

DFT meets OT

Worksheet 1 (January 17, 2018)

Problem 1

Consider the antisymmetrized product wave function Ψ 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 Ψ 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 Ψ (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 Ψ 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 Ψ 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)

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 ψ 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 γ 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)

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. 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 $x \in X$ $g_k(x) \uparrow f(x)$ (increasingly).

Hint: Show that $g(x) = \sup_{k \in \mathbb{N}} g_k(x)$ is l.s.c.

Problem 3

(a) Show that a coupling γ of two probability spaces (X, μ) and (Y, ν) is equivalent to:

(i) For all measurable sets $A \subset X$ and $B \subset Y$, one has $\gamma[A \times Y] = \mu[A]$ 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 μ_1 and μ_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 χ_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 γ concentrated in some hyperplane

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

then γ is an optimal coupling for $V_w^{SIL}[\rho]$. In this case, $\tilde{\gamma} \in \Pi_N(\rho)$ is optimal, if and only if, $\text{spt}(\tilde{\gamma}) \subset \{(\mathbf{r}_1, \dots, \mathbf{r}_N) \in \mathbb{R}^{dN} : \mathbf{r}_1 + \cdots + \mathbf{r}_N = \mathbf{k}\}$. 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 $C_w(\gamma) = \int_{(\mathbb{R}^d)^N} |\mathbf{r}_1 + \cdots + \mathbf{r}_N|^2 d\gamma$.

- (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*).