

# DFT meets OT

## Worksheet 1 (January 17, 2018)

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### Problem 1

Consider the antisymmetrized product wave function  $\Psi$  given in the lecture,

$$\Psi(\mathbf{x}_1, \dots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \sum_{\wp \in S_N} \text{sign}(\wp) \prod_{k=1}^N \psi_{\wp(k)}(\mathbf{x}_k) \quad \left( \mathbf{x}_k = (\mathbf{r}_k, \sigma_k) \right), \quad (1)$$

where  $\psi_1(\mathbf{x}) = \phi_1(\mathbf{r})\alpha(\sigma)$ ,  $\psi_2(\mathbf{x}) = \phi_1(\mathbf{r})\beta(\sigma)$ ,  $\psi_3(\mathbf{x}) = \phi_2(\mathbf{r})\alpha(\sigma)$ , etc.,

$$\alpha(\uparrow) = 1, \quad \alpha(\downarrow) = 0 \quad (\text{"spin up"}), \quad (2)$$

$$\beta(\uparrow) = 0, \quad \beta(\downarrow) = 1 \quad (\text{"spin down"}), \quad (3)$$

and the  $\phi_n(\mathbf{r})$  are the solutions of the **one-particle** Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + v(\mathbf{r}) \right\} \phi_n(\mathbf{r}) = \epsilon_n \phi_n(\mathbf{r}) \quad \left( \epsilon_1 \leq \epsilon_2 \leq \epsilon_3 \leq \dots \right). \quad (4)$$

(a) Show that  $\Psi$  is an eigenfunction of the non-interacting  $N$ -electron Hamiltonian

$$\hat{H}_N^{(0)}[v] = \sum_{i=1}^N \left\{ -\frac{\hbar^2}{2m} \nabla_i^2 + v(\mathbf{r}_i) \right\} \equiv \sum_{i=1}^N \hat{h}_i \quad (5)$$

to the eigenvalue  $E = 2 \sum_{n=1}^{N/2} \epsilon_n$ .

(b) Show that  $\Psi$  (for even  $N \in \{2, 4, 6, \dots\}$ ) has the electron density

$$\rho(\mathbf{r}) = 2 \sum_{n=1}^{N/2} |\phi_n(\mathbf{r})|^2. \quad (6)$$

Hint 1: For  $\mathbf{x} = (\mathbf{r}, \sigma)$ , use the notation  $\sum_{\sigma \in \{\uparrow, \downarrow\}} \int d^3r f(\mathbf{r}, \sigma) \equiv \int d^3x f(\mathbf{x})$ .

Hint 2: The single-particle wave functions  $\psi_k(\mathbf{x})$  are pairwise orthonormal,

$$\int d^3x \psi_k^*(\mathbf{x}) \psi_{k'}(\mathbf{x}) = \delta_{k,k'} \quad (k, k' \in \{1, \dots, N\}). \quad (7)$$

### Problem 2

Let  $\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$  be a (correctly antisymmetric) wave function for  $N = 2$  electrons.

(a) Which ones of the following terms can be evaluated without knowing  $\Psi$  explicitly?

$$|\Psi(\mathbf{r} \uparrow, \mathbf{r} \downarrow)|^2, \quad |\Psi(\mathbf{r} \uparrow, \mathbf{r} \uparrow)|^2, \quad \sum_{\sigma_1, \sigma_2} |\Psi(\mathbf{r}\sigma_1, \mathbf{r}\sigma_2)|^2. \quad (8)$$

As a region  $\Omega = \Omega_R(\mathbf{r}_0)$  in space, we consider a ball with radius  $R$  centered at  $\mathbf{r} = \mathbf{r}_0$ ,

$$\Omega_R(\mathbf{r}_0) = \left\{ \mathbf{r} \in \mathbb{R}^3 \mid |\mathbf{r} - \mathbf{r}_0| \leq R \right\}. \quad (9)$$

(b) Give a probability interpretation for the number

$$P_R(\mathbf{a}, \mathbf{b}; \sigma_1, \sigma_2) = \int_{\Omega_R(\mathbf{a})} d^3r_1 \int_{\Omega_R(\mathbf{b})} d^3r_2 |\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)|^2 \quad (10)$$

in the two cases (i)  $\Omega_R(\mathbf{a}) \cap \Omega_R(\mathbf{b}) = \emptyset$ , (ii)  $\mathbf{a} = \mathbf{b}$ .

