Stabilité en mécanique quantique

Jean DOLBEAULT

Ceremade, Université Paris Dauphine,
Place de Lattre de Tassigny,
75775 Paris Cédex 16, France

E-mail: dolbeaul@ceremade.dauphine.fr

http://www.ceremade.dauphine.fr/~dolbeaul/

A joint work in collaboration with
G. Rein, C. Cid, P. Felmer, E. Paturel and M. Loss
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Some issues on stability in quantum mechanics

I. Defocusing Nonlinear Schrödinger equation: confinement, stability and asymptotic stability - The "boson" case
[J.D., Rein], [Cid,J.D.]

II. Stability of mixed states and applications to molecular dynamics - The "fermion" case
[J.D., Felmer, Paturel, Rein]

III. Lieb-Thirring type inequalities
[J.D., Felmer, Loss, Paturel]

I. Defocusing Nonlinear Schrödinger equation: confinement, stability and asymptotic stability - The “boson” case

[Cid, J.D., Rein]

Nonlinear Schrödinger equation with confinement:

- Minimizers, Convexity
- Csiszár-Kullback type inequalities
- Nonlinear stability of NLS

Asymptotic stability and decay estimates (no confinement)

- Time-dependent rescalings
- Decay estimates
- Asymptotic nonlinear stability

Minimizers, Convexity

[Cid,J.D.] Let V be a nonnegative potential such that

$$\lim_{r\to+\infty} \operatorname{infess}_{|x|>r} V(x) = +\infty\ .$$

Assume that $p \in [1, \frac{d+2}{d-2})$ if $d \geq 3$ and $p \in [1, +\infty)$ if $d = 1$ or 2, and consider a minimizer ϕ_∞ of the functional

$$E[\phi] := \frac{A}{2} \int_{\mathbf{R}^d} |\nabla\phi|^2\, dx + \frac{B}{p+1} \int_{\mathbf{R}^d} |\phi|^{p+1}\, dx + \frac{1}{2} \int_{\mathbf{R}^d} V(x)|\phi|^2\, dx$$

with A, $B > 0$, under the constraint $\|\phi\|_{L^2(\mathbf{R}^d)} = 1$.
Euler-Lagrange equations:

$$-A\,\Delta\phi_\infty + B\,|\phi_\infty|^{p-1}\phi_\infty + V(x)\,\phi_\infty - \lambda\,\phi_\infty = 0 \qquad (1)$$

If V is radial and increasing, then the real positive solution ϕ_∞ has to be radial and strictly decreasing by [Gidas-Ni-Nirenberg79].

ϕ_∞ realizes the minimum of the functional

$$G[\phi] := F[\phi] - F[\phi_\infty] \ ,$$

where $F[\phi] := E[\phi] - \frac{\lambda}{2}\int_{\mathbf{R}^d} |\phi|^2 \ dx$. The functional G can be rewritten as

$$G[\phi] := F[\phi] - F[\phi_\infty] - DF[\phi_\infty] \cdot (\phi - \phi_\infty)$$

using the fact that $DF[\phi_\infty] = 0$.

$$\begin{aligned} G[\phi] = \ & \frac{A}{2}\int_{\mathbf{R}^d} |\nabla\phi - \nabla\phi_\infty|^2 \, dx \\ & + \frac{B}{p+1}\int_{\mathbf{R}^d} \Big(|\phi|^{p+1} - |\phi_\infty|^{p+1} - (p+1)|\phi_\infty|^{p-1}\phi_\infty \cdot (\phi - \phi_\infty) \Big) \, dx \\ & + \frac{1}{2}\int_{\mathbf{R}^d} V(x)|\phi - \phi_\infty|^2 \, dx - \frac{\lambda}{2}\int_{\mathbf{R}^d} |\phi - \phi_\infty|^2 \, dx \ . \end{aligned}$$

$\lambda < 0$: G is not a convex functional $\Longrightarrow$ introduce $\rho = |\phi|^2$, $\rho_\infty = |\phi_\infty|^2$, and $\mathfrak{F}[\rho] = F[\sqrt{\rho}]$

$$\mathcal{F}[\rho] = \frac{A}{2}\int_{\mathbf{R}^d} |\nabla\sqrt{\rho}|^2\,dx + \frac{B}{p+1}\int_{\mathbf{R}^d} \rho^{\frac{p+1}{2}}\,dx + \frac{1}{2}\int_{\mathbf{R}^d} V\rho\,dx - \frac{\lambda}{2}\int_{\mathbf{R}^d} \rho\,dx$$

[Benguria79,Benguria-Brezis-Lieb] With $\rho_t = t\rho_1 + (1-t)\rho_2$,

$$\frac{d^2}{dt^2}\int_{\mathbf{R}^d} \frac{|\nabla\rho_t|^2}{\rho_t}\,dx = \int_{\mathbf{R}^d} \frac{2}{\rho_t^3}\,|\rho_t\nabla(\rho_2-\rho_1) - (\rho_2-\rho_1)\nabla\rho_t|^2\,dx > 0\,.$$

$\mathcal{F}$ is strictly convex with a unique minimizer $\phi_\infty = \sqrt{\rho_\infty}$

$$-A\,\frac{\Delta(\sqrt{\rho_\infty})}{\sqrt{\rho_\infty}} + B\,\rho_\infty^{\frac{p-1}{2}} + V(x) - \lambda = 0\,. \qquad (2)$$

$$
\begin{aligned}
\mathcal{F}[\rho]-\mathcal{F}[\rho_\infty] &= \frac{A}{2}\int_{\mathbf{R}^d}\left(|\nabla\sqrt{\rho}|^2-|\nabla\sqrt{\rho_\infty}|^2\right)\,dx+\frac{B}{p+1}\int_{\mathbf{R}^d}\left(\rho^{\frac{p+1}{2}}-\rho_\infty^{\frac{p+1}{2}}\right)dx\\
&\qquad+\frac{1}{2}\int_{\mathbf{R}^d}(V-\lambda)(\rho-\rho_\infty)\,dx\\
&= \frac{A}{2}\int_{\mathbf{R}^d}\left(|\nabla\sqrt{\rho}|^2-|\nabla\sqrt{\rho_\infty}|^2\right)\,dx+\frac{B}{p+1}\int_{\mathbf{R}^d}\left(\rho^{\frac{p+1}{2}}-\rho_\infty^{\frac{p+1}{2}}\right)dx\\
&\qquad+\frac{1}{2}\int_{\mathbf{R}^d}\left(A\,\frac{\Delta\sqrt{\rho_\infty}}{\sqrt{\rho_\infty}}-B\,\rho_\infty{}^{\frac{p-1}{2}}\right)(\rho-\rho_\infty)\,dx\\
&= \frac{A}{2}\int_{\mathbf{R}^d}|\nabla\sqrt{\rho}-\sqrt{\frac{\rho}{\rho_\infty}}\,\nabla\sqrt{\rho_\infty}|^2\,dx\\
&\qquad+\frac{B}{p+1}\int_{\mathbf{R}^d}\left(\rho^{\frac{p+1}{2}}-\rho_\infty^{\frac{p+1}{2}}-\frac{p+1}{2}\rho_\infty^{\frac{p-1}{2}}(\rho-\rho_\infty)\right)dx\,.
\end{aligned}
$$

