Thermal effects in Hartree systems

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Gagliardo-Nirenberg inequalities for systems and Lieb-Thirring inequalities

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First eigenvalues and Gagliardo-Nirenberg inequalities (1)

Let $H = -\Delta + V$ in $\mathbb{R}^d$, $d > 1$ and consider $\lambda_1(V)$, its lowest eigenvalue

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

Consider the variational problem

$$C_1 = \sup_{\substack{V \in \mathcal{D}(\mathbb{R}^d) \\ V \leq 0}} \frac{|\lambda_1(V)|^\gamma}{\int_{\mathbb{R}^d} |V|^{\gamma + \frac{d}{2}} \, dx}$$

By density the minimization space can be extended to
$X_\gamma := \left\{ V \in L^{\gamma + \frac{d}{2}}(\mathbb{R}^d) \ : \ V \leq 0 \, , \ V \not\equiv 0 \ a.e. \right\}$

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

The variational problem amounts to

$$C_1 = \sup_{\substack{V \in X_\gamma \\ V \not\equiv 0 \ a.e.}} \ \sup_{\substack{u \in H^1(\mathbb{R}^d) \\ u \not\equiv 0 \ a.e.}} R(u,V)$$

Invariance under scalings: $\forall\,\lambda > 0$, if $u_\lambda = u(\lambda\,\cdot)$, $V_\lambda = \lambda^2 V(\lambda\,\cdot)$

$$R(u_\lambda, V_\lambda) = R(u,V)$$

Hint: optimize first on V. With $q := \frac{2\gamma+d}{2\gamma+d-2}$,

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

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

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

Theorem

Let $d \in \mathbb{N}^*$. For any $\gamma > \max(0, 1 - \frac{d}{2})$,

$$C_1 = \kappa_1(\gamma) \left[C_{\rm GN}(\gamma) \right]^{-\kappa_2(\gamma)}$$

$$\kappa_1(\gamma) = \frac{2\gamma}{d} \left(\frac{d}{2\gamma + d} \right)^{1+\frac{d}{2\gamma}} \quad \textit{and} \quad \kappa_2(\gamma) = 2 + \frac{d}{\gamma}$$

Range: $q := \frac{2\gamma+d}{2\gamma+d-2}$. For $\gamma > \max(0, 1 - d/2)$, $q > 1$ and $2\,q < \frac{2d}{d-2}$
Optimality:

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

First eigenvalues and Gagliardo-Nirenberg inequalities (2)

Consider now a nonnegative smooth potential $V \in \mathcal{C}^\infty(\mathbb{R}^d)$ such that

$$\lim_{|x|\to+\infty} V(x) = +\infty$$

and denote by $\lambda_1(V)$, $\lambda_2(V)$, ... the positive eigenvalues of $H := -\Delta + V$

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

Let

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

Second type Gagliardo-Nirenberg inequality:

$$C^*_{\rm GN}(\gamma) = \inf_{\substack{u \in H^1(\mathbb{R}^d),\; u \not\equiv 0 \; a.e. \\ \int_{\mathbb{R}^d} |u|^{2q}\,dx < \infty}} \frac{\|\nabla u\|_{L^2(\mathbb{R}^d)}^{\frac{d}{2\gamma}} \left(\int_{\mathbb{R}^d} |u|^{2q}\,dx\right)^{\frac{1}{2q}\left(1-\frac{d}{2\gamma}\right)}}{\|u\|_{L^2(\mathbb{R}^d)}}$$

With

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

Theorem

Let $d \in \mathbb{N}^*$. For any $\gamma > d/2$, for any $V \in Y_\gamma$,

$$[\lambda_1(V)]^{-\gamma} \le C_2 \int_{\mathbb{R}^d} V^{\frac{d}{2}-\gamma}\,dx$$

$$C_2 = \kappa_1(\gamma)\left[C^*_{\mathrm{GN}}(\gamma)\right]^{-\kappa_2(\gamma)}$$

where $\kappa_1(\gamma) = \frac{(2q)^{\gamma-\frac{d}{2}}(d(1-q))^{\frac{d}{2}}}{(d(1-q)+2q)^\gamma}$ *and* $\kappa_2(\gamma) = 2\gamma$

Notice that $q < 1$, and $2q > 1$ if and only if $\gamma > 1 + d/2$.

$$R(u,V) := \frac{\int_{\mathbb{R}^d} |u|^2\,dx \quad \left(\int_{\mathbb{R}^d} V^{\frac{d}{2}-\gamma}\,dx\right)^{\frac{1}{\gamma}}}{\int_{\mathbb{R}^d} |\nabla u|^2\,dx + \int_{\mathbb{R}^d} V\,|u|^2\,dx}$$

First eigenvalues and Gagliardo-Nirenberg inequalities (3)

$$\mathcal{C}_F^{(1)} = \sup_V \frac{F(\lambda_1(V))}{\int_{\mathbb{R}^d} G(V(x))\,dx} \leq 1$$

