

# Density Functional Theory for two-dimensional homogeneous materials

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**Goal:** study two-dimensional materials (embedded in 3d space).



≠ 2d material in 2d space (e.g. with the 2d Coulomb kernel).

**Questions:**

- What should be the size of the «simulation box»?
- What is the decay of the **electronic density** or **mean-field potential** away from the plane?

In this talk, we consider **homogeneous materials**, modelled by a charge density

$$\mu(x_1, x_2, x_3) = \mu(x_3) \in L^1(\mathbb{R}).$$

and study the properties of the electronic density in **Thomas-Fermi** and **Kohn-Sham** models.

**Remarks**

- Very crude approximation (we lose the microscopic details of the material);
- This model should have the correct decay properties away from the slab (the details *fade away*).

# Thomas-Fermi model

Recall the (three-dimensional) **Thomas-Fermi energy** (assume  $\mu \in C_0^\infty(\mathbb{R}^3)$ )

$$\forall \rho \in L^1(\mathbb{R}^3) \cap L^{5/3}(\mathbb{R}^3), \rho \geq 0, \quad \mathcal{E}_3^{\text{TF}}(\rho) := c_{\text{TF}} \int_{\mathbb{R}^3} \rho^{5/3} + \frac{1}{2} \mathcal{D}_3(\rho - \mu),$$

with the **three-dimensional Coulomb energy**

$$\mathcal{D}_3(f) := \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{f(x)f(y)}{|x-y|} dx dy.$$

The model is *convex* in  $\rho$ . In particular, if  $\mu$  satisfies some symmetries, then  $\rho$  satisfies the same symmetries.

If  $\mu$  only depends on  $x_3$ , we may assume that  $\rho$  also depends on  $x_3$  only.

We define the **Thomas-Fermi energy per unit surface**

$$\forall \rho \in L^1(\mathbb{R}) \cap L^{5/3}(\mathbb{R}), \quad \mathcal{E}_1^{\text{TF}}(\rho) := c_{\text{TF}} \int_{\mathbb{R}} \rho^{5/3} + \frac{1}{2} \mathcal{D}_1(\rho - \mu),$$

with the **one-dimensional Coulomb energy**

$$\mathcal{D}_1(f) := -2\pi \iint_{\mathbb{R} \times \mathbb{R}} f(x)f(y)|x-y| dx dy.$$

**Thomas-Fermi minimization** (for neutral systems only)

$$\rho_{\text{TF}} := \operatorname{argmin} \left\{ \mathcal{E}_1^{\text{TF}}(\rho), \rho \in L^1(\mathbb{R}) \cap L^{5/3}(\mathbb{R}), \rho \geq 0, \int_{\mathbb{R}} \rho = \int_{\mathbb{R}} \mu =: Z \right\}.$$

$$\rho_{\text{TF}} := \operatorname{argmin} \left\{ \mathcal{E}_1^{\text{TF}}(\rho), \rho \in L^1(\mathbb{R}) \cap L^{5/3}(\mathbb{R}), \rho \geq 0, \int_{\mathbb{R}} \rho = Z \right\}.$$

**Key remark:** It is a (very) simple model (one-dimensional, no derivatives, ...).

## Proposition

There is a unique minimizer  $\rho_{\text{TF}}$ . It is the (unique) solution to the Thomas-Fermi equation

$$\begin{cases} \frac{5}{3} c_{\text{TF}} \rho_{\text{TF}}^{2/3} = (\lambda - \Phi_{\text{TF}})_+ \\ -\Phi_{\text{TF}}'' = 4\pi(\rho_{\text{TF}} - \mu), \quad \Phi_{\text{TF}}'(\pm\infty) = 0, \quad \Phi_{\text{TF}}(0) = 0. \end{cases}$$

Here,  $\lambda \in \mathbb{R}$  is the *Fermi level*, chosen so that  $\int_{\mathbb{R}} \rho = Z$ , and  $\Phi_{\text{TF}}$  is defined as the unique solution of the second equation.

**Remark:** There is no *reference energy* in 1d (the 1d Green's function does not have a limit at infinity). Only the difference  $V_{\text{TF}} := \Phi_{\text{TF}} - \lambda$ , called the *mean-field potential*, makes sense.

The proof is similar to the ones of the *usual* Thomas–Fermi model (see [Lieb/Simon, Adv. Math. 23, 1977]).

