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23. Levy-Lieb density functional

22.2. Scaling properties of TF

Let $K=1$, $Z=N$. Denote $\rho_Z(x) = \frac{Z^2}{\gamma^3}\bar\rho(Z^{1/3}x/\gamma)$ and plug this into the TF functional. Then we get $\int \rho_Z = Z$, $Z=N$

$$\int \rho_Z(x)^{5/3} + \int \frac{Z}{|x|}\rho_Z(x) + \frac{1}{2}\iint \frac{\rho_Z(x)\rho_Z(y)}{|x-y|}\,dx\,dy =$$

$$= \int \left(\frac{Z^2}{\gamma^3}\right)^{5/3} \bar\rho^{5/3}(Z^{1/3}x/\gamma)\,dx + \int \frac{Z}{|x|}\frac{Z^2}{\gamma^3}\bar\rho(Z^{1/3}x/\gamma)\,dx$$

$$+ \frac{1}{2}\iint \frac{Z^4}{\gamma^6}\frac{\bar\rho(Z^{1/3}x/\gamma)\,\bar\rho(Z^{1/3}y/\gamma)}{|x-y|}\,dx\,dy =$$

$$= \iint \quad \frac{Z^{1/3}x}{\gamma} = \tilde{x}, \quad dx = \frac{\gamma^3}{Z}\,d\tilde{x} \quad \iint = Z^{7/3}\gamma^{-2}\int \tilde\rho^{5/3}(\tilde{x})\,d\tilde{x} +$$

$$+ \int \frac{Z^{4/3}}{\gamma|\tilde{x}|}\frac{Z^2}{\gamma^3}\cdot\frac{\gamma^3}{Z}\tilde\rho(\tilde{x})\,d\tilde{x} + \frac{1}{2}\frac{Z^4}{\gamma^6}\frac{\gamma^6}{Z^2}\iint d\tilde{x}\,d\tilde{y}\,\frac{Z^{1/3}}{\gamma}\frac{\tilde\rho(\tilde x)\tilde\rho(\tilde y)}{|\tilde{x}-\tilde{y}|}$$

$$= \frac{Z^{7/3}}{\gamma}\left[\frac{1}{\gamma}\int\tilde\rho^{5/3} + \int\frac{\tilde\rho}{|\tilde{x}|} + \frac{1}{2}\iint d\tilde{x}\,d\tilde{y}\,\frac{\tilde\rho(x)\tilde\rho(y)}{|\tilde{x}-\tilde{y}|}\right].$$

Setting $\gamma = C_{TF}$ we get

$$E_Z^{TF} = \left(\frac{e_0}{C_{TF}}\right) Z^{7/3} \qquad e_0$$

22.3 Scaling of H_N

Since we want to discuss the validity of TF approximation, in order to make connection to the many-body problem we need to rescale the Hamiltonian. The scaling of the TF functional suggest that the TF density lives on the scale $Z^{-1/3}$. Let us rescale H_N accordingly. We get:

$$H_N = \sum_{i=1}^{N}\left(-\Delta_{x_i} + \frac{Z}{|x_i|}\right) + \sum_{i<j} \frac{1}{|x_i - x_j|} = \left\{\left\{ y_i = Z^{1/3} x_i \right\}\right\} =$$

$$= \sum_{i=1}^{N}\left(Z^{2/3} - \Delta_{y_i} + \frac{Z^{4/3}}{|y_i|}\right) + \sum_{i<j} \frac{Z^{1/3}}{|y_i - y_j|} =$$

$$= Z^{4/3}\underbrace{\left[\sum_{i=1}^{N}\left(Z^{-2/3} - \Delta_{y_i} + \frac{1}{|y_i|}\right) + \frac{1}{Z}\sum_{i<j}\frac{1}{|y_i - y_j|}\right]}$$

$$\rightsquigarrow Z = N \Rightarrow \sum_{i=1}^{N}\left(N^{-2/3} - \Delta_{y_i} + \frac{1}{|y_i|}\right) + \frac{1}{N}\sum_{i<j}\frac{1}{|y_i - y_j|}$$

Note that in this scaling all terms are of order N! Indeed

kinetic: $\sum_{i=1}^{N} -\Delta_i \sim \rho^{5/3} \sim N^{5/3} \Rightarrow N^{-2/3}\sum -\Delta_i \sim N$

interaction: $\frac{1}{N}\sum_{i<j} \sim \frac{1}{N} \cdot \frac{N(N-1)}{2} \sim N$

Semiclassical ($h = N^{-1/3}$ in front of $-\Delta$) mean-field ($\lambda \sim \frac{1}{N}$) regime?