Duality condition to relate F and G... Optimization with respect to V

$$\kappa\,|\varphi|^2 - G'(V) = 0$$

$$\mathcal{C}_F^{(1)} = \sup_{\substack{\varphi \in H^1(\mathbb{R}^d) \\ \int_{\mathbb{R}^d} |\varphi|^2\,dx = 1}} \frac{F\left(\int_{\mathbb{R}^d} \left(|\nabla\varphi|^2 + |\varphi|^2\,(G')^{-1}(\kappa\,|\varphi|^2)\right)\,dx\right)}{\int_{\mathbb{R}^d} \left(G \circ (G')^{-1}\right)(\kappa\,|\varphi|^2)\,dx}$$

$$\kappa = \left(\mathcal{C}_F^{(1)}\right)^{-1} F'\left(\int_{\mathbb{R}^d} \left(|\nabla\varphi|^2 + |\varphi|^2\,(G')^{-1}(\kappa\,|\varphi|^2)\right)\,dx\right)$$

Logarithmic Sobolev inequality

A simple case: $q=1$ or $F(s)=e^{-s}$, $G(s)=(4\pi)^{-d/2}\,e^{-s}$

$$\mathcal{C}_F^{(1)} = \sup_{\substack{V,\,\varphi \\ \int_{\mathbb{R}^d}|\varphi|^2\,dx=1}} \frac{e^{-\int_{\mathbb{R}^d}(|\nabla\varphi|^2+V|\varphi|^2)\,dx}}{(4\pi)^{-d/2}\int_{\mathbb{R}^d}e^{-V}\,dx}$$

- The optimization with respect to V gives $V=-\log(|\varphi|^2)$
- The Lagrange multiplier $\kappa=1$ is such that $\int_{\mathbb{R}^d}e^{-V}\,dx=\int_{\mathbb{R}^d}|\varphi|^2\,dx=1$

This is equivalent to the usual logarithmic Sobolev inequality: for any $\varphi\in H^1(\mathbb{R}^d)$ such that $\int_{\mathbb{R}^d}|\varphi|^2\,dx=1$,

$$\int_{\mathbb{R}^d}|\varphi|^2\log(|\varphi|^2)\,dx+\log\left(\frac{(4\pi)^{d/2}}{\mathcal{C}_F^{(1)}}\right)\le\int_{\mathbb{R}^d}|\nabla\varphi|^2\,dx$$

Optimal functions φ are gaussian and $\mathcal{C}_F^{(1)}=\left(\frac{2}{e}\right)^d$

The inequality

$$e^{-\lambda_1(V)} \le (\pi\, e^2)^{-d/2} \int_{\mathbb{R}^d} e^{-V}\, dx$$

is equivalent to the logarithmic Sobolev inequality:
for any $\varphi \in H^1(\mathbb{R}^d)$ such that $\int_{\mathbb{R}^d} |\varphi|^2\, dx = 1$,

$$\int_{\mathbb{R}^d} |\varphi|^2 \log(|\varphi|^2)\, dx + \frac{d}{2} \log\left(\pi\, e^2\right) \le \int_{\mathbb{R}^d} |\nabla\varphi|^2\, dx$$

[Gross], [Carlen,Loss], [Bobkov,Götze]

Lieb-Thirring inequalities

Given a smooth bounded nonpositive potential V on $\mathbb{R}^d$, if

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

is the finite sequence of all negative eigenvalues of

$$H = -\Delta + V$$

then we have the Lieb-Thirring inequality

$$\sum_{i=1}^{N} |\lambda_i(V)|^\gamma \le C_{\mathrm{LT}}(\gamma) \int_{\mathbb{R}^d} |V|^{\gamma+\frac{d}{2}}\, dx \tag{1.1}$$

For $\gamma = 1$, $\sum_{i=1}^N |\lambda_i(V)|$ is the *complete ionization energy*
[...], [Laptev-Weidl] for $\gamma \ge 3/2$ the sharp constant is semiclassical
Lieb-Thirring conjecture: $d = 1$, $1/2 < \gamma < 3/2$, $C_{\mathrm{LT}}(\gamma) = C_1$

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

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

Theorem

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

$$\sum_{i=1}^N \lambda_i(V)^{-\gamma} \le \mathcal{C}(\gamma) \int_{\mathbb{R}^d} V^{\frac{d}{2}-\gamma}\, dx$$

$$\mathcal{C}(\gamma) = (2\pi)^{-d/2}\, \frac{\Gamma(\gamma - d/2)}{\Gamma(\gamma)}$$

Proof is based in an inequality by Golden, Thompson and Symanzik

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:

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

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

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

Generalization: Let f be a nonnegative function on $\mathbb{R}_+$ such that

$$\int_0^\infty f(t)\,\left(1+t^{-d/2}\right)\,\frac{dt}{t}<\infty$$

$$F(s):=\int_0^\infty e^{-t\,s}\,f(t)\,\frac{dt}{t}\quad\text{and}\quad G(s):=\int_0^\infty e^{-t\,s}\,(4\pi\,t)^{-d/2}\,f(t)\,\frac{dt}{t}$$

Theorem

Let V be in $L^1_{\rm loc}(\mathbb{R}^d)$ and bounded from below. If $G(V)\in L^1(\mathbb{R}^d)$, then

$$\sum_{i\in\mathbb{N}^*}F(\lambda_i(V))=\mathrm{tr}\left[F\left(-\Delta+V\right)\right]\le\int_{\mathbb{R}^d}G(V(x))\,dx$$