Theorem 1 *There exists a unique up to a constant phase factor (resp. unique) minimizer of* E *(resp.* $\mathcal{E}$*) under the constraint* $\|\phi\|_{L^2(\mathbf{R}^d)} = 1$ *(resp.* $\rho \geq 0$, $\|\rho\|_{L^1(\mathbf{R}^d)} = 1$*) that we shall denote by* ϕ_∞ *(resp.* ρ_∞*).*

Moreover, for any ϕ *such that* $\|\phi\|_{L^2(\mathbf{R}^d)} = 1$ *(resp. for any nonnegative* ρ *such that* $\|\rho\|_{L^1(\mathbf{R}^d)} = 1$*), provided* $\rho = |\phi|^2$*,*

$$E[\phi] - E[\phi_\infty] \geq \frac{A}{2}\int_{\mathbf{R}^d} \rho_\infty \left|\nabla\sqrt{\frac{\rho}{\rho_\infty}}\right|^2 dx + \frac{B}{p+1}\int_{\mathbf{R}^d}\left(\rho^{\frac{p+1}{2}} - \rho_\infty^{\frac{p+1}{2}} - \frac{p+1}{2}\rho_\infty^{\frac{p-1}{2}}(\rho - \rho_\infty)\right)dx$$

where equality holds for $\phi = \sqrt{\rho}$*.*

Limiting cases of Theorem 1

Case $A = 0$, $B > 0$: let ϕ_∞ and ρ_∞ be defined by

$$\phi_\infty(x) = \sqrt{\rho_\infty(x)} = \left[\frac{1}{B}(\lambda - V(x))_+\right]^{\frac{2}{p-1}},$$

Case $A > 0$, $B = 0$: let $\phi_\infty = \sqrt{\rho_\infty}$ be the first eigenfunction of the operator $(-A\,\Delta + V)$.

Csiszár-Kullback type inequalities

Consider a strictly convex function σ on $\mathbb{R}^+$, taking finite values on $(0,+\infty)$ and define on $L^1(\mathbb{R}^d)$ the functional

$$\Sigma[\rho] = \int_{\mathbb{R}^d} [\,\sigma(\rho) + V(\xi)\,\rho\,]\;dx - C$$

with C such that $\Sigma[\rho_\infty] = 0$.

Lemma 2 *[Caceres-Carrillo-J.D.] Assume that $d \geq 1$, $1 \leq p \leq 3$, $\max(1, 2/(4-p)) \leq s < 2$, and let $q = s(3-p)/(2-s)$. If $\kappa = \inf_{s>0} s^{-(p-3)/2}\sigma''(s) > 0$, then for any nonnegative function ρ in $L^1 \cap L^{(p+1)/2}(\mathbb{R}^d)$,*

$$\|\rho - \rho_\infty\|^2_{L^s(\mathbb{R}^d)} \leq \frac{1}{\kappa}\,\frac{2^{2(1+s)/s}}{p-1}\,K_q^{(3-p)/2}\,\Sigma[\rho]$$

where $K_q = \max\left\{\|\rho\|_{L^{q/2}(\mathbb{R}^d)}, \|\rho_\infty\|_{L^{q/2}(\mathbb{R}^d)}\right\}$.

Special case: $2s = q = p+1$.

Corollary 1 *With* $|\phi|^2 = \rho$, $|\phi_\infty|^2 = \rho_\infty$,

$$\frac{A}{2}\int_{\mathbb{R}^d}\left|\nabla\left(\sqrt{\tfrac{\rho}{\rho_\infty}}\right)\right|^2 \rho_\infty \, dx + \frac{C}{p+1}\|\rho - \rho_\infty\|^2_{L^{\frac{p+1}{2}}} \leq \mathcal{E}[\rho] - \mathcal{E}[\rho_\infty] \leq E[\phi] - E[\phi_\infty]$$

NONLINEAR STABILITY OF NLS

$$i\frac{\partial \phi}{\partial t} = -A\,\Delta\phi + B\,|\phi|^{p-1}\phi + V(x)\,\phi \qquad (3)$$

Existence: [Cazenave].

Corollary 2 *Consider a global in time solution of (3) with initial condition* $\phi_0 \in H^1(\mathbb{R}^d)$ *such that* $\sqrt{V}\,\phi_0 \in L^2(\mathbb{R}^d)$. *Then for any* $\epsilon > 0$, *there exists* $\delta > 0$ *such that*

$$E[\phi_0] - E[\phi_\infty] < \delta \quad \Longrightarrow \quad \|\,|\phi(\cdot,t)|^2 - |\phi_\infty|^2\|_{L^{\frac{p+1}{2}}(\mathbb{R}^d)} < \epsilon \quad \forall\, t > 0\,.$$

Asymptotic stability and decay estimates

Defocusing nonlinear Schrödinger equation (NLS)

$$i\,\psi_t = -\Delta\psi + |\psi|^{p-1}\psi \tag{4}$$

$p \in (1, p_*)$ with $p_* := 1 + 4/(d-2)$ if $d > 2$, $p_* := +\infty$ if $d = 1, 2$.
Define $p_c := 1 + 4/d < p_*$ as the critical exponent:
(i) *subcritical* case if $p \in (1, p_c)$,
(ii) *critical* case (or pseudo-conformal invariant case) if $p = p_c$,
(iii) *supercritical* case if $p \in (p_c, p_*)$.

$$\ddot{R}R = R^{-c_p-1} \quad \text{with } c_p = \min\left(\frac{d}{2}(p-1), 2\right), \quad R(0) = 1\,, \quad \dot{R}(0) = 0\,.$$

$$\psi(t,x) = R(t)^{-\frac{d}{2}} e^{\frac{i}{2}S(t)\,|x|^2} \phi\left(\tau(t), \frac{x}{R(t)}\right)$$