## Screening properties

Let  $f \in C_0^\infty(\mathbb{R})$  be such that  $\int_{\mathbb{R}} f = 0$ . The potential generated by  $f$  is formally

$$\Phi_f(x) := -2\pi \int_{\mathbb{R}} f(y)|x-y|dy.$$

We have  $\Phi_f(\infty) = 2\pi \int_{\mathbb{R}} f(y)ydy$  and  $\Phi_f(-\infty) = -2\pi \int_{\mathbb{R}} f(y)ydy$ .

The difference  $\Phi_f(\infty) - \Phi_f(-\infty) = 4\pi \int_{\mathbb{R}} f(y)ydy$  is called the **dipolar moment**.

### Proposition (perfect screening)

Assume  $|x|\mu(x) \in L^1(\mathbb{R})$ . Then  $|x|\rho_{\text{TF}}(x) \in L^1(\mathbb{R})$  as well, and the Thomas-Fermi potential  $V_{\text{TF}}$  satisfies

$$\lim_{x \rightarrow +\infty} V_{\text{TF}}(x) = \lim_{x \rightarrow -\infty} V_{\text{TF}}(x) = 0. \quad (\text{no dipolar moment.})$$

### Proposition (Sommerfeld estimates)

Assume  $\mu$  is compactly supported in  $[a, b]$ . Then, there is  $x_a, x_b \in \mathbb{R}$  so that

$$\forall x < a, \quad V_{\text{TF}}(x) = \frac{-c_1}{(x-x_a)^4}, \quad \text{and} \quad \rho_{\text{TF}}(x) = \frac{c_2}{(x-x_a)^6},$$

$$\forall x > b, \quad V_{\text{TF}}(x) = \frac{-c_1}{(x-x_b)^4}, \quad \text{and} \quad \rho_{\text{TF}}(x) = \frac{c_2}{(x-x_b)^6}.$$

with the constants  $c_1 := \frac{5^5 c_{\text{TF}}^3}{27\pi^2}$  and  $c_2 := \frac{5^6 c_{\text{TF}}^3}{27\pi^3}$ .

See [Sommerfeld, Zeitschrift für Physik 78(5-6) (1932)] and [Solovej, Ann. Math., (2003)] in the *usual* case.

# Interlude: the 1d Coulomb operator

For  $L > 0$ , we consider the  $L\mathbb{Z}^2$ -periodic Green's function  $G_L$ , solution to

$$-\Delta_3 G_L = 4\pi \sum_{(R_1, R_2) \in L\mathbb{Z}^2} \delta_{(R_1, R_2, 0)}.$$

A computation shows that (we write  $\mathbf{x} = (x_1, x_2)$ )

$$G_L(\mathbf{x}, x_3) = -\frac{2\pi}{L^2} |x_3| + \frac{2\pi}{L^2} \sum_{\mathbf{k} \in (2\pi/L)\mathbb{Z}^2 \setminus \{0\}} \frac{e^{-|\mathbf{k}| \cdot |x_3|}}{|\mathbf{k}|} e^{i\mathbf{k} \cdot \mathbf{x}}.$$

- We recognize the 1d Coulomb kernel in red.
- The other part is oscillating in  $\mathbf{x}$ , and exponentially decaying away from the slab («*details fade away*»).

If  $f(\mathbf{x}, x_3) = f(x_3)$  only depends on the third variable, then

$$\int_{[0, L]^2 \times \mathbb{R}} f(\mathbf{y}, y_3) G_L(\mathbf{x} - \mathbf{y}; x_3 - y_3) d\mathbf{y} dy_3 = -2\pi \int_{\mathbb{R}} f(y_3) |x_3 - y_3| dy_3.$$

and, with obvious notation,

$$\frac{1}{L^2} \mathcal{D}_{3, L}(f) = \mathcal{D}_1(f).$$



Define the **Hartree term**

$$\widetilde{\mathcal{D}}_1(f) := -2\pi \iint_{\mathbb{R} \times \mathbb{R}} f(x)f(y)|x-y|dx dy, \quad (\text{well-defined whenever } (1+|x|)f(x) \in L^1(\mathbb{R})).$$

**Warning:** The map  $f \mapsto \widetilde{\mathcal{D}}_1(f)$  is **not** convex.

$$\widetilde{\mathcal{D}}_1(tf + (1-t)g) - t\widetilde{\mathcal{D}}_1(f) - (1-t)\widetilde{\mathcal{D}}_1(g) = -t(1-t)\widetilde{\mathcal{D}}_1(f-g).$$

If  $f - g =: h$  is positive pointwise, then  $\widetilde{\mathcal{D}}_1(f-g) = \widetilde{\mathcal{D}}_1(h) < 0$ .