23. Levy-Lieb density functional

Recall the representability theorem (without proof) which stated that if $0 \le \rho \in L^1(\mathbb{R}^d)$, $\int \rho = N$, then there exists a normalized wave function $\psi_N \in L^2_a(\mathbb{R}^{dN})$ such that $\rho_{\psi_N} = \rho$. One can choose ψ_N to be a Slater determinant.

Because of that we can write

$$E_N = \inf_{\|\psi_N\|_{L^2_a}=1} \langle \psi_N, H_N \psi_N \rangle = \inf_{\substack{\rho \ge 0 \\ \int \rho = N}} \inf_{\substack{\|\psi_N\|_2 = 1 \\ \rho_{\psi_N} = \rho}} \langle \psi_N, H_N \psi_N \rangle$$

This motivates the definition of the Levy-Lieb density functional:

$$\boxed{\mathcal{L}_N(\rho) = \inf_{\substack{\|\psi_N\|_{L^2_a}=1 \\ \rho_{\psi_N} = \rho}} \langle \psi_N, H_N \psi_N \rangle \quad \forall \rho \ge 0 : \int \rho = N}$$

The discussion in the previous section suggests that for

$$H_N = \sum_{i=1}^{N} \left(-h^2 \Delta_{x_i} + v(x_i) \right) + \lambda \sum_{i<j} w(x_i - x_j)$$

we have

$$\mathcal{E}_N(\rho) \sim K_{cl}\, h^2 \int_{\mathbb{R}^3} \rho^{1+\frac{2}{3}} + \int_{\mathbb{R}^3} V\rho + \frac{1}{2} \iint \rho(x)\, \rho(y)\, w(x-y)$$

As we will show, the Thomas–Fermi approximation is correct to leading order for

$$h \sim N^{-1/3}, \quad \lambda \sim \frac{1}{N}, \quad N \to \infty.$$

23.1 Convergence of the kinetic density functional

Let us introduce $f_{\Psi_N} = \dfrac{\rho_{\Psi_N}}{N}$, $f \geq 0$, $\int f = 1$.

$$K_d^{cl} = \frac{d}{d+2} \frac{(2\pi)^2}{|B_{\mathbb{R}^d}(0,1)|^{2/d}} = \frac{d}{d+2} \frac{(2\pi)^2}{\pi} \Gamma\left(1+\frac{d}{2}\right)^{2/d}$$

Thm

•) If the normalized wave functions $\Psi_N \in L^2_a(\mathbb{R}^{dN})$ satisfy $f_{\Psi_N} \to f$ weakly in $L^{1+\frac{2}{d}}(\mathbb{R}^d)$, then

$$\liminf_{N\to\infty} \frac{1}{N^{1+2/d}} \langle \Psi_N, \sum_{i=1}^N -\Delta_i \Psi_N \rangle \geq K_d^{cl} \int_{\mathbb{R}^d} f^{1+2/d}$$

•) For every $0 \leq f \in L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$, $\int f = 1$

there exist Slater determinants $\Psi_N \in L^2_a(\mathbb{R}^{dN})$ such that $f_{\Psi_N} \to f$ strongly in $L^1(\mathbb{R}^d) \cap L^{1+2/d}(\mathbb{R}^d)$ and

$$\limsup_{N\to\infty} \frac{1}{N^{1+2/d}} \langle \Psi_N, \sum -\Delta_i \Psi_N \rangle \leq K_d^{cl} \int f^{1+2/d}$$

Proof (sketch)

Lower bound: for every $0 \le U$ we can write

$$\frac{1}{N^{1+2/d}} \langle \psi_N, \sum -\Delta_i \psi_N \rangle = \frac{1}{N^{1+2/d}} \operatorname{Tr}\left[(-\Delta - N^{2/d} U)\gamma_{\psi_N}^{(1)}\right] + \int U f_{\psi_N}$$

By Pauli's exclusion principle $0 \le \gamma_{\psi_N}^{(1)} \le 1$ and Weyl's law on the sum of negative eigenvalues

$$\operatorname{Tr}\left((-\Delta - N^{2/d} U)\gamma_{\psi_N}^{(1)}\right) \ge \operatorname{Tr}\left[-\Delta - N^{2/d} U\right]_- =$$

$$= -L_{1,d}^{cl} \int_{\mathbb{R}^d} |N^{2/d} U|^{1+\frac{d}{2}} + o\left((N^{2/d})^{1+\frac{d}{2}}\right)$$