Time-dependent rescalings [J.D.,Rein]. Rescaled equation:

$$i\dot\tau\phi_\tau = -\frac{1}{R^2}\Delta\phi + R^{-\frac{d}{2}(p-1)}|\phi|^{p-1}\phi + \frac{R^2}{2}(\dot S + 2S^2)|\xi|^2\phi + i\left(\frac{\dot R}{R} - 2S\right)\left(\frac{d}{2}\,\phi + \xi\cdot\nabla\phi\right),$$

Choice: $S = \dot R/2R$,

$$\dot\tau = \frac{1}{2}\ddot R R = R^{-c_p} \quad \text{where } c_p = \min\left(\frac{d}{2}(p-1), 2\right).$$

Thus $c_p = d(p-1)/2$ if p is subcritical and $c_p = 2$ if p is critical or supercritical, and ϕ solves the equation

$$i\phi_\tau = -R^{c_p-2}\Delta\phi + R^{c_p-\frac{d}{2}(p-1)}|\phi|^{p-1}\phi + \frac{1}{2}|\xi|^2\,\phi\,. \qquad (5)$$

$$\lim_{t\to+\infty}\tau(t) = \tau_\infty > 0\,,$$

where $\tau_\infty = +\infty$ if $p \le 1 + 2/d$ and $\tau_\infty < +\infty$ if $p > 1 + 2/d$.

Energy functional:

$$E(\tau) = \frac{1}{2} R^{c_p - 2} \int_{\mathbf{R}^d} |\nabla\phi|^2 d\xi + \frac{1}{4} \int_{\mathbf{R}^d} |\xi|^2 |\phi|^2 d\xi + \frac{R^{c_p - \frac{d}{2}(p-1)}}{p+1} \int_{\mathbf{R}^d} |\phi|^{p+1} d\xi$$

$$E' = -\dot{R} R^{2c_p - 1} \left(\frac{2-c_p}{2R^2} \int_{\mathbf{R}^d} |\nabla\phi|^2 d\xi + \frac{d\,(p-1) - 2\,c_p}{2\,(p+1)\,R^{d\,(p-1)/2}} \int_{\mathbf{R}^d} |\phi|^{p+1} d\xi \right)$$

Case $p \geq p_c$:

$$R^2 \int_{\mathbf{R}^d} \left| \nabla\psi - \frac{i\dot{R}}{2R}\,\psi x \right|^2 \, dx = \frac{1}{2} \int_{\mathbf{R}^d} |\nabla\phi|^2 \, d\xi \leq E(\tau) \leq E(0) \, .$$

$$\int_{\mathbf{R}^d} |\nabla|\psi|\,|^2 \, dx = \int_{\mathbf{R}^d} \left| \nabla |e^{-\frac{i\dot{R}}{2R}|x|^2} \psi| \right|^2 \, dx \leq \int_{\mathbf{R}^d} \left| \nabla\psi - \frac{i\dot{R}}{2R}\, x\,\psi \right|^2 \, dx$$

Case $p \leq p_c$:

$$\frac{1}{p+1} R^{d(p+1)\left(\frac{1}{2}-\frac{1}{p+1}\right)} \int_{\mathbf{R}^d} |\psi|^{p+1} dx = \frac{1}{p+1} \int_{\mathbf{R}^d} |\phi|^{p+1} d\xi \leq E(0) \; ,$$

$$\frac{1}{2} R^{\frac{d}{2}(p-1)} \int_{\mathbf{R}^d} |\nabla \psi - \frac{i\dot{R}}{2R} x\, \psi|^2 \, dx = \frac{1}{2} R^{c_p - 2} \int_{\mathbf{R}^d} |\nabla \phi|^2 \, d\xi \leq E(0) \; .$$

Decay estimates

Theorem 3 *Assume that $p \in (1, p_*)$, $r \in [2, p_* + 1)$. Let ψ be a solution of (4) with an initial data $\psi_0 \in H^1(\mathbb{R}^d)$ such that $(1 + |\cdot|^2)^{1/2}\,\psi_0 \in L^2(\mathbb{R}^d)$. Then there exists a constant $C > 0$ such that*

$$\|\psi(t,\cdot)\|_{L^r(\mathbb{R}^d)} \leq C R(t)^{-d\left(\frac{1}{2}-\frac{1}{r}\right)(1-\epsilon)} \quad \forall\, t \geq 0\,,$$

where $\epsilon = 0$ if $p \in [p_c, p_*)$ or $r \in [2, p+1]$, and $\epsilon = \frac{(r-(p+1))(4-d(p-1))}{(r-2)(4-d(p-1)+2(p-1))}$ otherwise. Moreover C depends only on d, p, r and

$$E_0 := \frac{1}{2}\|\nabla\psi_0\|^2_{L^2} + \frac{1}{4}\|\,|x|\,\psi_0\|^2_{L^2} + \frac{1}{p+1}\|\psi_0\|^{p+1}_{L^{p+1}}\,.$$

Asymptotic nonlinear stability

Theorem 4

$$\| \, |\psi|^2 - |\psi_\infty|^2 \|^2_{L^{(p+1)/2}(\mathbb{R}^d)} \leq C \, \epsilon \, R(t+t_0)^{-2d(p-1)/(p+1)}$$

where $\psi_\infty(t,x) = \frac{1}{R(t)^{d/2}} \phi_\infty(\frac{x}{R(t)})$.

Other example: the logarithmic NLS [Cid,J.D.]

$$i\psi_t = -\Delta\psi + \log(|\psi|^2)\,\psi\,, \quad \psi_{|t=0} = \psi_0\,.$$

II. Stability of mixed states an applications to molecular dynamics - The "fermion" case

[J.D., Felmer, Paturel, Rein]

- One-particle linear Schrödinger equation: free energy and stability
- N-particles Schrödinger equation
- Stability for the Hartree-Fock model with temperature

An extension of the results of [Markowich-Rein-Wolansky]

One-particle linear Schrödinger equation

Consider the linear Schrödinger equation

$$i\partial_t \psi = -\Delta\psi + V\,\psi\,, \quad x \in \mathbb{R}^d\,,\ t > 0 \tag{1}$$

Let

$$E(\psi) := \int_{\mathbb{R}^d} \left(|\nabla\psi|^2 + V\,|\psi|^2\right) dx$$

Assume that V is a potential such that for any $i \in \mathbb{N}$,

$$\lambda_i := \inf_{\substack{(\psi_j)_{j=1}^i \in (L^2(\mathbb{R}^d))^i \\ (\psi_j,\psi_k)_{L^2} = \delta_{jk}}} \ \sup_{\substack{\psi \in \mathrm{Vect}(\psi_j)_{j=1}^i \\ \|\psi\|_{L^2}}} E(\psi)$$

is a nondecreasing sequence such that for any $i \in \mathbb{N}$, there exists a $j \in \mathbb{N}$ with $j > i$ such that $\lambda_j > \lambda_i$: *Assumption (H1)*