We define a **regularized** version of the Hartree term,

$$\mathcal{D}_1(f) := 4\pi \int_{\mathbb{R}} \frac{|\widehat{f}(k)|^2}{k^2} dk = 4\pi \int_{\mathbb{R}} |W_f|^2(x) dx, \quad \text{with } W_f(x) := \int_{-\infty}^x f(y) dy.$$

This is well-defined whenever  $W_f \in L^2(\mathbb{R})$ . In particular,  $W(\infty) = \int_{\mathbb{R}} f = 0$  (**neutral system only**).

## Lemma

- The map  $f \mapsto \mathcal{D}_1(f)$  is strictly convex on  $\mathcal{C} := \{f \in L^1(\mathbb{R}), W_f \in L^2(\mathbb{R})\}$ .
- If  $f \in \mathcal{C}$  satisfies  $|x|f(x) \in L^1(\mathbb{R})$ , then  $\mathcal{D}_1(f) = \widetilde{\mathcal{D}}_1(f)$ .
- If  $f \in \mathcal{C}$ , then  $\mathcal{D}_1(f) = 4\pi \iint_{(\mathbb{R}_+)^2 \cup (\mathbb{R}_-)^2} \min\{|x|, |y|\} f(x)f(y) dx dy = \int_{\mathbb{R}} f(x)\Phi_f(x) dx$ .

**Idea of the proof.**  $|x| + |y| - |x - y| = \begin{cases} 2 \min\{|x|, |y|\} & \text{on } (\mathbb{R}_+)^2 \cup (\mathbb{R}_-)^2 \\ 0 & \text{else.} \end{cases}$

# Kohn-Sham models (reduced Hartree-Fock)

**One-body density matrix:**  $\gamma \in \mathcal{S}(L^2(\mathbb{R}^3))$  satisfying the Pauli principle  $0 \leq \gamma \leq 1$ .

For *homogeneous* 2d materials, we request that  $\gamma$  commutes with all  $\mathbb{R}^2$  translations:

$$\forall \mathbf{R} \in \mathbb{R}^2 \subset \mathbb{R}^3, \quad \tau_{\mathbf{R}}\gamma = \gamma\tau_{\mathbf{R}}, \quad \text{with} \quad \tau_{\mathbf{R}}f(\mathbf{x}, x_3) := f(\mathbf{x} - \mathbf{R}, x_3).$$

Equivalently,  $\gamma(\mathbf{x}, x_3; \mathbf{y}, y_3) = \gamma(\mathbf{x} - \mathbf{y}, x_3; \mathbf{0}, y_3) =: \gamma(\mathbf{x} - \mathbf{y}, x_3, y_3)$ .

For such one-body density matrix, the **density**  $\rho_\gamma(\mathbf{x}, x_3) := \gamma(\mathbf{x}, x_3; \mathbf{x}, x_3)$  satisfies

$$\rho_\gamma(\mathbf{x}, x_3) = \rho_\gamma(x_3).$$

**Trace per unit surface.** Set  $\Gamma := [0, 1]^2 \times \mathbb{R} \subset \mathbb{R}^3$  (tube),

$$\underline{\text{Tr}}(\gamma) := \text{Tr}_3(\mathbf{1}_\Gamma \gamma \mathbf{1}_\Gamma) = \int_{\mathbb{R}} \rho_\gamma(x_3) dx_3.$$

**reduced Hartree-Fock energy per unit surface**

$$\mathcal{E}_3^{\text{rHF}}(\gamma) := \frac{1}{2} \underline{\text{Tr}}(-\Delta_3 \gamma) + \frac{1}{2} \mathcal{D}_1(\rho_\gamma - \mu).$$