(c) Provided that  $\Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2)$  is a continuous function of both  $\mathbf{r}_1 \in \mathbb{R}^3$  and  $\mathbf{r}_2 \in \mathbb{R}^3$ , determine the limit

$$p(\mathbf{a}, \mathbf{b}; \sigma_1, \sigma_2) = \lim_{R \rightarrow 0} \frac{P_R(\mathbf{a}, \mathbf{b}; \sigma_1, \sigma_2)}{\left(\frac{4\pi}{3}R^3\right)^2}. \quad (11)$$

(d) What can you tell about the quantities

$$p(\mathbf{a}, \mathbf{a}; \uparrow, \uparrow), \quad p(\mathbf{a}, \mathbf{a}; \uparrow, \downarrow). \quad (12)$$

What is the probability (density) for finding the two electrons on top of each other?

### Problem 3

The most general form of a wave function for  $N = 2$  electrons is

$$\begin{aligned} \Psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2) = & \psi_1(\mathbf{r}_1, \mathbf{r}_2)\alpha(\sigma_1)\alpha(\sigma_2) + \psi_2(\mathbf{r}_1, \mathbf{r}_2)\alpha(\sigma_1)\beta(\sigma_2) \\ & + \psi_3(\mathbf{r}_1, \mathbf{r}_2)\beta(\sigma_1)\alpha(\sigma_2) + \psi_4(\mathbf{r}_1, \mathbf{r}_2)\beta(\sigma_1)\beta(\sigma_2), \end{aligned}$$

with the spin functions  $\alpha(\sigma)$  and  $\beta(\sigma)$  from Eqs. (2) and (3).

(a) Using the short-hand notations  $\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(1, 2)$  and  $\chi(\sigma_1, \sigma_2) = \chi(1, 2)$ , find the conditions on the functions  $\psi_k(\mathbf{r}_1, \mathbf{r}_2)$  ( $k = 1, 2, 3, 4$ ) that make  $\Psi$  antisymmetric.

(b) For non-interacting electrons, we expect the product form

$$\psi_k(\mathbf{r}_1, \mathbf{r}_2) = A_k \phi_1(\mathbf{r}_1) \phi_2(\mathbf{r}_2) + B_k \phi_2(\mathbf{r}_1) \phi_1(\mathbf{r}_2), \quad (13)$$

with  $\int d^3r |\phi_1(\mathbf{r})|^2 = \int d^3r |\phi_2(\mathbf{r})|^2 = 1$ .

What can you tell about the values of the coefficients  $A_k, B_k$  in the following cases?

(i)  $\phi_1(\mathbf{r}) = \phi_2(\mathbf{r}) \equiv \phi(\mathbf{r})$ .

(ii)  $\int d^3r \phi_1^*(\mathbf{r}) \phi_2(\mathbf{r}) = 0$ .

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## Worksheet 2 (January 29, 2018)

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### Problem 1

- (a) Show that the function  $v : \mathbb{R}^3 \setminus \{0\} \rightarrow \mathbb{R}$ ,  $v(\mathbf{r}) = -\frac{1}{|\mathbf{r}|}$  belongs to  $L^{3/2}(\mathbb{R}^3) \oplus L^\infty(\mathbb{R}^3)$ .
- (b) Consider the energy function for the Hydrogen atom ( $N = 1$ ).

$$E[\psi] = \sum_{s \in \mathbb{Z}_2} \int_{\mathbb{R}^3} |\nabla \psi(\mathbf{r}, s)|^2 - \frac{1}{|\mathbf{r}|} |\psi(\mathbf{r}, s)|^2 d\mathbf{r}.$$

Show that the above energy is not well-defined in  $L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ .

(Hint: Consider the function  $\psi(r, s) = (2\pi)^{-1/2} \delta_{1/2}(s) e^{-|r|}/|r|$ .

Show that  $\psi \in L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$  with  $\|\psi\|_{L^2} = 1$ , but not in  $H^1(\mathbb{R}^3 \times \mathbb{Z}_2)$ . Conclude by comparing with the right-hand term.)

### Problem 2

Consider  $\rho : \mathbb{R}^3 \rightarrow \mathbb{R}$  a probability density and a (admissible) function  $\psi \in H^1((\mathbb{R}^3 \times \mathbb{Z}_2)^N)$  such that  $\|\psi\|_{L^2} = 1$ ,  $\psi \mapsto \rho$  and  $\psi$  is anti-symmetric.

