DFT meets OT

Worksheet 1 (January 17, 2018)

Problem 1

Consider the antisymmetrized product wave function Ψ given in the lecture,

$$\Psi(\mathbf{x}_1, ..., \mathbf{x}_N) \;=\; \frac{1}{\sqrt{N!}} \sum_{\wp \in S_N} \mathrm{sign}(\wp) \prod_{k=1}^{N} \psi_{\wp(k)}(\mathbf{x}_k) \qquad \Big(\mathbf{x}_k = (\mathbf{r}_k, \sigma_k)\Big), \tag{1}$$

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.,

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

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

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

$$\Big\{-\frac{\hbar^2}{2m}\nabla^2 + v(\mathbf{r})\Big\}\phi_n(\mathbf{r}) \;=\; \epsilon_n\,\phi_n(\mathbf{r}) \qquad \Big(\epsilon_1 \le \epsilon_2 \le \epsilon_3 \le ...\Big). \tag{4}$$

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

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

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

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

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

Hint 1: For $\mathbf{x} = (\mathbf{r}, \sigma)$, use the notation $\sum_{\sigma\in\{\uparrow,\downarrow\}}\int \mathrm{d}^3r\, f(\mathbf{r},\sigma) \equiv \int \mathrm{d}^3x\, f(\mathbf{x})$.
Hint 2: The single-particle wave functions $\psi_k(\mathbf{x})$ are pairwise orthonormal,

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

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?

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

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

$$\Omega_R(\mathbf{r}_0) \;=\; \Big\{ \mathbf{r} \in \mathbb{R}^3 \;\Big|\; |\mathbf{r} - \mathbf{r}_0| \leq R \Big\}. \tag{9}$$

(b) Give a probability interpretation for the number

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

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

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

(d) What can you tell about the quantities

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

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

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

with $\int \mathrm{d}^3r\,|\phi_1(\mathbf{r})|^2 = \int \mathrm{d}^3r\,|\phi_2(\mathbf{r})|^2 = 1$.
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) $\int \mathrm{d}^3r\,\phi_1^*(\mathbf{r})\,\phi_2(\mathbf{r}) = 0$.

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Worksheet 2 (January 29, 2018)

Problem 1

(a) Show that the function $v : \mathbb{R}^3 \backslash \{0\} \to \mathbb{R}, v(\mathbf{r}) = -\dfrac{1}{|\mathbf{r}|}$ 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 $\rho : \mathbb{R}^3 \to \mathbb{R}$ 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

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

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

(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

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

(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 Lorenzian density $\rho : \mathbb{R} \to \mathbb{R}$, $\rho(r) = \frac{1}{\pi(1+r^2)}$ 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, $\gamma_f = (Id, f)_\sharp \rho$) is not in $H^1(\mathbb{R}^2, \mathbb{R})$.
(Hint: Draw the graph $\{(r, f(r)) \in \mathbb{R}^2 : r \in \mathbb{R}\backslash\{0\}\}$. Write the definition of the gradient of γ at a point $(r, f(r))$).

Problem 4

(a) Give an example of a function $g : \mathbb{R} \to \mathbb{R}$ 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 $g : X \to \mathbb{R} \cup \{+\infty\}$ 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 $g : X \to \mathbb{R} \cup \{+\infty\}$ 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 $g : X \to \mathbb{R} \cup \{+\infty\}$ 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 $\inf g \le g_k(x) \le g(x)$. 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 $d(y_k, x) \le \frac{\ell+1/k-g(y_k)}{k} \le \frac{C}{k}$, thanks to the lower bound on g and to $\ell < \infty$. Hence we know $y_k \to x$. Yet, we have $g_k(x) + 1/k \ge g(y_k)$ and we get $\lim_k g_k(x) \ge \liminf_k g(y_k) \ge g(x)$. This proves $\ell \ge g(x)$. 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_α 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 $x_n \to x$ and write $g_\alpha(x) \le \liminf_n g_\alpha(x_n) \le_n g(x_n)$. Then pass to the sup in α and get $g(x) \le \liminf_n g(x_n)$. It is also possible to check the same fact using epigraphs: indeed, a function is lower semi-continuous if and only if its epigraph $\{(x, t) : t \ge g(x)\} \subset X \times \mathbb{R}$ is closed, and the epigraph of the sup is the intersection of the epigraphs.

Problem 3

(a) Show that a coupling 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 $\mu_1, \ldots, \mu_N \in \mathcal{P}(\mathbb{R}^d)$. Show that if $\gamma \in \Pi_N^{sym}(\mathbb{R}^{dN}, \mu_1, \ldots, \mu_N)$ then $(e_i)_\sharp \gamma = \mu_1, \forall i = 1, \ldots, N$. Conclude that $\Pi_N^{sym}(\mathbb{R}^{dN}, \mu_1, \ldots, \mu_N) = \Pi_N^{sym}(\mathbb{R}^{dN}, \mu_1)$.

Problem 4

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

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

$$= \sup \left\{ N \int_{\mathbb{R}^d} u(\mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} : u \in L^1(\mathbb{R}^d, \rho), u(\mathbf{r}_1) + \cdots + u(\mathbf{r}_N) \leq V_{ee}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \right\}.$$

Problem 5

Let $N = 2$, $\mu_1 = \rho_1 \mathcal{L}, \mu_2 = \rho_2 \mathcal{L}$ probabilities in $\mathbb{R}$ and $V_a(r_1, r_2) = |r_1 - r_1|^2$ 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 $\gamma_T = (Id, T)_\sharp \mu_1 = \mu_2$, where $T : \mathbb{R} \to \mathbb{R}$ 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 $T_\sharp \mu_1 = \mu_2$ 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 $\rho : \mathbb{R}^d \to \mathbb{R}$ 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 $V_w : (\mathbb{R}^d)^N \to \mathbb{R}$ the repulsive harmonic interaction

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

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

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

(a1) Show that

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

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

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

admits a maximizer and exhibit a measure of type $\gamma_T = (Id, T_1, T_2, \ldots, T_{N-1})_\sharp \rho = \rho$ 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, $\mathrm{spt}(\tilde{\gamma}) \subset \{(\mathbf{r}_1, \ldots, \mathbf{r}_N) \in \mathbb{R}^{dN} : \mathbf{r}_1 + \cdots + \mathbf{r}_N = k\}$. 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 $\gamma_h = (Id, h)_\sharp \rho$ is optimal for $V_w^{SIL}[\rho]$ where $h : \mathbb{R} \to \mathbb{R}$ is the reflection map $h(r) = 1 - r$.
HINT: Compute the constant $k = N \int r \rho(r) dr$ in this case.
Show that $h_\sharp \rho = \rho$, $r_1 + h(r_1) = 1$ and use the part (b*).