Weyl's law $\operatorname{Tr}|(-\Delta + \lambda V)_-| = L_{1,d}^{cl} \int |\lambda V_-|^{1+\frac{d}{2}} + o(\lambda^{1+\frac{d}{2}})$ as $\lambda \to \infty$

gives the asymptotics with equality and error term whereas LT inequality gives inequality (but with the constant ?).

$$= N^{1+2/d}\left(-L_{1,d}^{d} \int U^{1+\frac{d}{2}} + o(1)_{N\to\infty}\right)$$

Moreover, using $f_{\psi_N} \to f$ in $L^{1+2/d}(\mathbb{R}^d)$ we find that

$$\int U f_{\psi_N} \to \int U f.$$

$$L_{1,d}^{d} = \frac{1}{(4\pi)^{d/2}\,\Gamma(2+\frac{d}{2})}$$

Thus

$$\liminf_{N\to\infty} \frac{1}{N^{1+2/d}} \langle \psi_N, \sum -\Delta_i \psi_N \rangle \ge -L_{1,d}^{cl} \int_{\mathbb{R}^d} U^{1+\frac{d}{2}} + \int U f.$$

Choosing $U = \text{const.} f^{2/d}$ we conclude

$$\ge \left(-L_{1,d}^{cl} c^{1+\frac{d}{2}} + c\right) \int f^{1+\frac{2}{d}}$$

Problem: can K_d be reached there? (I am not sure)

Upper bound

We see from the lower bound that one could expect it is good to use Weyl's Law. But the proof of Weyl's law makes it difficult to satisfy the Slater determinant condition. Hence, more direct approach:

Step 1. (Slaters on cubes)

Consider the Dirichlet Laplacian $-\Delta$ on $Q = [0,L]^d$. Its eigenvalues $\left|\frac{\pi k}{L}\right|^2$, $k \in \mathbb{N}^d$ with eigenfct's

$$u_k(x) = \prod_{i=1}^{d} \sqrt{\frac{2}{L}} \sin\left(\frac{\pi k^i x^i}{L}\right).$$

Ground state of $\sum_{j=1}^{N} (-\Delta_{x_j})$ is the Slater determinant φ_N^S. Then

$$\frac{1}{N^{1+2/d}} \langle \varphi_N^S, \sum_{j=1}^{N} (-\Delta_{x_j}) \varphi_N^S \rangle = \frac{1}{N^{1+2/d}} \sum_{k \in S_N} \left|\frac{\pi k}{L}\right|^2 \longrightarrow \frac{K_d^d}{|Q|^{2/d}}$$

and

$$\rho_{\varphi_N^S} = \frac{1}{N} \sum_{\substack{\text{first } N \\ \text{eigenfct}}} |u_k|^2 \longrightarrow \frac{1_Q}{|Q|} \quad \text{in } L^p(Q)$$

Step 2.

Let $f \geq 0$, $\int f = 1$, $f \in L^1 \cap L^{1+2/d}$, $\{Q\}$ family of disjoint cubes (see later for precise conditions).

Consider cubes s.t. $\displaystyle\int_Q f > 0$.

We can find $M_Q \in \left(N \int_Q f - 1, N \int_Q f + 1\right)$

such that $\displaystyle\sum_Q M_Q = N \int f = N$.

For every Q, consider the first M_Q eigenfcts $\{u_j^Q\}_{j=1}^{M_Q}$ of the Dirichlet Laplacian $-\Delta$ on Q. We extend those fcts by 0 outside Q to become elements of $H_0^1(\mathbb{R}^d)$. Since the cubes are disjoint, the N functions $\displaystyle\bigcup_Q \{u_j^Q\}$ are orthonormal in $L^2(\mathbb{R}^d)$. Let φ_N^S be a Slater determinant made of those fcts. Then in the limit as $N \to \infty$, using

$$\frac{M_Q}{N} \to \int_Q f > 0$$

and the calculation in Step 1 for each cube, we get

$$\frac{1}{N^{1+2/d}} \left\langle \varphi_N^S, \sum^N -\Delta_{x_i} \varphi_N^S \right\rangle = \frac{1}{N^{1+2/d}} \sum_Q \sum_{i=1}^{M_Q} \| \nabla u_i^Q \|^2$$