$(\lambda_i)_{i\in\mathbb{N}}$ is a sequence of eigenvalues counted with multiplicity. Let $(\psi_i)_{i\in\mathbb{N}}$ be the associated eigenstates:

$$(\psi_i, \psi_j)_{L^2(\mathbb{R}^d)} = \delta_{ij} \quad \forall\, i\,,\; j \in \mathbb{N}\;.$$

Free energy functional $\mathcal{F} : [0, +\infty)^{\mathbb{N}} \times (L^2(\mathbb{R}^d))^{\mathbb{N}} \ni\to \mathbb{R}$

$$\mathcal{F}(\nu, \psi) := \sum_{i\in\mathbb{N}} \left(\beta(\nu_i) + \nu_i\, E(\psi_i)\right)$$

Here β is a convex nonnegative and nondecreasing function such that $\lim_{\nu\to 0} \beta(\nu) = 0$ (at least when there is a confining potential): *Assumption (H2)*. Then $\lambda \mapsto (\beta')^{-1}(\lambda - \lambda_i)$ is an increasing function.

Assumption (H3) (on V and β): $\exists\lambda \in \mathbb{R}$ such that

$$\nu_i = (\beta')^{-1}(\lambda - \lambda_i)\;, \quad \sum_{i\in\mathbb{N}} \nu_i = 1\;, \quad \sum_{i\in\mathbb{N}} \beta(\nu_i) < \infty\;, \quad \sum_{i\in\mathbb{N}} \nu_i\, \lambda_i < \infty$$

$$\mathcal{F}(\nu,\psi) := \sum_{i=1}^{N} \left(\beta(\nu_i) + \nu_i\, E(\psi_i)\right)$$

$$E(\psi_i) := \int_{\mathbb{R}^d} \left(|\nabla\psi_i|^2 + V\,|\psi_i|^2\right) dx$$

Lemma 5 *There exists a minimizer* $(\bar\nu,\bar\psi) \in [0,+\infty)^{\mathbb{N}} \times (L^2(\mathbb{R}^d))^{\mathbb{N}}$ *of* $\mathcal{F}$ *under the constraints*

$$\sum_{i\in\mathbb{N}} \nu_i = 1 \quad \textit{and} \quad (\psi_i,\psi_j)_{L^2(\mathbb{R}^d)} = \delta_{ij} \quad \forall\, i\,,\; j \in \mathbb{N}\,.$$

$$\bar\nu_i = (\beta')^{-1}(\lambda - \lambda_i)$$

and the sequence $\bar\psi = (\bar\psi_i)_{i\in\mathbb{N}}$ *is unique up to any unitary transformation which leaves all eigenspaces of* $-\Delta + V$ *invariant.*

Lemma 6 *For any* $(\nu, \psi) \in [0, +\infty)^{\mathbb{N}} \times (L^2(\mathbb{R}^d))^{\mathbb{N}}$

$$\mathcal{F}(\nu, \psi) = \sum_{i \in \mathbb{N}} (\beta(\nu_i) - \beta(\bar{\nu}_i) - \beta'(\bar{\nu}_i)(\nu_i - \bar{\nu}_i)) + \sum_{i \in \mathbb{N}} \nu_i \, (E(\psi_i) - E(\bar{\psi}_i)) \, .$$

If $\psi = (\psi_i)_{i \in \mathbb{N}} \in (L^2(\mathbb{R}^d))^{\mathbb{N}}$ *satisfies the orthogonality conditions*

$$(\psi_i, \psi_j)_{L^2(\mathbb{R}^d)} = \delta_{ij} \quad \forall \, i \, , \; j \in \mathbb{N} \, .$$

and is ordered such that $(E(\psi_i))_{i \in \mathbb{N}}$ *is a nondecreasing sequence, then for any* $i \in \mathbb{N}$

$$E(\psi_i) - E(\bar{\psi}_i) = \int_{\mathbb{R}^d} (|\nabla \psi_i - \nabla \bar{\psi}_i|^2 + V \, |\psi_i - \bar{\psi}_i|^2 - \lambda_i \, |\psi_i - \bar{\psi}_i|^2) \, dx \quad (2)$$

is nonnegative.

For an orthogonal sequence $\psi = (\psi_i)_{i \in \mathbb{N}} \in (L^2(\mathbb{R}^d))^{\mathbb{N}}$, define

$$\mathsf{d}_i(\psi_i, \bar{\psi}_i) := E(\psi_i) - E(\bar{\psi}_i) \, .$$

$$\begin{aligned} \mathsf{d}((\nu,\psi),(\bar\nu,\bar\psi)) &= \mathcal{F}(\nu,\psi) - \mathcal{F}(\bar\nu,\bar\psi) \\ &= \sum_{i\in\mathbb{N}} \left(\beta(\nu_i) - \beta(\bar\nu_i) - \beta'(\bar\nu_i)(\nu_i - \bar\nu_i)\right) + \sum_{i\in\mathbb{N}} \nu_i \, \mathsf{d}_i(\psi_i,\bar\psi_i)\,. \end{aligned}$$

defines a "distance" on $(0,+\infty)^{\mathbb{N}} \times (L^2(\mathbb{R}^d))^{\mathbb{N}}/\mathcal{U}_V$ where $\mathcal{U}_V$ is the the group of unitary transformations that leave invariant all eigenspaces of $-\Delta + V$.

Theorem 7 *Let $(\nu,\psi^0) \in [0,+\infty)^{\mathbb{N}} \times (L^2(\mathbb{R}^d))^{\mathbb{N}}$ be such that*

$$\sum_{i\in\mathbb{N}} \nu_i = 1 \quad \textit{and} \quad \|\psi_i\|_{L^2} = 1 \quad \forall\, i \in \mathbb{N}$$

If $\psi_i(x,t)$ is the solution to Equation (1) with initial data ψ_i^0, then

$$d((\nu,\psi(\cdot,t)),(\bar\nu,\bar\psi)) = d((\nu,\psi^0),(\bar\nu,\bar\psi))\,.$$

N-PARTICLES SCHRÖDINGER EQUATION

Consider now an N-particles wave function $\psi(x_1, x_2, \dots, x_N; t)$ defined on $(\mathbb{R}^d)^N \times \mathbb{R}^+$ and evolving under the action of a Schrödinger operator:

$$i\partial_t \psi = -\sum_{i=1}^{N} \Delta_{x_i}\psi + V\,\psi\,, \quad x \in \mathbb{R}^d,\ t > 0 \tag{3}$$

Case of interest in molecular dynamics:

$$V(x_1, x_2, \dots, x_N) = \sum_{k=1}^{M} \frac{Z_k}{|x - \bar{x}_k|} + \sum_{i,j=1,\dots,N} \frac{1}{|x_i - x_j|}\,. \tag{4}$$

By Pauli's exclusion principle, the N-particles wave function is antisymmetric:the natural space is $\Lambda^N(\mathbb{R}^3)$, which is invariant under the evolution according to (3).