If $F(s)=s^{-\gamma}$, then $G(s)=\frac{\Gamma(\gamma-\frac d2)}{(4\pi)^{\frac d2}\,\Gamma(\gamma)}\,s^{\frac d2-\gamma}$

If $F(s)=e^{-s}$, then $f(s)=\delta(s-1)$ and $G(s)=(4\pi)^{-d/2}\,e^{-s}$

$$\sum_{i\in\mathbb{N}^*}e^{-\lambda_i(V)}\le\frac{1}{(4\pi)^{d/2}}\int_{\mathbb{R}^d}e^{-V(x)}\,dx$$

Stability for the linear Schrödinger equation

$E[\psi] := \int_{\mathbb{R}^d} (|\nabla\psi|^2 + V\,|\psi|^2)\,dx$, eigenvalues of $H := -\Delta + V$

$$\lambda_i(V) := \inf_{\substack{F \subset L^2(\mathbb{R}^d) \\ \dim(F) = i}} \sup_{\psi \in F} E[\psi]$$

The eigenfunction $\bar\psi_i$ form an orthonormal sequence:

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

Free energy of the *mixed state* $(\boldsymbol{\nu}, \boldsymbol{\psi}) = ((\nu_i)_{i\in\mathbb{N}^*}, (\psi_i)_{i\in\mathbb{N}^*})$:

$$\mathcal{F}[\boldsymbol{\nu}, \boldsymbol{\psi}] := \sum_{i\in\mathbb{N}^*} \beta(\nu_i) + \sum_{i\in\mathbb{N}^*} \nu_i\, E[\psi_i]$$

Assumption (H) holds if β is a strictly convex function, $\beta(0) = 0$,

$$\Big|\sum_{i\in\mathbb{N}^*} \beta(\bar\nu_i)\Big| < \infty \quad \text{and} \quad \Big|\sum_{i\in\mathbb{N}^*} \bar\nu_i\, \lambda_i(V)\Big| < \infty$$

where $\bar\nu_i := (\beta')^{-1}(-\lambda_i(V))$ for any $i \in \mathbb{N}^*$

A discrete Csiszár-Kullback inequality

Lemma

Under Assumption (H)*, if* $\boldsymbol{\psi} = (\psi_i)_{i\in\mathbb{N}^*}$ *is an orthonormal sequence,*

$$\mathcal{F}_n[\boldsymbol{\nu},\boldsymbol{\psi}] - \mathcal{F}_n[\bar{\boldsymbol{\nu}},\bar{\boldsymbol{\psi}}]$$

$$= \sum_{i=1}^n \Big(\beta(\nu_i) - \beta(\bar\nu_i) - \beta'(\bar\nu_i)(\nu_i - \bar\nu_i)\Big) + \sum_{i=1}^n \nu_i \Big(E[\psi_i] - E[\bar\psi_i]\Big)$$

Corollary

Assume that $\inf_{s>0}\beta''(s)\,s^{2-p} =: \alpha > 0$, $p\in[1,2]$. *If* $\sum_{i\in\mathbb{N}^*}\beta(\nu_i)$ *and* $\sum_{i\in\mathbb{N}^*}\nu_i\,\beta'(\bar\nu_i)$ *are absolutely convergent, then* $(\nu_i-\bar\nu_i)_{i\in\mathbb{N}^*}\in\ell^p$ *and*

$$\sum_{i\in\mathbb{N}^*}\Big(\beta(\nu_i)-\beta(\bar\nu_i)-\beta'(\bar\nu_i)(\nu_i-\bar\nu_i)\Big) \ge \frac{\alpha\,\|\boldsymbol{\nu}-\bar{\boldsymbol{\nu}}\|_{\ell^p}^2}{2^{2/p}}\cdot\min\Big\{\|\boldsymbol{\nu}\|_{\ell^p}^{p-2},\|\bar{\boldsymbol{\nu}}\|_{\ell^p}^{p-2}\Big\}$$

Examples

To various functions β with $-F(s) = (\beta \circ (\beta')^{-1})(-s) + s\,(\beta')^{-1}(-s)$ correspond various generalized Lieb-Thirring inequalities

Example 1. Let $m > 1$ and consider $\beta(\nu) := (m-1)^{m-1} m^{-m}\,\nu^m$. With $\beta'(\nu) = (m-1)^{m-1} m^{1-m}\,\nu^{m-1} = -\lambda$ and $m = \frac{\gamma}{\gamma-1}$, we get:

$$-(\beta(\nu) + \lambda\,\nu) = F(\lambda) = (-\lambda)^\gamma$$

The case $\gamma \in (0,1)$ is formally covered by

$$\beta(\nu) := -(1-m)^{m-1} |m|^{-m}\,\nu^m$$

with $m \in (-\infty, 0)$, $m = \frac{\gamma}{\gamma-1}$ again and $F(s) = (-s)^\gamma$, but in this case, β is not convex and the free energy $\mathcal{F}$ cannot be defined as above.