**Remark:** This energy still depends on the three-dimensional object  $\gamma \in \mathcal{S}(L^2(\mathbb{R}^3))$ .

**Can we find a *reduced one-dimensional model*?**

**Minimization set** =  $\mathcal{P} \cap \{\gamma, \text{Tr}(\gamma) = Z\}$  (**neutrality condition**) with

$$\mathcal{P} := \{\gamma \in \mathcal{S}(L^2(\mathbb{R}^3)), \quad 0 \leq \gamma \leq 1, \quad \forall \mathbf{R} \in \mathbb{R}^2, \tau_{\mathbf{R}}\gamma = \gamma\tau_{\mathbf{R}}\}.$$

### Theorem (DG, Lahbabi, Maichine, 2021)

Introduce  $\mathcal{G} := \{G \in \mathcal{S}(L^2(\mathbb{R})), \quad G \geq 0, \quad \text{Tr}_1(G) < \infty\}$ . Then, for any (representable) density  $\rho$ ,

$$\inf \left\{ \frac{1}{2} \text{Tr}(-\Delta_3 \gamma), \quad \gamma \in \mathcal{P}, \quad \rho_\gamma = \rho \right\} = \inf \left\{ \frac{1}{2} \text{Tr}_1(-\Delta_1 G) + \pi \text{Tr}(G^2), \quad G \in \mathcal{G}, \quad \rho_G = \rho \right\}.$$

#### Remarks:

- Works for general Kohn-Sham models (assuming *no «in-plane» symmetry breaking*).
- The new minimization problem is set on operators acting on  $L^2(\mathbb{R}^1)$ .
- **There is no Pauli principle for  $G$** . It is replaced by a penalization term  $+\pi \text{Tr}(G^2)$  in the energy.
- The term  $\text{Tr}(G^2)$  is sometime called the **Tsallis** or **Rényi** entropy.

#### Constrained-search

$$\begin{aligned} \inf_{\gamma} \{ \mathcal{E}_3^{\text{rHF}}(\gamma) \} &= \inf_{\rho} \left\{ \frac{1}{2} \mathcal{D}_1(\rho - \mu) + \inf_{\gamma \rightarrow \rho} \left\{ \frac{1}{2} \text{Tr}(-\Delta_3 \gamma) \right\} \right\} \\ &= \inf_{\rho} \left\{ \frac{1}{2} \mathcal{D}_1(\rho - \mu) + \inf_{G \rightarrow \rho} \left\{ \frac{1}{2} \text{Tr}_1(-\Delta_1 G) + \pi \text{Tr}_1(G^2) \right\} \right\} = \inf_G \mathcal{E}_1^{\text{rHF}}(G) \end{aligned}$$

with the **reduced rHF model**

$$\mathcal{E}_1^{\text{rHF}}(G) := \frac{1}{2} \text{Tr}_1(-\Delta_1 G) + \pi \text{Tr}_1(G^2) + \frac{1}{2} \mathcal{D}_1(\rho_G - \mu).$$

### Proof of the theorem

Consider  $\mathcal{F} : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$  the partial Fourier transform

$$(\mathcal{F}f)(\mathbf{k}, x_3) = \frac{1}{(2\pi)} \int_{\mathbb{R}^2} e^{i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}, x_3) d\mathbf{x}.$$

**Bloch theory.** Since  $\gamma \in \mathcal{P}$  commutes with  $\mathbb{R}^2$ -translations, there is  $\{\gamma_{\mathbf{k}}\}_{\mathbf{k} \in \mathbb{R}^2}$  with  $\gamma_{\mathbf{k}} \in \mathcal{S}(L^2(\mathbb{R}))$  so that

$$\boxed{\mathcal{F}\gamma\mathcal{F}^{-1} = \int_{\mathbb{R}^2}^{\oplus} \gamma_{\mathbf{k}} d\mathbf{k}}, \quad \text{in the sense} \quad (\mathcal{F}\gamma f)(\mathbf{k}, \cdot) = \gamma_{\mathbf{k}} [(\mathcal{F}f)(\mathbf{k}, \cdot)].$$

We have

$$0 \leq \gamma_{\mathbf{k}} \leq 1, \quad \rho_{\gamma} = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \rho_{\gamma_{\mathbf{k}}} \quad \text{and} \quad \underline{\text{Tr}}(\gamma) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_1(\gamma_{\mathbf{k}}).$$

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Now, we set

$$\boxed{G := \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \gamma_{\mathbf{k}} d\mathbf{k}}, \quad \text{in the sense} \quad Gf = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} (\gamma_{\mathbf{k}} f) d\mathbf{k}.$$