Stability for the Hartree-Fock model with temperature

Ansatz (zero-temperature Hartree-Fock model): replace $\Lambda^N(\mathbb{R}^3)$ by

$$X := \{\psi = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \mathcal{S}_N} \varepsilon(\sigma) \prod_{1 \le i,j \le N} \psi_i(x_{\sigma(j)}) \ : \ (\psi_i, \psi_j)_{L^2(\mathbf{R}^d)} = \delta_{ij}\}$$

$$\begin{aligned} E^{\mathrm{HF}}(\psi_1, \psi_2, \ldots, \psi_N) \ = \ & \sum_{1 \le i \le N} \int_{\mathbf{R}^3} |\nabla \psi_i|^2 \, dx \\ & + \sum_{1 \le i,j \le N} \int_{\mathbf{R}^3} (\frac{1}{2}|\psi_j|^2 * \frac{1}{|x|} - \sum_{k=1}^{M} \frac{Z_k}{|x - \bar{x}_k|}) \, |\psi_i|^2 \, dx \\ & - \frac{1}{2} \sum_{1 \le i,j \le N} \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \frac{\psi_i(x)\psi_i(y)\psi_j(x)\psi_j(y)}{|x - y|} \, dx \, dy \end{aligned}$$

Evolution equation:

$$i\partial_t\psi_i = -\Delta\psi_i - \sum_{k=1}^{M}\frac{Z_k}{|x-\bar{x}_k|}\,\psi_i \;+\; \frac{1}{2}\Big(\sum_{1\le j\le N}|\psi_j|^2\Big)*\frac{1}{|x|}\,\psi_i \qquad (5)$$

$$-\;\frac{1}{2}\sum_{1\le j\le N}\int_{\mathbb{R}^3}\frac{\psi_i(y)\psi_j(y)}{|x-y|}\,dy\,\psi_j(x)$$

Hartree-Fock model with temperature:

$$i\partial_t\psi_i = -\Delta\psi_i - \sum_{k=1}^{M}\frac{Z_k}{|x-\bar{x}_k|}\,\psi_i \;+\; \frac{1}{2}\rho(x)*\frac{1}{|x|}\,\psi_i \qquad (6)$$

$$-\;\frac{1}{2}\sum_{1\le j\le N}\int_{\mathbb{R}^3}\frac{\rho(x,y)\,\psi_i(y)}{|x-y|}\,dy$$

$$\rho(x,y) = \sum_{j\in\mathbb{N}}\nu_j\,\psi_j(x)\,\psi_j(y)\,, \qquad \rho(x) = \rho(x,x)$$

Free energy:

$$\mathcal{F}(\nu,\psi) := \sum_{i\in\mathbb{N}} \beta(\nu_i) + E_\nu^{\mathsf{HF}}(\psi)\ .$$

Lemma 8 *Under Assumption (H2),* $\mathcal{F}(\nu,\psi)$ *has a minimizer under the constraints*

$$\sum_{i\in\mathbb{N}} \nu_i = 1 \quad \textit{and} \quad (\psi_i,\psi_j)_{L^2(\mathbb{R}^d)} = \delta_{ij} \quad \forall\ i\ ,\ j\in\mathbb{N}\ ,$$

which can be written as

$$\begin{aligned}&\nu_i = \beta(\lambda-\lambda_i)\ ,\\ &-\Delta\,\psi_i + \Big(\rho * \tfrac{1}{|x|} - \textstyle\sum_{k=1}^M \tfrac{Z_k}{|x-\bar{x}_k|}\Big)\,\psi_i - \int_{\mathbb{R}^3} \tfrac{\rho(x,y)}{|x-y|}\,\psi_i(y)\,dy = \lambda_i\,\psi_i\end{aligned} \tag{7}$$

$$\mathsf{e}_\rho(\psi) := \int_{\mathbb{R}^3} |\nabla\psi|^2\,dx \;+\; \int_{\mathbb{R}^3} \Big(\rho * \frac{1}{|x|} - \sum_{k=1}^{M} \frac{Z_k}{|x-\bar{x}_k|}\Big)\,|\psi|^2\,dx$$
$$-\;\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \psi(x)\,\psi(y)\,\frac{\rho(x,y)}{|x-y|}\,dx\,dy\;.$$

$\lambda_i = \mathsf{e}_\rho(\psi_i)\;,\quad E_\nu^{\mathsf{HF}} = \sum_{i\in\mathbb{N}} \nu_i\,\mathsf{e}_\rho(\psi_i)$ and $\mathsf{d}_i(\psi_i,\bar{\psi}_i) := \mathsf{e}_\rho(\psi_i) - \mathsf{e}_{\bar\rho}(\bar{\psi}_i)$

Lemma 9 *Let $(\nu,\psi^0)\in[0,+\infty)^{\mathbb{N}}\times(L^2(\mathbb{R}^d))^{\mathbb{N}}$ and assume that*

$$\sum_{i\in\mathbb{N}}\nu_i = 1 \quad \textit{and} \quad \|\psi_i\|_{L^2} = 1 \quad \forall\, i\in\mathbb{N}\;.$$

If $(\mathsf{e}_\rho(\psi_i)_i)_{i\in\mathbb{N}}$ is nondecreasing, then $\mathsf{d}_i(\psi_i,\bar{\psi}_i)$ is nonnegative.