- (a) Show that

$$\int_{\mathbb{R}^{3N}} \sum_{i=1}^N v(\mathbf{r}_i) \rho^\psi(\mathbf{r}_1, \dots, \mathbf{r}_N) d\mathbf{r}_1 \dots d\mathbf{r}_N = N \int_{\mathbb{R}^3} v(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r},$$

where  $\rho^\psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{s_1, \dots, s_N \in \mathbb{Z}_2} |\psi(\mathbf{r}_1, s_1, \dots, \mathbf{r}_N, s_N)|^2$ .

- (b) Denote by  $A[\rho] = \int_{\mathbb{R}^3} v(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r}$ . Consider  $\rho_\epsilon(\mathbf{r}) = \rho(\mathbf{r}) + \epsilon \xi(\mathbf{r})$  with  $\xi(\mathbf{r}) \geq 0$  and  $\int_{\mathbb{R}^3} \xi(\mathbf{r}) d\mathbf{r} = 0$ . Compute the limit

$$\lim_{\epsilon \rightarrow 0} \frac{A[\rho_\epsilon] - A[\rho]}{\epsilon}.$$

- (c) Show that  $\rho \geq 0$ ,  $\|\rho\|_{L^1} = 1$  and  $\sqrt{\rho} \in H^1(\mathbb{R}^3)$ .

(Hint: Use Cauchy-Schwarz and notice that  $|\nabla \sqrt{g}|^2 = \frac{|\nabla g|^2}{4g}$ .)

### Problem 3

- (a) Consider the Lorentzian density  $\rho : \mathbb{R} \rightarrow \mathbb{R}$ ,  $\rho(r) = \frac{1}{\pi(1+r^2)}$  and the associate co-motion function  $f(r) = -1/r$ . Show that the *SCE*-ansatz  $\gamma_f(r_1, r_2) = \delta(r_2 - f(r_1))\rho(r_1)$  (or, equivalently,  $\gamma_f = (Id, f)_\# \rho$ ) is not in  $H^1(\mathbb{R}^2, \mathbb{R})$ . (Hint: Draw the graph  $\{(r, f(r)) \in \mathbb{R}^2 : r \in \mathbb{R} \setminus \{0\}\}$ . Write the definition of the gradient of  $\gamma$  at a point  $(r, f(r))$ ).

### Problem 4

- (a) Give an example of a function  $g : \mathbb{R} \rightarrow \mathbb{R}$  that is lower-semi continuous but not continuous. Justify your example.
- (b) Suppose  $X$  is a metric space (if you prefer you can assume  $X = \mathbb{R}^d$ ). If  $g : X \rightarrow \mathbb{R} \cup \{+\infty\}$  is lower semi-continuous and  $X$  is compact, then there exists  $\bar{x} \in X$  such that  $g(\bar{x}) = \min\{g(x) : x \in X\}$ .

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## Worksheet 3 (February 6, 2018)

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### Problem 1

Consider  $X = \mathbb{R}^d$ . Prove that  $C_0(\mathbb{R}^d)$  is a closed subset of the Banach Space  $(C_b(\mathbb{R}^d), \|\cdot\|_\infty)$ , where  $\|\cdot\|_\infty$  denotes the sup-norm.

### Problem 2

Suppose  $g : X \rightarrow \mathbb{R} \cup \{+\infty\}$  be a lower semi-continuous function and **bounded from below**. Show that, there exists a sequence  $(g_k)_{k \in \mathbb{N}}$  such that for every  $k$ ,  $g_k$  is  $k$ -Lipschitz and for every  $x \in X$   $g_k(x) \uparrow g(x)$  (increasingly).

*The goal of this exercise is to show a characterization of lower semi-continuity. We will give a complete explanation below.*

**Claim 1:** Let  $g : X \rightarrow \mathbb{R} \cup \{+\infty\}$  be a function bounded from below. Then  $g$  is l.s.c. if and only there exists a sequence  $g_k$  of  $k$ -Lipschitz functions such that for every  $x \in X$ ,  $g_k(x)$  converges increasingly to  $g(x)$