Example 2. For $m \in (0,1)$ and $\beta(\nu) := -(1-m)^{m-1} m^{-m}\,\nu^m$, with $\beta'(\nu) = -(1-m)^{m-1} m^{1-m}\,\nu^{m-1} = -\lambda$ and $m = \frac{\gamma}{\gamma+1}$, we get: $F(\lambda) = \lambda^{-\gamma}$

Example 3. If $\beta(\nu) := \nu \log \nu - \nu$, then $\beta'(\nu) = \log \nu = -\lambda$

$$\sum_{i \in \mathbb{N}^*} e^{-\lambda_i(V)} \leq \frac{1}{(4\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-V(x)}\, dx$$

This case can formally be seen as the limit case $m \to 1$ in Examples 1 and 2. Here $F(s) = e^{-s}$, $G(s) = (4\pi)^{-d/2}\, e^{-s}$

Example 4. If $\beta(\nu) := \nu \log \nu + (1-\nu) \log(1-\nu)$, then $\beta'(\nu) = \log\left(\frac{\nu}{1-\nu}\right) = -\lambda$ and $F(s) = \log(1 + e^{-s})$

$$\sum_{i \in \mathbb{N}^*} \log\left(1 + e^{-\lambda_i(V)}\right) \leq \int_{\mathbb{R}^d} G(V(x))\, dx$$

Interpolation: Gagliardo-Nirenberg inequalities for systems

Assume that $H = -\Delta + V$ has an infinite sequence $(\lambda_i(V))_{i\in\mathbb{N}^*}$ of eigenvalues. Let F and G be such that

$$\sum_{i\in\mathbb{N}^*} F(\lambda_i(V)) = \mathrm{tr}\left[F\left(-\Delta+V\right)\right] \le \int_{\mathbb{R}^d} G(V(x))\,dx$$

Let $\bar\lambda := \lim_{i\to\infty} \lambda_i(V) \le \infty$ and assume that

$$\mathrm{Spectrum}(-\Delta+V)\cap(-\infty,\bar\lambda) = \{\lambda_i(V)\ :\ i\in\mathbb{N}^*\}$$

Define $\sigma(s) := -F'(s)$ and $\beta(s) := -\int_0^s \sigma^{-1}(t)\,dt$. Notice that

$$F(s) = \int_s^{\bar\lambda} \sigma(t)\;dt = \int_s^{\bar\lambda} (\beta')^{-1}(-t)\;dt = -\min_{\nu>0}\left[\beta(\nu)+\nu\,s\right]$$

$$\sum_{i\in\mathbb{N}^*} \nu_i \int_{\mathbb{R}^d} \left(|\nabla\psi_i|^2 + V\,|\psi_i|^2\right)\,dx + \sum_{i\in\mathbb{N}^*} \beta(\nu_i) + \int_{\mathbb{R}^d} G(V(x))\,dx \geq 0$$

for any sequence of nonnegative occupation numbers $(\nu_i)_{i\in\mathbb{N}^*}$ and any sequence $(\psi_i)_{i\in\mathbb{N}^*}$ of orthonormal $L^2(\mathbb{R}^d)$ functions

Method: For fixed $\boldsymbol{\nu} = (\nu_i)_{i\in\mathbb{N}^*}$, $\boldsymbol{\psi} = (\psi_i)_{i\in\mathbb{N}^*}$

$$K[\boldsymbol{\nu},\boldsymbol{\psi}] := \int_{\mathbb{R}^d} \sum_{i\in\mathbb{N}^*} \nu_i\,|\nabla\psi_i|^2\,dx \quad \text{and} \quad \rho := \sum_{i\in\mathbb{N}^*} \nu_i\,|\psi_i|^2$$

$$H(s) := -\left[G\circ(G')^{-1}(-s) + s\,(G')^{-1}(-s)\right]$$

Assume that G' is invertible and optimize on V: The optimal potential V has to satisfy

$$G'(V) + \rho = 0$$

$$\int_{\mathbb{R}^d} V\,\rho\,dx + \int_{\mathbb{R}^d} G(V(x))\,dx = -\int_{\mathbb{R}^d} H(\rho(x))\,dx$$

Theorem

$$K[\boldsymbol{\nu},\boldsymbol{\psi}]+\sum_{i\in\mathbb{N}^*}\beta(\nu_i)\geq\int_{\mathbb{R}^d}H(\rho)\,dx$$

with $\rho=\sum_{i\in\mathbb{N}^*}\nu_i\,|\psi_i|^2$

Here $(\nu_i)_{i\in\mathbb{N}^*}$ *is any nonnegative sequence of occupation numbers and* $(\psi_i)_{i\in\mathbb{N}^*}$ *is any sequence of orthonormal* $L^2(\mathbb{R}^d)$ *functions*

Example 1. Let $m>1$ (standard Lieb-Thirring inequality) and consider $\beta(\nu):=c_m\,\nu^m$, $c_m:=(m-1)^{m-1}m^{-m}$, $m=\frac{\gamma}{\gamma-1}$, $F(s)=(-s)^\gamma$ and $G(s)=C_{\rm LT}(\gamma)(-s)^{\gamma+d/2}$

$$q:=\frac{2\gamma+d}{2\gamma+d-2}\quad\text{and}\quad\mathcal{K}^{-1}:=q\,[C_{\rm LT}(\gamma)\,(\gamma+d/2)]^{q-1}$$