Theorem 10 *Consider* $(\nu, \psi^0) \in [0, +\infty)^{\mathbb{N}} \times (L^2(\mathbb{R}^d))^{\mathbb{N}}$ *and assume that*

$$\sum_{i \in \mathbb{N}} \nu_i = 1 \quad \text{and} \quad \|\psi_i\|_{L^2} = 1 \quad \forall\, i \in \mathbb{N}\ .$$

Let ψ *be the solution of (6) with initial data* ψ_i^0*. Let* $\sigma(t,i)$ *be a reordering such that* $(e_{\rho(\cdot,t)}(\psi_i(\cdot,t))_i)_{i\in\mathbb{N}}$ *is nondecreasing for any* $t \geq 0$*. Then*

$$\begin{aligned}\mathcal{F}(\nu, \psi(\cdot,t)) - \mathcal{F}(\bar{\nu}, \bar{\psi}) \;=\; & \sum_{i\in\mathbb{N}} \left(\beta(\nu_{\sigma(t,i)}) - \beta(\bar{\nu}_i) - \beta'(\bar{\nu}_i)(\nu_{\sigma(t,i)} - \bar{\nu}_i)\right) \\ & + \sum_{i\in\mathbb{N}} \nu_{\sigma(t,i)}\, d_i(\psi_{\sigma(t,i)}, \bar{\psi}_i)\end{aligned}$$

does not depend on t

and measures the distance between $((\nu(t), \psi(t))_i)_{i\in\mathbb{N}}$ *and* $((\bar{\nu}, \bar{\psi})_i)_{i\in\mathbb{N}}$

III. Lieb-Thirring type inequalities

[J.D., Felmer, Paturel, Loss]

Lieb-Thirring type inequalities and "the stability of matter" in quantum mechanics.

Let V be a smooth bounded nonpositive potential on $\mathbb{R}^d$,
$H_V = -\frac{\hbar^2}{2m}\Delta + V$ with eigenvalues

$$\lambda_1(V) < \lambda_2(V) \leq \lambda_3(V) \leq \ldots \lambda_N(V) < 0$$

The *Lieb-Thirring inequality.*

$$\sum_{i=1}^{N} |\lambda_i(V)|^\gamma \leq C_{\mathsf{LT}}(\gamma) \int_{\mathbb{R}^d} |V|^{\gamma+\frac{d}{2}}\, dx \tag{1}$$

$\gamma = 1$: the sum $\sum_{i=1}^{N} |\lambda_i(V)|$ is the *complete ionization energy,*
[Hundertmark-Laptev-Weidl00,Laptev-Weidl00]

The *Lieb-Thirring conjecture*

$$C_{\mathrm{LT}}(\gamma) = C^{(1)}_{\mathrm{LT}}(\gamma) := \inf_{\substack{V \in \mathcal{D}(\mathbb{R}^d) \\ V \leq 0}} \frac{|\lambda_1(V)|^\gamma}{\int_{\mathbb{R}^d} |V|^{\gamma+\frac{d}{2}}\, dx}\,. \tag{2}$$

Plan

- Connection of the best constant $C^{(1)}_{\mathrm{LT}}(\gamma)$ with the best constant in Gagliardo-Nirenberg inequalities
- A new inequality of Lieb-Thirring type
- The "dual" case in Gagliardo-Nirenberg inequalities

Connection with Gagliardo-Nirenberg inequalities

(Usual case of the Lieb-Thirring inequalities)

$$X_\gamma := \left\{ V \in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d) \ : \ V \geq 0 \, , \ V \not\equiv 0 \ a.e. \right\}$$

Best constant in the Lieb-Thirring inequality:

$$C^{(1)}_{\mathsf{LT}}(\gamma) = \sup_{\substack{V \in X_\gamma \\ V \geq 0, \ V \not\equiv 0 \ a.e.}} \frac{|\lambda_1(-V)|^\gamma}{\int_{\mathbb{R}^d} V^{\gamma+\frac{d}{2}} \, dx} \, .$$

where

$$\lambda_1(-V) = \inf_{\substack{u \in H^1(\mathbb{R}^d) \\ u \not\equiv 0 \ a.e.}} \frac{\int_{\mathbb{R}^d} |\nabla u|^2 \, dx - \int_{\mathbb{R}^d} V \, |u|^2 \, dx}{\int_{\mathbb{R}^d} |u|^2 \, dx} \, .$$

Gagliardo-Nirenberg inequality:

$$C_{\mathsf{GN}}(\gamma) = \inf_{\substack{u \in H^1(\mathbb{R}^d) \\ u \not\equiv 0\ a.e.}} \frac{\|\nabla u\|_{L^2(\mathbf{R}^d)}^{\frac{d}{2\gamma+d}} \|u\|_{L^2(\mathbf{R}^d)}^{\frac{2\gamma}{2\gamma+d}}}{\|u\|_{L^{2\frac{2\gamma+d}{2\gamma+d-2}}(\mathbf{R}^d)}} . \qquad (3)$$

Theorem 11 *Let $d \in \mathbb{N}$, $d \geq 1$. For any $\gamma > 1 - \frac{d}{2}$,*

$$C_{\mathsf{LT}}^{(1)}(\gamma) = \kappa_1(\gamma) \left[C_{\mathsf{GN}}(\gamma)\right]^{-\kappa_2(\gamma)} , \qquad (4)$$

where $\kappa_1(\gamma) = \frac{2}{d} \left(\frac{d}{2\gamma+d}\right)^{1+\frac{d}{2\gamma}}$ and $\kappa_2(\gamma) = 2 + \frac{d}{\gamma}$. Moreover, the constant $C_{\mathsf{LT}}^{(1)}(\gamma)$ is optimal and achieved by a unique pair of functions (u, V), up to multiplications by a constant, scalings and translations.

The scaling invariance can be made clear by redefining

$$[C_{\mathsf{LT}}^{(1)}(\gamma)]^{\frac{1}{\gamma}} = \sup_{\substack{V \in X_\gamma \\ V \geq 0,\ V \not\equiv 0\ a.e.}} \ \sup_{\substack{u \in H^1(\mathbb{R}^d) \\ u \not\equiv 0\ a.e.}} R(u,V)$$

where

$$R(u,V) = \frac{\int_{\mathbf{R}^d} V\,|u|^2\,dx - \int_{\mathbf{R}^d} |\nabla u|^2\,dx}{\int_{\mathbf{R}^d} |u|^2\,dx \quad \|V\|_{L^{\gamma+\frac{d}{2}}(\mathbf{R}^d)}^{1+\frac{d}{2\gamma}}}\ .$$

Note indeed that $\lambda_1(V) \leq 0$, and $R(u,V)$ is invariant under the transformation

$$(u,V) \mapsto (u_\lambda = u(\lambda\,\cdot),\ V_\lambda = \lambda^2 V(\lambda\,\cdot))\ ,$$

i.e.,

$$R(u_\lambda, V_\lambda) = R(u,V) \quad \forall\,\lambda > 0\ .$$

Proof of Theorem 11. By Hölder's inequality,

$$\int_{\mathbf{R}^d} V\,|u|^2\,dx \le A\,\|u\|^2_{L^{2q}(\mathbf{R}^d)}, \quad A = \|V\|_{L^{\gamma+\frac{d}{2}}(\mathbf{R}^d)}, \quad q = \frac{2\gamma+d}{2\gamma+d-2}\,.$$