Given  $g$  lower semi-continuous and bounded from below, let us define

$$g_k(x) = \inf_y (g(y) + kd(x, y)).$$

These functions are  $k$ -Lipschitz continuous since  $x \mapsto g(y) + kd(x, y)$  is  $k$ -Lipschitz. For fixed  $x$ , the sequence  $g_k(x)$  is increasing and we have  $\inf g \leq g_k(x) \leq g(x)$ . We just need to prove that  $\ell := \lim_k g_k(x) = \sup_k g_k(x) = g(x)$ . Suppose by contradiction  $\ell < g(x)$ , which implies in particular  $\ell < +\infty$ . For every  $k$ , let us choose a point  $y_k$  such that  $g(y_k) + kd(y_k, x) < g_k(x) + 1/k$ . We get  $d(y_k, x) \leq \frac{\ell + 1/k - g(y_k)}{k} \leq \frac{C}{k}$ , thanks to the lower bound on  $g$  and to  $\ell < \infty$ . Hence we know  $y_k \rightarrow x$ . Yet, we have  $g_k(x) + 1/k \geq g(y_k)$  and we get  $\lim_k g_k(x) \geq \liminf_k g(y_k) \geq g(x)$ . This proves  $\ell \geq g(x)$ . Finally, the functions  $g_k$  may be made bounded by taking  $g_k \wedge k \equiv \max\{g_k, k\}$ .

The other implication is simpler, since the functions  $g_k$  are continuous, hence lower semi-continuous, and  $g$  is the sup of  $g_k$  (see claim 2, below).

**Claim 2:** If  $g_\alpha$  is an arbitrary family of lower semi-continuous functions on  $X$ , then  $g = \sup_\alpha g_\alpha$  (i.e.  $g(x) := \sup_\alpha g_\alpha(x)$ ) is also lower semi-continuous.

*Proof* - Take  $x_n \rightarrow x$  and write  $g_\alpha(x) \leq \liminf_n g_\alpha(x_n) \leq_n g(x_n)$ . Then pass to the sup in  $\alpha$  and get  $g(x) \leq \liminf_n g(x_n)$ . It is also possible to check the same fact using epigraphs: indeed, a function is lower semi-continuous if and only if its epigraph  $\{(x, t) : t \geq g(x)\} \subset X \times \mathbb{R}$  is closed, and the epigraph of the sup is the intersection of the epigraphs.

### Problem 3

(a) Show that a coupling  $\gamma$  of two probability spaces  $(X, \mu)$  and  $(Y, \nu)$  is equivalent to:

(i) For all measurable sets  $A \subset X$  and  $B \subset Y$ , one has

$$\gamma[A \times Y] = \mu[A] \text{ and } \gamma[X \times B] = \nu[B].$$

(ii) For all integrable measurable functions  $u, v$  on  $X, Y$ ,

$$\int_{X \times Y} (u(x) + v(y)) d\gamma(x, y) = \int_X u(x) d\mu(x) + \int_Y v(y) d\nu(y).$$

(b) Consider  $\mu_1, \dots, \mu_N \in \mathcal{P}(\mathbb{R}^d)$ . Show that if  $\gamma \in \Pi_N^{sym}(\mathbb{R}^{dN}, \mu_1, \dots, \mu_N)$  then  $(e_i)_\# \gamma = \mu_i, \forall i = 1, \dots, N$ . Conclude that  $\Pi_N^{sym}(\mathbb{R}^{dN}, \mu_1, \dots, \mu_N) = \Pi_N^{sym}(\mathbb{R}^{dN}, \mu_1)$ .

### Problem 4

Consider the Kantorovich dual of  $V_{ee}^{SIL}[\rho]$ . Show that

$$\begin{aligned} \sup \left\{ \sum_{i=1}^N \int_{\mathbb{R}^d} u_i(\mathbf{r}_i) \rho(\mathbf{r}_i) d\mathbf{r}_i : \forall i \ u_i \in L^1(\mathbb{R}^d, \rho), u_1(\mathbf{r}_1) + \dots + u_N(\mathbf{r}_N) \leq V_{ee}(\mathbf{r}_1, \dots, \mathbf{r}_N) \right\} = \\ = \sup \left\{ N \int_{\mathbb{R}^d} u(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} : u \in L^1(\mathbb{R}^d, \rho), u(\mathbf{r}_1) + \dots + u(\mathbf{r}_N) \leq V_{ee}(\mathbf{r}_1, \dots, \mathbf{r}_N) \right\}. \end{aligned}$$

### Problem 5

Let  $N = 2$ ,  $\mu_1 = \rho_1 \mathcal{L}, \mu_2 = \rho_2 \mathcal{L}$  probabilities in  $\mathbb{R}$  and  $V_a(r_1, r_2) = |r_1 - r_2|^2$  the attractive harmonic interaction. Consider the following problem.

$$\inf_{\gamma \in \Pi(\mathbb{R}^2, \mu_1, \mu_2)} \int_{\mathbb{R} \times \mathbb{R}} |r_1 - r_2|^2 d\gamma(r_1, r_2)$$

(a) Argue that the above problem has a minimizer.