Corollary

For any $m\in(1,+\infty)$,

$$K[\boldsymbol{\nu},\boldsymbol{\psi}]+c_m\sum_{i\in\mathbb{N}^*}\nu_i^m\geq\mathcal{K}\int_{\mathbb{R}^d}\rho^q\,dx$$

$$\Big(K[\boldsymbol{\nu},\boldsymbol{\psi}]\Big)^\theta\Big(\sum_{i\in\mathbb{N}^*}\nu_i^m\Big)^{(1-\theta)}\geq\mathcal{L}\int_{\mathbb{R}^d}\rho^q\,dx\,,\quad\theta=\frac{d}{2(\gamma-1)+d}$$

The case $m=\frac{\gamma}{\gamma-1}\in(-\infty,0)$, which corresponds to $\gamma\in(0,1)$, $q\in(1+d/2,d/(d-2))$, $\beta(\nu):=c_m\,\nu^m$, is not covered

Example 2. $m \in (0,1)$, $\beta(\nu) := -c_m\,\nu^m$, $c_m := (1-m)^{m-1} m^{-m}$, $m = \frac{\gamma}{\gamma+1}$, $F(\lambda) = \lambda^{-\gamma}$ and $G(s) = \mathcal{C}(\gamma)\, s^{d/2-\gamma}$

$$q := \frac{2\gamma - d}{2(\gamma+1) - d} \in (0,1) \quad \text{and} \quad \mathcal{K}^{-1} := q\,[\mathcal{C}(\gamma)\,(\gamma - d/2)]^{q-1}$$

Notice that $\gamma > d/2 \;\Rightarrow\; m \in (d/(d+2), 1)$

Corollary

For any $m \in (\frac{d}{d+2}, 1)$,

$$K[\boldsymbol{\nu}, \boldsymbol{\psi}] + \mathcal{K} \int_{\mathbb{R}^d} \rho^q\, dx \geq c_m \sum_{i\in\mathbb{N}^*} \nu_i^m$$

Scale invariant version:

$$\Big(K[\boldsymbol{\nu}, \boldsymbol{\psi}]\Big)^{\theta} \left(\int_{\mathbb{R}^d} \rho^q\, dx\right)^{(1-\theta)} \geq \mathcal{L} \sum_{i\in\mathbb{N}^*} \nu_i^m$$

with $\theta = \frac{d}{2(\gamma+1)}$

Example 3. If $\beta(\nu) := \nu \log \nu - \nu$, then $\beta'(\nu) = \log \nu = -\lambda$, $F(s) = e^{-s}$ and $G(s) = (4\pi)^{-d/2} e^{-s}$

Corollary

$$K[\boldsymbol{\nu}, \psi] + \sum_{i \in \mathbb{N}^*} \nu_i \log \nu_i \geq \int_{\mathbb{R}^d} \rho \log \rho \, dx + d/2 \log(4\pi) \int_{\mathbb{R}^d} \rho \, dx$$

$$\int_{\mathbb{R}^d} \rho \log \rho \, dx \leq \sum_{i \in \mathbb{N}^*} \nu_i \log \nu_i + \frac{d}{2} \log \left(\frac{e}{2\pi \, d} \, \frac{K[\boldsymbol{\nu}, \psi]}{\int_{\mathbb{R}^d} \rho \, dx} \right) \int_{\mathbb{R}^d} \rho \, dx$$

Trace operators and compactness properties

J. Dolbeault, P. Felmer, and J. Mayorga-Zambrano. *Compactness properties for trace-class operators and applications to quantum mechanics.* Monatshefte für Mathematik, 155 (1): 43–66, 2008

Lieb-Thirring and Gagliardo-Nirenberg inequalities

$\Omega \subset \mathbb{R}^d$ bounded domain
Let g be a non-negative function on $\mathbb{R}_+$ such that

$$\int_0^\infty g(t)\,\left(1+t^{-d/2}\right)\,\frac{dt}{t} < \infty$$

and consider F and G such that

$$F(s) = \int_0^\infty e^{-t\,s}\,g(t)\,\frac{dt}{t}\,, \quad G(s) = \int_0^\infty e^{-t\,s}\,(4\pi\,t)^{-d/2}\,g(t)\,\frac{dt}{t}$$

$F, G : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ are convex non-increasing

Theorem

Let $V \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ be a potential bounded from below. Assume moreover that $G(V)$ is in $\mathrm{L}^1(\Omega)$. Then we have

$$\sum_{i\in\mathbb{N}} F(\lambda_{V,i}) = \mathrm{Tr}\left[F\left(-\Delta + V\right)\right] \le \int_\Omega G(V(x))\,dx$$

Example

If $V \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ is a non-negative potential such that $V^{\frac{d}{2}-\gamma}$ is in $L^1(\Omega)$, then

$$\mathrm{Tr}\left[(-\Delta+V)^{-\gamma}\right]=\sum_{i\in\mathbb{N}}(\lambda_{V,i})^{-\gamma}\leq\frac{\Gamma(\gamma-\frac{d}{2})}{(4\pi)^{d/2}\,\Gamma(\gamma)}\int_\Omega V^{\frac{d}{2}-\gamma}\,dx$$