$$= \sum_Q \left[\frac{1}{M_Q^{1+2/d}} \sum_{i=1}^{M_Q} \| \nabla u_i^Q \|^2 \right] \left(\frac{M_Q}{N} \right)^{1+2/d} \longrightarrow \sum_Q \frac{K_d^{cl}}{|Q|^{2/d}} \left| \int_Q f \right|^{1+\frac{2}{d}}$$

$$= K_d^{cl} \sum_Q |Q| \left(\frac{1}{|Q|} \int_Q f \right)^{1+2/d} \leq K_d^{cl} \sum_Q \int_Q f^{1+2/d} \leq K_d^{cl} \int_{\mathbb{R}^d} f^{1+2/d}$$

and

$$f_{\varphi_N^S} = \frac{1}{N}\sum_Q \sum_{i=1}^{M_Q} |u_i^Q|^2 = \sum_Q \sum_{i=1}^{M_Q} \frac{|u_i^Q|^2}{M_Q} \cdot \frac{M_Q}{N} \underset{(*)}{\longrightarrow} \sum_Q \frac{1\!\!1_Q}{|Q|}\int_Q f$$

Step 3.

Since $f \in L^1 \cap L^{1+2/d}$, $\forall k \geq 1$ $\exists$ family of disjoint cubes $\{Q\}$ such that

$$\| f - \sum_Q 1\!\!1_Q \bar{f}^Q \|_{L^1} + \| f - \sum_Q 1\!\!1_Q \bar{f}^Q \|_{L^{1+2/d}} \leq k^{-1}$$

Here

$$\bar{f}^Q = \frac{1}{|Q|}\int_Q f .$$

Using this collection of cubes, for every $N \geq 1$ we can construct a Slater determinant φ_N^k as in the previous step. Thus there exists $N_k > 0$ such that for every $N \geq N_k$

$$\frac{1}{N^{1+2/d}} \langle \varphi_N^k , \sum_{i=1}^N -\Delta_{x_i} \varphi_N^k \rangle \leq K_d^{cl} \int_{\mathbb{R}^d} f^{1+2/d} + \frac{1}{k}$$

and, using (*),

$$\| f_{\varphi_N^k} - \sum_Q 1\!\!1_Q \bar{f}^Q \|_{L^1} + \| f_{\varphi_N^k} - \sum_Q 1\!\!1_Q \bar{f}^Q \|_{L^{1+2/d}} \leq k^{-1}$$

By triangle inequality, for $N > N_k$,

$$\| f_{\varphi_N^k} - f \|_{L^1} + \| f_{\varphi_N^k} - f \|_{L^{1+2/d}} \leq 2k^{-1}$$

To finish the proof one does a diagonal argument to pick $k = k_N \to \infty$, $N > N_{k_N}$ and sets

$$\psi_N = \psi_N^{k_N}$$

In particular

$$\frac{1}{N^{1+2/d}} \langle \psi_N, \sum_{i=1}^{N} -\Delta_{x_i} \psi_N \rangle \leq K_d^{\,cl} \int_{\mathbb{R}^d} f^{1+2/d} + k_N^{-1} \to K_d^{\,cl} \int_{\mathbb{R}^d} f^{1+\frac{2}{d}}$$

and

$$\| f_{\psi_N} - f \|_{L^1} + \| f_{\psi_N} - f \|_{L^{1+2/d}} \leq 2 k_N^{-1} \to 0 \qquad \square$$

Conjecture:

$$K_d^{\,cl} \int_{\mathbb{R}^d} \rho_{\psi_N}^{1+2/d} \leq \langle \psi_N, \sum_{i=1}^{N} -\Delta_{x_i} \psi_N \rangle \leq K_d^{\,cl} \int \rho_{\psi_N}^{1+2/d} + \int_{\mathbb{R}^d} | \nabla \sqrt{\rho_{\psi_N}} |^2$$

$$\iff K_d^{\,cl} \int_{\mathbb{R}^d} f_{\psi_N}^{1+2/d} \leq \frac{1}{N^{1+2/d}} \langle \psi_N, \sum_{i=1}^{N} (-\Delta_{x_i}) \psi_N \rangle \leq K_d^{\,cl} \int_{\mathbb{R}^d} f_{\psi_N}^{1+2/d} + N^{-2/d} \int_{\mathbb{R}^d} | \nabla \sqrt{f_{\psi_N}} |^2$$

where the lower bound holds for all $d \geq 3$ (Lieb-Thirring conjecture!) and upper bound $\forall d \geq 1$.

Upper bound has been proven in 1958 for $d = 1$ by March and Young, but does not extend to higher dimensions.