We have

$$G \geq 0, \quad \rho_G = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \rho_{\gamma_{\mathbf{k}}} = \rho_{\gamma}, \quad \text{Tr}_1(G) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \text{Tr}_1(\gamma_{\mathbf{k}}) = \underline{\text{Tr}}(\gamma).$$

## Kinetic energy

Since  $\mathcal{F}(-\Delta_3)\mathcal{F}^{-1} = |\mathbf{k}|^2 + (-\Delta_1)$ ,

$$\begin{aligned}\underline{\text{Tr}}(-\Delta_3\gamma) &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} (|\mathbf{k}|^2 \text{Tr}(\gamma_{\mathbf{k}}) + \text{Tr}_1(-\Delta_1\gamma_{\mathbf{k}})) d\mathbf{k} \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} |\mathbf{k}|^2 \text{Tr}(\gamma_{\mathbf{k}}) d\mathbf{k} + \text{Tr}_1(-\Delta_1 G).\end{aligned}$$

Write  $G = \sum g_j |\phi_j\rangle\langle\phi_j|$ , with  $g_j \geq 0$  and  $\sum g_j = \text{Tr}_1(G)$ , and define

$$\boxed{m_j(\mathbf{k}) := \langle\phi_j, \gamma_{\mathbf{k}}\phi_j\rangle}, \quad \text{so that } 0 \leq m_j(\mathbf{k}) \leq 1 \quad \text{and} \quad \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} m_j(\mathbf{k}) d\mathbf{k} = g_j.$$

Then

$$\begin{aligned}\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} |\mathbf{k}|^2 \text{Tr}(\gamma_{\mathbf{k}}) d\mathbf{k} &= \frac{1}{(2\pi)^2} \sum_j \int_{\mathbb{R}^2} |\mathbf{k}|^2 m_j(\mathbf{k}) d\mathbf{k} \\ &\geq \frac{1}{(2\pi)^2} \sum_j \min \left\{ \int_{\mathbb{R}^2} |\mathbf{k}|^2 m(\mathbf{k}) d\mathbf{k}, 0 \leq m(\mathbf{k}) \leq 1, \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} m(\mathbf{k}) d\mathbf{k} = g_j \right\}.\end{aligned}$$

«Bathtub principle»: the minimum is obtained for  $m_j^*(\mathbf{k}) = \mathbb{1}(|\mathbf{k}| < k_j)$  with  $k_j = 2\sqrt{\pi g_j}$ .

This proves

$$\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} |\mathbf{k}|^2 \text{Tr}(\gamma_{\mathbf{k}}) d\mathbf{k} \geq 2\pi \sum_j g_j^2 = 2\pi \text{Tr}_1(G^2).$$

Conversely, given  $G = \sum_j g_j |\phi_j\rangle\langle\phi_j|$ , we have equality for  $\gamma^*$  defined by

$$\gamma^* := \int_{\mathbb{R}^2}^{\oplus} \gamma_{\mathbf{k}}^*, \quad \text{with } \gamma_{\mathbf{k}}^* := \sum_j m_j^*(\mathbf{k}) |\phi_j\rangle\langle\phi_j|. \quad \square$$

We now study the one-dimensional minimization problem

$$\inf \left\{ \frac{1}{2} \text{Tr}_1(-\Delta G) + \pi \text{Tr}_1(G^2) + \frac{1}{2} \mathcal{D}_1(\rho_G - \mu), \quad G \in \mathcal{S}(L^2(\mathbb{R})), G \geq 0, \text{Tr}_1(G) = Z \right\}.$$

## Proposition

There is a unique minimizer  $G_*$ . This minimizer satisfies the Euler-Lagrange equations

$$\begin{cases} G_* = \frac{1}{2\pi}(\lambda - H_*)_+ \\ H_* := -\frac{1}{2}\Delta + \Phi_* \\ -\Phi_*'' = 4\pi(\rho_* - \mu), \quad \Phi_*'(\pm\infty) = 0, \quad \Phi_*(0) = 0. \end{cases}$$

## Remarks

- The problem is **strictly** convex in  $G$ , due to the  $\text{Tr}_1(G^2)$  term (hence uniqueness of the minimizer).
- We have  $G_* = \frac{1}{2\pi}(\lambda - H_*)_+$  instead of the usual  $\gamma_* = \mathbb{1}(\lambda - H_* > 0)$ .
- In particular, since  $\lambda \mapsto \text{Tr}(\lambda - H_*)_+$  is **strictly** increasing, the Fermi level is unique.