Hint: Use the direct method of Calculus of Variations.

(b) Assume that  $\mu_1$  and  $\mu_2$  are, respectively, the uniform measure in  $[0, 1]$  and  $[1, 2]$ , i.e.  $\rho_1 = \chi_{[0,1]}$  and  $\rho_2 = \chi_{[1,2]}$ , where  $\chi_A$  is the characteristic function of a set  $A \subset \mathbb{R}$ . Show that the coupling  $\gamma_T = (Id, T)_\# \mu_1 = \mu_2$ , where  $T : \mathbb{R} \rightarrow \mathbb{R}$  is the translation  $T(r_1) = r_1 + 1$ , is an optimal coupling in the above minimization problem (we can show that this is the unique one).

Hint: Use Jensen's inequality to show that the value of  $C_a(\gamma)$  must be  $\geq$  than a constant  $A$ . Show that  $T_\# \mu_1 = \mu_2$  and therefore  $\gamma_T \in \Pi(\mathbb{R}^2, \mu_1, \mu_2)$ .

Compute the value of the integral  $\int_{\mathbb{R}^2} |r_1 + T(r_1)|^2 dr_1$  for the translation map defined above.

## Problem 6

Suppose  $\rho : \mathbb{R}^d \rightarrow \mathbb{R}$  is a probability density such that  $\int_{\mathbb{R}^d} |\mathbf{r}|^2 \rho(\mathbf{r}) d\mathbf{r} < +\infty$  (finite second moments) and denote by  $V_w : (\mathbb{R}^d)^N \rightarrow \mathbb{R}$  the repulsive harmonic interaction

$$V_w(\mathbf{r}_1, \dots, \mathbf{r}_N) = - \sum_{1 \leq i < j \leq N} |\mathbf{r}_i - \mathbf{r}_j|^2.$$

Consider the strong-interaction limit functional for the repulsive harmonic interaction

$$V_w^{SIL}[\rho] = \inf_{\gamma \in \Pi_N(\rho)} \int_{(\mathbb{R}^d)^N} V_w(\mathbf{r}_1, \dots, \mathbf{r}_N) d\gamma(\mathbf{r}_1, \dots, \mathbf{r}_N).$$

(a1) Show that

$$\int_{(\mathbb{R}^d)^N} V_w(\mathbf{r}_1, \dots, \mathbf{r}_N) d\gamma(\mathbf{r}_1, \dots, \mathbf{r}_N) = \int_{(\mathbb{R}^d)^N} |\mathbf{r}_1 + \dots + \mathbf{r}_N|^2 d\gamma(\mathbf{r}_1, \dots, \mathbf{r}_N) + C,$$

where  $C$  is a constant that can be computed explicitly. Argue to conclude that  $V_w^{SIL}[\rho]$  admits a minimizer.

(a2) Show that the problem

$$\sup_{\gamma \in \Pi_N(\rho)} \int_{(\mathbb{R}^d)^N} V_w(\mathbf{r}_1, \dots, \mathbf{r}_N) d\gamma(\mathbf{r}_1, \dots, \mathbf{r}_N).$$

admits a maximizer and exhibit a measure of type  $\gamma_T = (Id, T_1, T_2, \dots, T_{N-1})_{\#} \rho = \rho$  maximizing the above functional.

(b\*) Show that if there exists a plan  $\gamma$  concentrated in some hyperplane

$$\{\mathbf{r}_1 + \dots + \mathbf{r}_N = \mathbf{k}\}, \quad \mathbf{k} \in \mathbb{R}^d$$

then  $\gamma$  is an optimal coupling for  $V_w^{SIL}[\rho]$ . In this case,  $\tilde{\gamma} \in \Pi_N(\rho)$  is optimal, if and only if,  $\text{spt}(\tilde{\gamma}) \subset \{(\mathbf{r}_1, \dots, \mathbf{r}_N) \in \mathbb{R}^{dN} : \mathbf{r}_1 + \dots + \mathbf{r}_N = \mathbf{k}\}$ . In particular, the constant  $k$  can be computed explicitly  $k = N \int_{\mathbb{R}^d} \mathbf{r} \rho(\mathbf{r}) d\mathbf{r}$ .