Example

If $V \in \mathrm{L}^1_{\mathrm{loc}}(\Omega)$ is bounded from below and such that $e^{-V}\in L^1(\Omega)$ and $F(s)=e^{-s}$ for any $s\in\mathbb{R}$, then $G(s)=(4\pi)^{-d/2}\,e^{-s}$ and

$$\mathrm{Tr}\left[e^{-\Delta+V}\right]=\sum_{i\in\mathbb{N}}e^{-\lambda_{V,i}}\leq\frac{1}{(4\pi)^{d/2}}\int_\Omega e^{-V}\,dx$$

Theorem

Let V be a potential verifying appropriate integrability conditions. Let β be an entropy generating function, F the free energy, and G a strictly convex function with F and G related as above, then

$$\mathrm{Tr}\left[F(-\Delta+V)\right] \le \int_\Omega G(V(x))\,dx$$

If τ is such that $G(s)=\tau^*(-s)$ for any $s\in\mathbb{R}$, where τ and τ^* are related according to a modified Legendre-Fenchel transformation, then for any $L\in\mathcal{H}^1_+$ (trace-class with finite kinetic energy), we have

$$\mathcal{K}(L)+\mathcal{H}_\beta(L) \ge \int_\Omega \tau(\rho_L)\,dx$$

Compactness results

Theorem

Consider $d \geq 2$, and assume that $m \in (d/(d+2), 1)$. Let $\{L_n\}_{n\in\mathbb{N}}$ be a sequence in $\mathcal{H}^1_+$ such that

$$K_\infty \equiv \sup_{n\in\mathbb{N}} \mathcal{K}(L_n) < \infty$$

Then $\{\|L_n\|_1\}_{n\in\mathbb{N}}$ is bounded and $\sup_{n\in\mathbb{N}} \sum_{i\in\mathbb{N}} |\nu_i^n|^m < \infty$. Moreover, up to a subsequence, $\lim_{n\to\infty} \nu_i^n = \bar{\nu}_i$, for all $i \in \mathbb{N}$ and

1. *If $\bar{\nu}_i \neq 0$ for all $i \in \mathbb{N}$, then $\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^m = \sum_{i\in\mathbb{N}} |\bar{\nu}_i|^m$*
2. *For any $m' \in (m, 1]$, $\lim_{n\to\infty} \sum_{i\in\mathbb{N}} |\nu_i^n|^{m'} = \sum_{i\in\mathbb{N}} |\bar{\nu}_i|^{m'}$*
3. *Up to a subsequence, $\{L_n\}_{n\in\mathbb{N}}$ converges in trace norm $\|\cdot\|_1$ to some operator $\bar{L} \in \mathcal{H}^1_+$, whose eigenvalues are $\{\bar{\nu}_i^n\}_{i\in\mathbb{N}}$*

Orbitally stable states in generalized Hartree-Fock theory: the repulsive case

- J. Dolbeault, P. Felmer, and M. Lewin.
Orbitally stable states in generalized Hartree-Fock theory.
Mathematical Models and Methods in Applied Sciences, 19 (3): 347–367, 2009.

- P.A. Markowich, G. Rein, G. Wolansky.
Existence and Nonlinear Stability of Stationary States of the Schrödinger-Poisson System. Journal of Statistical Physics, Vol. 106, Nos. 5/6, March 2002

- We consider *free energy* functionals[1] of the form

$$\gamma \mapsto \mathcal{E}^{\mathrm{HF}}(\gamma) - T\,S(\gamma)$$

where $\mathcal{E}^{\mathrm{HF}}$ is the Hartree-Fock energy and the entropy takes the form

$$S(\gamma) := -\,\mathrm{tr}\,(\beta(\gamma))$$

for some convex function β on $[0,1]$. Has the free energy a minimizer ? The Hartree-Fock energy $\mathcal{E}^{\mathrm{HF}}(\gamma)$ is

$$\mathrm{tr}\,((-\Delta)\,\gamma) - Z\int_{\mathbb{R}^3}\frac{\rho_\gamma(x)}{|x|}\,dx + \frac{1}{2}\,D(\rho_\gamma,\rho_\gamma) - \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\gamma(x,y)|^2}{|x-y|}\,dx\,dy$$

with $D(f,g) := \iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{f(x)\,g(y)}{|x-y|}\,dx\,dy$ (*direct term* of the interaction). The last term is the *exchange term*

- Evolution is described by the *von Neumann equation*

$$i\,\frac{d\gamma}{dt} = [H_\gamma,\gamma]$$

Here H_γ is a self-adjoint operator depending on γ but not on β. Orbital stability of the solution obtained by minimization ?