## Proposition

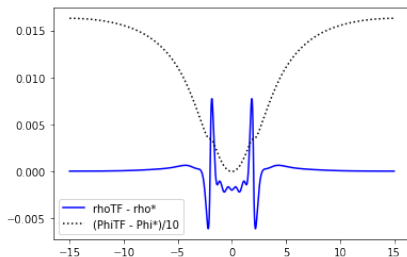
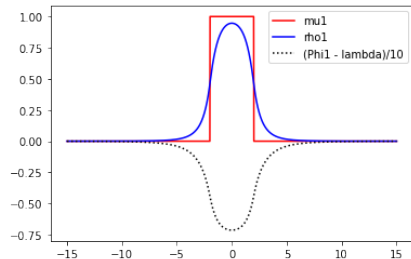
Assume  $|x|^3 \mu(x) \in L^1(\mathbb{R})$ . Then, if  $|x|^3 \rho(x) \in L^1(\mathbb{R})$  as well,  $G_*$  is finite rank, and its density  $\rho_*$  is exponentially decaying away from the slab.

# Numerical illustrations



## Numerical results 1

$$\mu_1(x) = \mathbb{1}(|x| < 2)$$

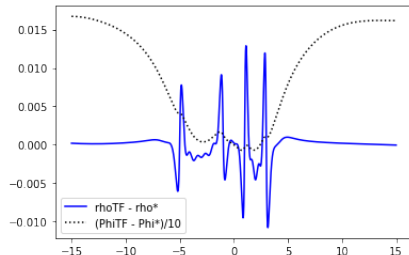
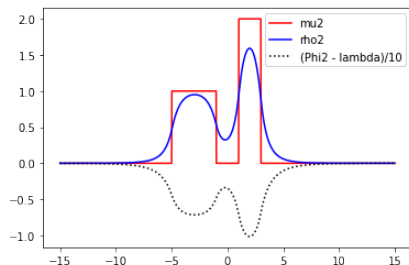


### Remarks

- The Thomas-Fermi density  $\rho_{TF}$  and rHF density  $\rho_*$  are **very** close!
- The optimal  $G_*$  has 15 positive eigenvalues. The largest one is around 1.07.

## Numerical results 2 (with dipolar moment)

$$\mu_2(x) = \mathbb{1}(-5 < x < -2) + 2 \cdot \mathbb{1}(1 < x < 3)$$

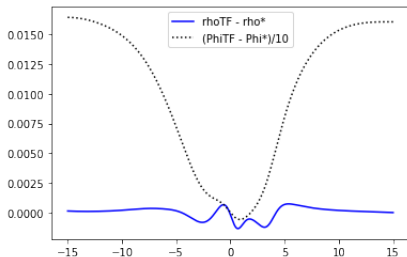
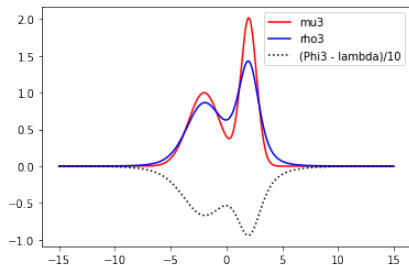


### Remarks

- The Thomas-Fermi density  $\rho_{TF}$  and rHF density  $\rho_*$  are **very** close!
- The optimal  $G_*$  has 17 positive eigenvalues. The largest one is around 1.44.
- The *screening* in the rHF model is close to perfect!

## Numerical results 3 (smooth case)

$$\mu_3(x) = e^{-\frac{1}{4}(x+2)^2} + 2 \cdot e^{-(x-2)^2}.$$

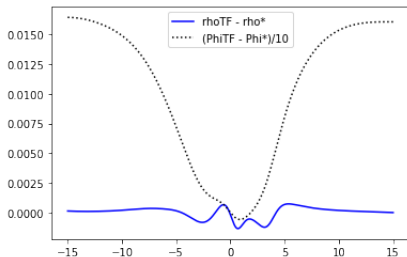
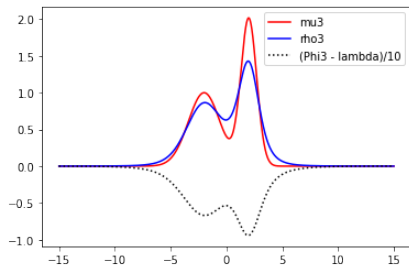


