mathrm{d}\mathbb{P}_n = \sum_{n>1} \int_{\Omega^n} h(\sum_{i=1}^{n} x_i) \mathrm{d}\mathbb{P}_n - \sum_{n>1} n^2 \int_{\Omega} x^2 \mathrm{d}\rho_{\mathbb{P}_n}.$$

Moreover, the worst is coming...

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Proposition

Let $c_n(x_1, \cdots, x_n) = -\sum_{i<j} w(x_i, x_j)$ *such that* $\int_{\Omega^2} w(x,y) d\rho(x) d\rho(y) > 0$, *then*

$$\inf(GC) = -\infty.$$

Sketch of proof: Choose $\mathbb{P}$ s.t.

- $\mathbb{P}_K = Z_K \left(\frac{\rho^{\otimes^K}}{\bar{N}K} \right)$ with $Z_K = \frac{K! K^{K-1}}{\bar{N}^{K-1}}$;
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Then,

$$\mathbb{P}(c) = -\frac{K-1}{2\langle N \rangle} \underbrace{\int_{\Omega^2} w(x,y) d\rho(x) d\rho(y)}_{>0}$$

Remark: take $w(x,y) = |x-y|^2$!

The Entropic Grand Canonical OT

Let us consider the Poisson GC state $\mathbb{G}_\rho$ given by

$$\mathbb{G}_{\rho,0} = e^{-\rho(\Omega)},\ \mathbb{G}_{\rho,n} = e^{-\rho(\Omega)}\frac{\rho^{\otimes n}}{n!},$$

then the entropic Grand-Canonical problem at $T > 0$ reads

$$\mathcal{F}_T(\rho) := \inf_{\mathbb{P}\in\Pi_{GC}(\rho)}\{\mathbb{P}(c) + T\mathcal{H}(\mathbb{P},\mathbb{G}_\rho)\},$$

where $\mathbb{P}(c) := \sum_{n>1}\int_{\Omega^n} c_n(x_1,\cdots,x_n)\mathrm{d}\mathbb{P}_n$

Some results:

- $\mathcal{F}_T(\rho)$ admits a unique minimizer $\mathbb{P}^{(T)}$ for all $T > 0$.
- we have $\lim_{T\to 0^+}\mathcal{F}_T(\rho) = \inf_{\substack{\mathbb{P}\in\Pi_{GC}(\rho)\\ \mathcal{H}(\mathbb{P},\mathbb{G}_\rho)<\infty}} \mathbb{P}(c)$
- Assume that $\mathbb{G}_\rho(c) < \infty$ then $\lim_{T\to\infty}\mathcal{F}_T(\rho) = \mathbb{G}_\rho(c)$

Thank You!!

Given the partition function for a measurable potential ϕ

$$Z_{T,\rho}(\phi) := e^{-\frac{c_0}{T}-\rho(\Omega)} + \sum_{n\geq 1} \frac{e^{-\rho(\Omega)}}{n!} \int_{\Omega^n} \exp\left(\frac{-c_n + \sum_{j=1}^n \phi(x_j)}{T}\right) d\rho^{\otimes n}.$$

Then one can prove strong duality,

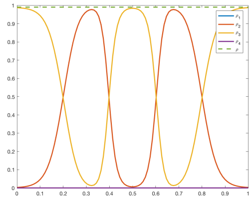
$$\mathcal{F}_T(\rho) = \sup_{\int e^{-\phi/T}<\infty} \left\{ \int \phi d\rho - T \log Z_T(\phi) \right\},$$

and existence of an optimal potential such that unique minimiser of $\mathcal{F}_T(\rho)$ is given by the Gibbs state $\mathbb{P}_\phi$

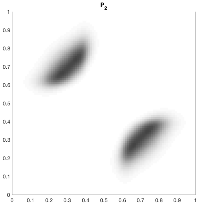
$$\mathbb{P}_{\phi,0} = \frac{e^{-\frac{c_0}{T}-\rho(\Omega)}}{Z_{T,\rho}(\phi)}, \qquad \mathbb{P}_{\phi,n} = \frac{e^{\frac{-c_n+\sum_{j=1}^n \phi(x_j)}{T}-\rho(\Omega)}\rho^{\otimes n}}{Z_{T,\rho}(\phi) n!}.$$

Numerical test, Coulomb $d = 1$ with entropic regularization

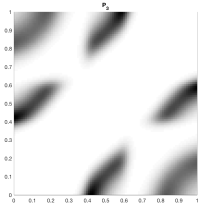
$d = 1$, $\langle N \rangle = 2.5$, $\rho(x) = \langle N \rangle \chi_{[0,1]}(x)$ and the Coulomb potential.



densities of $\mathbb{P}_n$



$\mathbb{P}_2$



$\mathbb{P}_3$