[1] P.-L. Lions '88

Assumptions on the entropy term

(A1) β is a strictly convex C^1 function on $(0,1)$

(A2) $\beta(0)=0$ and $\beta\geq 0$ on $[0,1]$

Fermions !... we introduce a modified Legendre transform of β

$$g(\lambda):=\operatorname*{argmin}_{0\leq\nu\leq 1}\left(\lambda\,\nu+\beta(\nu)\right)$$

$$g(\lambda)=\sup\left\{\inf\left\{(\beta')^{-1}(-\lambda),\,1\right\},\;0\right\}$$

Notice that g is a nonincreasing function with $0\leq g\leq 1$. Also define

$$\beta^*(\lambda):=\lambda\,g(\lambda)+(\beta\circ g)(\lambda)$$

(A3) β is a nonnegative C^1 function on $[0,1)$ and $\beta'(0)=0$ (no loss of generality)

(A4) $\sum_{j\geq 1} j^2\left|\beta^*\left(-Z^2/(4\,T\,j^2)\right)\right|<\infty$

The ground state free energy is finite (the eigenvalues of $-\Delta-Z/|x|$ are $-Z^2/(4\,j^2)$, with multiplicity j^2)

From well-posedness...

A typical example is

$$\beta(\nu) = \nu^m$$

which satisfies (A1)–(A4) as long as $1 < m < 3$. In this special case

$$g(\lambda) = \begin{cases} \min\left\{\left(\frac{-\lambda}{m}\right)^{\frac{1}{m-1}}, 1\right\} & \text{if} \quad \lambda < 0 \\ 0 & \text{otherwise} \end{cases}$$

and

$$\beta^*(\lambda) = -(m-1)\left(\frac{-\lambda}{m}\right)^{\frac{m}{m-1}} \quad \text{if} \quad -m < \lambda < 0$$

Space of operators

$$\mathfrak{H} := \left\{\gamma : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \mid \gamma = \gamma^*,\ \gamma \in \mathfrak{S}_1,\ \sqrt{-\Delta}\,|\gamma|\,\sqrt{-\Delta} \in \mathfrak{S}_1\right\}$$

...

The Banach space $\mathfrak{H}$ is equipped with the norm

$$\|\gamma\|_{\mathfrak{H}} = \mathrm{tr}\,|\gamma| + \mathrm{tr}\left(\sqrt{-\Delta}\,|\gamma|\,\sqrt{-\Delta}\right)$$

$\mathcal{K} := \{\gamma \in \mathfrak{H} \mid 0 \le \gamma \le 1\}$ is a convex closed subset of $\mathfrak{H}$
Since β is convex and $\beta(0) = 0$, we have $0 \le \beta(\nu) \le \beta(1)\,\nu$ on $[0,1]$
For any $\gamma \ge 0$, $0 \le \beta(\gamma) \le \beta(1)\,\gamma \Longrightarrow \beta(\gamma) \in \mathfrak{S}_1$ when $\gamma \in \mathfrak{S}_1$

$$\mathrm{tr}\left((-\Delta)\,\gamma\right) := \mathrm{tr}\left(\sqrt{-\Delta}\,\gamma\,\sqrt{-\Delta}\right) \in \mathbb{R} \cup \{+\infty\}$$

Density of charge: $\rho_\gamma(x) = \gamma(x,x) \in L^1(\mathbb{R}^3)$
By the spectral decomposition of γ

$$\forall\,\gamma \in \mathcal{K}\,, \qquad \left\|\nabla\sqrt{\rho_\gamma}\right\|^2_{L^2(\mathbb{R}^3)} \le \mathrm{tr}\left(\sqrt{-\Delta}\,\gamma\,\sqrt{-\Delta}\right)$$

Hence we have $\left\|\sqrt{\rho_\gamma}\right\|^2_{H^1(\mathbb{R}^3)} \le \|\gamma\|_{\mathfrak{H}}$
and, as a consequence, $\rho_\gamma \in L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3) \subset L^{6/5}(\mathbb{R}^3)$,
$\int_{\mathbb{R}^3} \frac{\rho_\gamma(x)}{|x|}\,dx < \infty$ and $D(\rho_\gamma, \rho_\gamma) < \infty$

… to the minimization of the free energy

By the Hardy-Littlewood-Sobolev inequality and the Cauchy-Schwarz inequality

$$|\gamma(x,y)|^2 \leq \rho_\gamma(x)\,\rho_\gamma(y) \quad \text{for a.e. } (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3$$

so that

$$\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\gamma(x,y)|^2}{|x-y|}\,dx\,dy \leq D(\rho_\gamma,\rho_\gamma) < \infty\,.$$

The free energy $\mathcal{E}_Z^\beta$ is well-defined on $\mathcal{K}$. We are interested in minimizing it under a constraint corresponding to the closed convex subset

$$\mathcal{K}_q := \{\gamma \in \mathcal{K} \mid \operatorname{tr}\gamma = q\}$$

Define

$$I_Z^\beta(q) := \inf\left\{\mathcal{E}_Z^\beta(\gamma) \mid \gamma \in \mathcal{K} \text{ and } \operatorname{tr}(\gamma) = q\right\}$$

$$I_Z^\beta := \inf\left\{\mathcal{E}_Z^\beta(\gamma) \mid \gamma \in \mathcal{K}\right\} = \inf_{q\geq 0} I^\beta(q)$$

Minimization of the free energy

Theorem (Minimization for the generalized HF model)