HINT: Use Jensen's inequality to compute  $C_w(\gamma) = \int_{(\mathbb{R}^d)^N} |\mathbf{r}_1 + \dots + \mathbf{r}_N|^2 d\gamma$ .

(c) Consider the case when  $N = 2$  and  $\rho = \chi_{[0,1]} \mathcal{L}$  (uniform measure in the unit interval in  $\mathbb{R}$ ). Show that the coupling  $\gamma_h = (Id, h)_{\#} \rho$  is optimal for  $V_w^{SIL}[\rho]$  where  $h : \mathbb{R} \rightarrow \mathbb{R}$  is the reflection map  $h(r) = 1 - r$ .

HINT: Compute the constant  $k = N \int r \rho(r) dr$  in this case.

Show that  $h_{\#} \rho = \rho$ ,  $r_1 + h(r_1) = 1$  and use the part (b\*).

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## Worksheet 4 (February 19, 2018)

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### Problem 1

Let  $V : \mathbb{R}^{dN} \rightarrow \mathbb{R} \cup \{+\infty\}$  be a lower semi-continuous functions and bounded from below. Remember the following definitions:

$$(\mathcal{MK}_N) \quad \min \left\{ \int_{\mathbb{R}^{dN}} V(x_1, \dots, x_N) d\gamma(x_1, \dots, x_N) : \gamma \in \Pi_N(\mu) \right\}.$$

$$(\mathcal{MK}_N^{sym}) \quad \min \left\{ \int_{\mathbb{R}^{dN}} V(x_1, \dots, x_N) d\gamma(x_1, \dots, x_N) : \gamma \in \Pi_N^{sym}(\mu) \right\}.$$

$$(\mathcal{M}_N) \quad \inf \left\{ \int_{(\mathbb{R}^d)^N} V(\mathbf{r}, \mathbf{f}_1(x), \dots, \mathbf{f}_{N-1}(x)) d\rho(x) dx : \mathbf{f}_{i\#}\mu = \mu, \forall i \in I \right\}.$$

$$(\mathcal{M}_N^{cyc}) \quad \inf \left\{ \int_{(\mathbb{R}^d)^N} V(\mathbf{r}, \mathbf{f}(x), \mathbf{f}^{(2)}(x), \dots, \mathbf{f}^{(N-1)}(x)) d\rho(x) dx : \mathbf{f}_{\#}\mu = \mu, \mathbf{f}^{(N)} = id \right\}.$$

Observe that

- (i)  $\min(\mathcal{MK}_N^{sym}) = (\mathcal{MK}_N)$ .
- (ii)  $\inf(\mathcal{M}_N) \leq \inf(\mathcal{M}_N^{cyc})$ .
- (iii)  $\min(\mathcal{MK}_N^{sym}) \leq \inf(\mathcal{M}_N^{cyc})$ .

Prove that:

$$\inf(\mathcal{M}_N) = \inf(\mathcal{M}_N^{cyc}) \quad \text{if and only if} \quad \inf(\mathcal{MK}_N) = \inf(\mathcal{M}_N^{cyc})$$

### Problem 2

Show that

- (i) If  $g : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$  is a convex function, then  $g : \mathbb{R}^d \rightarrow \mathbb{R}$  is continuous.
- (ii) Let  $(g_k)_k$  a sequence of continuous affine functions  $g_k : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ . Show that  $g := \sup_k g_k$  is convex and lower semi-continuous.
- (iii) Show that the sub-differential of  $g : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$ ,  $g(x) = |x|^2$ , is

$$\partial g(x) = \begin{cases} 1 & \text{if } x > 0 \\ -1 & \text{if } x < 0 \\ [-1, 1] & \text{if } x = 0 \end{cases}$$



### Problem 3

Compute the Legendre transform of the functions  $g, h : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{+\infty\}$ , where

$$g(x) = \frac{\|x\|^p}{p}, p \geq 1 \quad \text{and} \quad h(x) = e^x.$$

### Problem 4

Consider the functional  $J_\epsilon[\rho]$  defined by the strong-interaction limit functional with an Entropic penalization.