With $x = \frac{\|u\|_{L^{2q}(\mathbf{R}^d)}}{\|u\|_{L^2(\mathbf{R}^d)}}$ and $\theta = \frac{d}{2\gamma+d}$, the Gagliardo-Nirenberg inequality (3) can be rewritten as

$$\frac{\|\nabla u\|_{L^2(\mathbf{R}^d)}}{\|u\|_{L^2(\mathbf{R}^d)}} \ge [C_{\mathsf{GN}}(\gamma)\,x]^{\frac{1}{\theta}}$$

so that

$$R(u,V) \le \frac{A\,x^2 - [C_{\mathsf{GN}}(\gamma)]^{\frac{2}{\theta}}\,x^{\frac{2}{\theta}}}{A^{1+\frac{d}{2\gamma}}}$$

Optimize on x.

The estimate is achieved:

$$V^{\gamma+\frac{d}{2}-1} = |u|^2 \quad \Longleftrightarrow \quad V = V_u = |u|^{\frac{4}{2\gamma+d-2}} = |u|^{2(q-1)}\,, \qquad (5)$$

where u is a solution of

$$\Delta u + |u|^{2(q-1)} u - u = 0 \quad \text{in} \quad \mathbb{R}^d\,.$$

Up to a scaling, these two equations are the Euler-Lagrange equations corresponding to the maximization in V and u.
Gagliardo-Nirenberg inequality:

$$R(u,V) \le R(u,V_u) = \frac{\int_{\mathbf{R}^d} u^{2q}\,dx - \int_{\mathbf{R}^d} |\nabla u|^2\,dx}{\int_{\mathbf{R}^d} u^2\,dx \left(\int_{\mathbf{R}^d} u^{2q}\,dx\right)^{\frac{1}{\gamma}}}$$

□

A new inequality of Lieb-Thirring type

Let V be a nonnegative unbounded smooth potential on $\mathbb{R}^d$: the eigenvalues of H_V are

$$0 < \lambda_1(V) < \lambda_2(V) \leq \lambda_3(V) \leq \ldots \lambda_N(V) \ldots$$

Main Theorem

For any $\gamma > d/2$, for any nonnegative $V \in C^\infty(\mathbb{R}^d)$ such that $V^{d/2-\gamma} \in L^1(\mathbb{R}^d)$,

$$\sum_{i=1}^{N} \lambda_i(V)^{-\gamma} \leq C_{\mathrm{LT,d}}(\gamma) \int_{\mathbb{R}^d} V^{\frac{d}{2}-\gamma}\, dx.$$

Theorem 12 *An inequality by Golden, Thompson and Symanzik* [Symanzik, B. Simon] *Let V be in $L^1_{\mathrm{loc}}(\mathbb{R}^d)$ and bounded from below. Assume moreover that $e^{-t\,V}$ is in $L^1(\mathbb{R}^d)$ for any $t > 0$. Then*

$$\mathrm{Tr}\left(e^{-t\,(-\Delta+V)}\right) \le (4\pi t)^{-\frac{d}{2}} \int_{\mathbb{R}^d} e^{-t\,V(x)}\,dx\ . \tag{6}$$

Proof. The usual proof is based on the Feynman-Kac formula. Here: an elementary approach.

$$G(x,t) = (4\pi t)^{-\frac{d}{2}}\,e^{-\frac{|x|^2}{4t}}\ , \quad e^{t\Delta} f = G(\cdot,t) * f\ .$$

Trotter's formula:

$$e^{-t(-\Delta+V)} = \lim_{n\to\infty}\left(e^{\frac{t}{n}\Delta}\,e^{-\frac{t}{n}V}\right)^n$$

Compute the trace...

$$\ldots = \quad \int_{(\mathbf{R}^d)^n} dx\, dx_1\, dx_2 \ldots\, dx_n\, G\left(\frac{t}{n}, x - x_1\right)\, e^{-\frac{t}{n}V(x_1)}\, G\left(\frac{t}{n}, x_1 - x_2\right)$$
$$\cdot e^{-\frac{t}{n}V(x_2)} \ldots\ldots\; G\left(\frac{t}{n}, x_n - x\right)\, e^{-\frac{t}{n}V(x)}\ .$$

Notation $x = x_0 = x_{n+1}$:

$$\int_{(\mathbf{R}^d)^n} dx_0\, dx_1\, dx_2 \ldots\, dx_n\; \prod_{j=0}^{n} G\left(\frac{t}{n}, x_j - x_{j+1}\right)\; e^{-\frac{t}{n}\sum_{k=0}^{n-1} V(x_k)}\ .$$

Convexity of $x \mapsto e^{-x}$:

$$e^{-\frac{t}{n}\sum_{k=0}^{n-1} V(x_k)} \leq \frac{1}{n}\sum_{k=0}^{n-1} e^{-t\,V(x_k)}\ .$$

Main ingredient:

$$\int_{(\mathbf{R}^d)^{n-1}} dx_0\, dx_1\, dx_2 \ldots\, dx_{k-1}\, dx_{k+1} \ldots\, dx_n \, \prod_{j=0}^{n} G\left(\frac{t}{n}, x_j - x_{j+1}\right)$$

$$= \quad G(t, x_k - x_k) = (4\pi t)^{-\frac{d}{2}} \,.$$

$$\mathrm{Tr}\left(e^{\frac{t}{n}\Delta}\, e^{-\frac{t}{n}V}\right)^n \le \frac{1}{n}\sum_{k=0}^{n-1}\int_{(\mathbf{R}^d)^n} dx_0\, dx_1\, dx_2 \ldots\, dx_n$$

$$\cdot \prod_{j=0}^{n} G\left(\frac{t}{n}, x_j - x_{j+1}\right)\, e^{-t\,V(x_k)}$$

$$= (4\pi t)^{-\frac{d}{2}} \int_{(\mathbf{R}^d)^2} e^{-t\,V(x)}\, dx$$

□

Proof of the Main Theorem. By definition of the Γ function, for any $\gamma > 0$ and $\lambda > 0$,

$$\lambda^{-\gamma} = \frac{1}{\Gamma(\gamma)} \int_0^{+\infty} e^{-t\lambda}\, t^{\gamma-1} dt\,.$$