### Remarks

- The Thomas-Fermi density  $\rho_{TF}$  and rHF density  $\rho_*$  are **extremely** close!
- The optimal  $G_*$  has 19 positive eigenvalues. The largest one is around 1.32.
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**Thank you for your attention**

# A Lieb-Thirring type inequality

### General dimension

Let  $\gamma \in \mathcal{S}(L^2(\mathbb{R}^{s+d}))$  be translationally invariant in its first  $s$  variables, and so that  $0 \leq \gamma \leq 1$ . Then there is  $G \in \mathcal{S}(L^2(\mathbb{R}^d))$  so that  $\rho_\gamma = \rho_G$  and

$$\underline{\text{Tr}}(-\Delta_{s+d}\gamma) \geq \text{Tr}_d(-\Delta_d G) + 2c_{\text{TF}}(s)\text{Tr}_d(G^{1+\frac{2}{s}}).$$

Conversely, for each  $G$ , there is a  $\gamma$  such that we have equality.

If there is equality, the «Lieb-Thirring» inequality for  $\gamma$  gives

$$\text{Tr}_d(-\Delta_d G) + 2c_{\text{TF}}(s)\text{Tr}_d(G^{1+\frac{2}{s}}) = \underline{\text{Tr}}(-\Delta_{s+d}\gamma) \geq K_{\text{LT}}(d+s) \int_{\mathbb{R}^d} \rho_G^{1+\frac{2}{d+s}}.$$

After optimization over scaling  $\lambda \mapsto \lambda G$ , we obtain

### Theorem (Lieb-Thirring type inequality)

There is a constant  $K$  so that, for all  $G \in \mathcal{S}(L^2(\mathbb{R}^d))$  with  $G \geq 0$ , and for all  $s \in \mathbb{N}$ ,

$$K \left( \int_{\mathbb{R}^d} \rho_G^{1+\frac{2}{s+d}} \right)^{1+\frac{s}{d}} \leq \left( \text{Tr}_d(G^{1+\frac{s}{d}}) \right)^{s/d} \text{Tr}_d(-\Delta_d G).$$

This type of inequalities was recently studied in [Frank/Gontier/Lewin, Commun. Math. Phys. 384 (2021)].

### Theorem (Frank, DG, Lewin, 2021)

For all  $d \geq 1$  and all  $1 \leq p \leq 1 + \frac{2}{d}$ , there is an optimal constant  $K_{p,d}$  so that, for all  $G \in \mathcal{S}(L^2(\mathbb{R}^d))$ ,

$$K_{p,d} \left( \int_{\mathbb{R}^d} \rho_G^p \right)^{\theta_1} \leq (\text{Tr}_d(G^q))^{\theta_2} \text{Tr}_d(-\Delta_d G), \quad \text{where } q := \frac{2p + d - dp}{2 + d - dp}.$$

In addition,  $K_{p,d}$  is the **dual constant** of the usual Lieb-Thirring constant  $L_{\gamma,d}$ , in the sense

$$K_{p,d} (L_{\gamma,d})^{\frac{2}{d}} = \left( \frac{\gamma}{\gamma + \frac{d}{2}} \right)^{\frac{2\gamma}{d}} \left( \frac{d}{2\gamma + d} \right), \quad \text{with } \gamma + \frac{d}{2} = \frac{p}{p-1}, \quad \text{so that } \frac{\gamma}{\gamma-1} = q.$$

The previous case corresponds to  $p = 1 + \frac{2}{d+s}$ , which gives  $\gamma = 1 + \frac{s}{2}$ .

In particular,  $\gamma \geq \frac{3}{2}$ : the best constant is the **semi-classical** one.

In other words, for all  $d \in \mathbb{N}$  and  $s \in \mathbb{N}$ ,

$$\frac{1}{2} \text{Tr}_d(-\Delta_d G) + c_{\text{TF}}(s) \text{Tr}_d(G^{1+\frac{2}{s}}) \geq c_{\text{TF}}(d+s) \int_{\mathbb{R}^d} \rho_G^{1+\frac{2}{d+s}}.$$

**The reduced rHF energy is greater than the reduced Thomas–Fermi one.**