$$J_\epsilon[\rho] = \inf_{\gamma \in \Pi_N(\rho)} J_\epsilon[\gamma] = \inf_{\gamma \in \Pi(\rho)} \int_{\mathbb{R}^{dN}} V_{ee} d\gamma + \epsilon E_N(\gamma),$$

where

$$E_N(\gamma) = \begin{cases} \int_{\mathbb{R}^{dN}} \gamma \log(\gamma) dx_1 \dots dx_N & , \gamma \text{ is a.c.} \\ +\infty & , \text{ otherwise} \end{cases}$$

We remind that *a.c.* stands for *absolutely continuous*, i.e. there exists a density function  $h(x_1, \dots, x_N)$  such that  $\gamma(x_1, \dots, x_N) = h(x_1, \dots, x_N) dx_1 \dots dx_N = h \mathcal{L}^{dN}$ .

- (a) Show that  $J_\epsilon[\rho]$  admits a minimizer.  
(use the Direct method of Calculus of Variations).
- (b) Show that the minimizer is unique.  
*Hint: prove that the functional  $C(\gamma) + \epsilon H_N(\gamma)$  is strictly convex.*
- (c) Show that (formally) the dual problem associated to  $J_\epsilon[\rho]$  is given by

$$\sup \left\{ N \int_{\mathbb{R}^d} \rho(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} : u(\mathbf{r}_1) + \dots + u(\mathbf{r}_N) \leq V + \gamma(\ln \gamma) \right\}.$$

**For make the notation simpler, you can consider the case when  $N = 2$ .**

### Problem 5

The goal of this exercise is to provide a rigorous justification for an example introduced by Michael Seidl in the first part of the course. Suppose  $\rho : \mathbb{R} \rightarrow \mathbb{R}$  is given by the Lorentzian density ( $d = 1$ ):  $\rho(x) = \frac{1}{\pi} \frac{1}{1+x^2}$ .

- (i) ( $N = 2$ ) Compute the co-motion function  $f(x)$  associated to the strong-interaction limit functional, i.e.  $f : \mathbb{R} \rightarrow \mathbb{R}$  such that

$$V_{ee}^{SIL}[\rho] = \min \left\{ \int_{\mathbb{R} \times \mathbb{R}} \frac{1}{|x_1 - x_2|} d\gamma(x_1, x_2) : \gamma \in \Pi_2(\rho) \right\} = \int_{\mathbb{R}} \frac{1}{|x - f(x)|} \rho(x) dx.$$

– Does  $f \in C^1(\mathbb{R})$ ? Plot the graph of  $f$  and do a sketch of the set

$$\{(x, \gamma(x, f(x))) \in \mathbb{R}^3 : x \in \mathbb{R}\}.$$

(ii) Show that, there exist a function  $u : \mathbb{R} \rightarrow \mathbb{R}$  such that

$$u(x_1) + u(x_2) \leq \frac{1}{|x_1 - x_2|}, \quad \forall (x_1, x_2) \in \mathbb{R} \times \mathbb{R}.$$

and

$$u(x) + u(f(x)) = \frac{1}{|x - f(x)|}, \text{ for almost every } x \in \text{spt}(\gamma)^1.$$

– Compute such a function  $u$ . Does  $u \in C_b(\mathbb{R})$ ? Plot the graph of  $u$ .

(iii) Compute the curvature of the curve  $t \in \mathbb{R} \mapsto (t, f(t)) \in \mathbb{R}^2$ .

## Problem 6

Now we fix  $N = 3$  and consider the uniform measure on the unit interval  $\mu = \chi_{[0,1]} \mathcal{L}$ . Notice that, contrary to the previous exercise, the measure  $\mu$  has compact support.

(i) Compute the co-motion functions  $f, f^2 : \mathbb{R} \rightarrow \mathbb{R}$  associated to

$$V_{ee}^{SIL}[\mu] = \min \left\{ \int_{\mathbb{R} \times \mathbb{R} \times \mathbb{R}} \frac{1}{|x_1 - x_2|} + \frac{1}{|x_1 - x_3|} + \frac{1}{|x_2 - x_3|} d\gamma(x_1, x_2, x_3) : \gamma \in \Pi_3(\mu) \right\}.$$

Show that  $f^3 = id$ .

(ii) Compute the Kantorovich potentials  $u$  associated to  $V_{ee}^{SIL}[\mu]$ .