The operator $-\Delta + V$ is essentially self-adjoint on $L^2(\mathbb{R}^d)$, and positive:

$$\mathrm{Tr}\left((-\Delta + V)^{-\gamma}\right) = \frac{1}{\Gamma(\gamma)} \int_0^{+\infty} \mathrm{Tr}\left(e^{-t(-\Delta+V)}\right)\, t^{\gamma-1} dt\,.$$

Using (6), since $V^{\frac{d}{2}-\gamma} \in L^1(\mathbb{R}^d)$, we get

$$\begin{aligned} \mathrm{Tr}\left((-\Delta + V)^{-\gamma}\right) &\leq \frac{1}{\Gamma(\gamma)} \int_0^{+\infty} \int_{\mathbb{R}^d} (4\pi t)^{-\frac{d}{2}} e^{-tV(x)}\, t^{\gamma-1} dx\, dt \\ &\leq \frac{\Gamma(\gamma - \frac{d}{2})}{(4\pi)^{\frac{d}{2}} \Gamma(\gamma)} \int_{\mathbb{R}^d} V(x)^{\frac{d}{2}-\gamma} dx\,. \end{aligned}$$

□

The "dual" case in Gagliardo-Nirenberg inequalities

Let $V \in \mathcal{C}^\infty(\mathbb{R}^d)$ such that $\lim_{|x|\to+\infty} V(x) = +\infty$ and denote by $\lambda_1(V)$, $\lambda_2(V)$, ... $\lambda_N(V)$ the positive eigenvalues of $-\Delta + V$.

$$Y_\gamma = \left\{ V^{\frac{d}{2}-\gamma} \in L^1(\mathbb{R}^d) \ : \ V \geq 0 \, , \ V \not\equiv +\infty \ a.e. \right\}$$

Second type Gagliardo-Nirenberg inequalities:

$$C_{\mathrm{GN,d}}(\gamma) = \inf_{\substack{u \in H^1(\mathbb{R}^d) \\ u \not\equiv 0 \ a.e. \\ \int_{\mathbb{R}^d} |u|^{2q} \, dx < \infty}} \frac{\|\nabla u\|_{L^2(\mathbb{R}^d)}^{\frac{d(1-q)}{d(1-q)+2q}} \, \|u\|_{L^{2q}(\mathbb{R}^d)}^{\frac{2q}{d(1-q)+2q}}}{\|u\|_{L^2(\mathbb{R}^d)}} \tag{7}$$

with $q := \frac{2\gamma - d}{2(\gamma+1)-d} \in (0, 1)$.

Theorem 13 *Let $d \in \mathbb{N}$, $d \geq 1$. For any $\gamma > 1 - \frac{d}{2}$, there exists a positive constant $C^{(1)}_{\mathsf{LT,d}}(\gamma)$ such that, for any $V \in Y_\gamma$,*

$$\lambda_1(V)^{-\gamma} \leq C^{(1)}_{\mathsf{LT,d}}(\gamma) \int_{\mathbb{R}^d} V^{\frac{d}{2}-\gamma}\, dx \,. \tag{8}$$

The optimal value of $C^{(1)}_{\mathsf{LT,d}}(\gamma)$ is such that

$$C^{(1)}_{\mathsf{LT,d}}(\gamma) = \kappa_1(\gamma)\,[C_{\mathsf{GN,d}}(\gamma)]^{-\kappa_2(\gamma)} \,, \tag{9}$$

where, with $q := \frac{2\gamma-d}{2\gamma-d+2}$,

$$\kappa_1(\gamma) = \frac{(2q)^{\gamma-\frac{d}{2}}(d(1-q))^{\frac{d}{2}}}{(d(1-q)+2q)^{\gamma}} \quad \text{and} \quad \kappa_2(\gamma) = 2\gamma \,.$$

Moreover, the constant $C^{(1)}_{\mathsf{LT,d}}(\gamma)$ is achieved by a unique pair of functions (u, V), up to multiplications by a constant, scalings and translations.

Notice that if $\gamma > 1 - \frac{d}{2}$, then $2q > 1$.

$$C^{(1)}_{\mathrm{LT}}(\gamma) \quad := \quad \sup_{\substack{V \in Y_\gamma \\ V \geq 0,\ V \not\equiv 0\ a.e.}} \quad \frac{[\lambda_1(V)]^{-\gamma}}{\int_{\mathbb{R}^d} V^{\frac{d}{2}-\gamma}\, dx} \,.$$

Scaling invariance:

$$[C^{(1)}_{\mathrm{LT,d}}(\gamma)]^{\frac{1}{\gamma}} \quad = \quad \sup_{\substack{V \in X_\gamma \\ V \geq 0,\ V \not\equiv 0\ a.e.}} \quad \sup_{\substack{u \in H^1(\mathbb{R}^d) \\ u \not\equiv 0\ a.e.}} \quad R(u,V)$$

$R(u,V) := \frac{\int_{\mathbb{R}^d} |u|^2\, dx \quad \|V^{-1}\|^{1-\frac{d}{2\gamma}}_{L^{\gamma-\frac{d}{2}}(\mathbb{R}^d)}}{\int_{\mathbb{R}^d} |\nabla u|^2\, dx + \int_{\mathbb{R}^d} V\, |u|^2\, dx}$ is invariant under the transformation

$$(u,V) \mapsto (u_\lambda = u(\lambda\,\cdot),\ V_\lambda = \lambda^2 V(\lambda\,\cdot)) \,.$$

Proof of Theorem 13. By Hölder's inequality,

$$\int_{\mathbf{R}^d} u^{2q}\,dx = \int_{\mathbf{R}^d} u^{2q}\,V^q . V^{-q}\,dx \le \left(\int_{\mathbf{R}^d} V\,|u|^2\,dx\right)^q \left(\int_{\mathbf{R}^d} V^{-\frac{q}{1-q}}\,dx\right)^{1-q} .$$

With $C := \left(\int_{\mathbf{R}^d} V^{-\frac{q}{1-q}}\,dx\right)^{-\frac{1-q}{q}} = \|V^{-1}\|_{L^{\gamma-\frac{d}{2}}(\mathbf{R}^d)}$, this means that

$$R(u,V) \le \frac{\|u\|^2_{L^2(\mathbf{R}^d)} \quad C^{1-\frac{d}{2\gamma}}}{\|\nabla u\|^2_{L^2(\mathbf{R}^d)} + C\,\|u\|^2_{L^2(\mathbf{R}^d)}} .$$

Optimize $R(u,V)$ under the scaling $\lambda \mapsto \lambda^{-d/2} u(\cdot/\lambda)$. □

Remark 1 Optimal functions are explicitly known only for $d = 1$. *Solutions have compact support and minimal ones are radially symmetric and unique up to translations.*