Assume that β satisfies **(A1)–(A4)** *for some $T > 0$.*

1. *For every $q \geq 0$, the following statements are equivalent:*
   (i) *all minimizing sequences $(\gamma_n)_{n\in\mathbb{N}}$ for $I_Z^\beta(q)$ are precompact in $\mathcal{K}$,*
   (ii) *$I_Z^\beta(q) < I_Z^\beta(q')$ for all q, q' such that $0 \leq q' < q$*
2. *Any minimizer γ of $I_Z^\beta(q)$ satisfies the self-consistent equation*

$$\gamma = g\big((H_\gamma - \mu)/T\big)\,, \quad H_\gamma = -\Delta - \frac{Z}{|x|} + \rho_\gamma * |\cdot|^{-1} - \frac{\gamma(x,y)}{|x-y|}$$

   for some $\mu \leq 0$
3. *The minimization problem $I_Z^\beta(q)$ has no minimizer if $q \geq 2\,Z + 1$*
4. *Problem I_Z^β always has a minimizer $\bar\gamma$. It satisfies the self-consistent equation*

Back to the linear case

We now recall the properties of the linear case corresponding to

$$\mathcal{F}^{\beta}_{Z}(\gamma) := \mathrm{tr}\left((-\Delta)\,\gamma\right) - Z\int_{\mathbb{R}^3}\frac{\rho_\gamma(x)}{|x|}\,dx + T\;\mathrm{tr}\left(\beta(\gamma)\right)$$

A straightforward minimization gives

$$\inf_{\gamma\in\mathcal{K}}\mathcal{F}^{\beta}_{Z}(\gamma) = \sum_{j\geq 1} j^2\,\beta^*\left(\frac{\lambda_j}{T}\right) > -\infty$$

where $\lambda_j = -\frac{Z^2}{4\,j^2}$ are the negative eigenvalues of $-\Delta - Z/|x|$ with multiplicity j^2
The trace

$$q^{\rm lin}_{\rm max}(T) := \mathrm{tr}\Big(g\left(\tfrac{1}{T}\left(-\Delta - \tfrac{Z}{|x|}\right)\right)\Big) = \sum_{j\geq 1} j^2\,g\left(\frac{\lambda_j}{T}\right) \in (0,\infty]$$

could in principle be infinite

Then the minimization problem with constraint $\inf_{\gamma\in\mathcal{K}_q}\mathcal{F}_Z^\beta(\gamma)$ admits a minimizer for all $q\geq 0$ if $q_{\max}^{\rm lin}=\infty$, whereas it has a minimizer if and only if $q\in[0,q_{\max}^{\rm lin}]$ if $q_{\max}^{\rm lin}<\infty$. In all cases, this minimizer solves the equation

$$\gamma=g\left(\tfrac{1}{T}(-\Delta-\tfrac{Z}{|x|}-\mu)\right)$$

for some $\mu\leq 0$, a Lagrange multiplier which is chosen to ensure that the condition $\operatorname{tr}\gamma=q$ is satisfied

$\mu\mapsto q(\mu):=\operatorname{tr}(g((-\Delta-Z/|x|-\mu)/T))$ is non decreasing and satisfies $q(\mu)=0$ for $\mu<0$, $|\mu|$ large enough and $q(\mu)\to q_{\max}^{\rm lin}$ when $\mu\to 0$

If $\beta(\nu) = \nu^m$, we see that $q_{\max}^{\rm lin} < \infty$ if and only if $m < 5/3$, as summarized in Table 1. For $T > Z^2/(4\,m)$,

$$q_{\max}^{\rm lin}(T) = \left(\frac{Z^2}{4\,T\,m}\right)^{\frac{1}{m-1}} \sum_{j\geq 1} j^{2-\frac{2}{m-1}} = \left(\frac{Z^2}{4\,T\,m}\right)^{\frac{1}{m-1}} \zeta\left(2\,\frac{m-2}{m-1}\right)$$

where ζ denotes the Riemann zeta function

<table>
<tr><th>$1 < m < 5/3$</th><th>$5/3 \leq m < 3$</th><th>$m \geq 3$</th></tr>
<tr><td>$q_{\max}^{\rm lin}(T) < \infty$
Existence iff
$0 \leq q \leq q_{\max}^{\rm lin}(T)$</td><td>$q_{\max}^{\rm lin}(T) = \infty$
Existence
$\forall\, q \geq 0$</td><td rowspan="2">Linear energy unbounded from below</td></tr>
<tr><td colspan="2">Linear energy bounded from below</td></tr>
</table>

Table: Existence and non-existence of minimizers with a finite trace for $\beta(\nu) = \nu^m$

A criterion for existence

Proposition

Assume that β satisfies **(A1)–(A4)** *for some $T > 0$. Then the minimization problem $I_Z^\beta(q)$ has no solution if $q \geq q_{\max}^{\mathrm{lin}}$*

Proposition

Assume that β satisfies **(A1)–(A4)** *for some $T > 0$. Then for all q such that*

$$0 \leq q \leq \min \left\{ \sum_{j \geq 1} g \left(\frac{-(Z-q)^2}{4\,T\,j^2} \right) \,,\, Z \right\}$$

Condition $I_Z^\beta(q) < I_Z^\beta(q')$ in the theorem on the minimization of the free energy *is satisfied*

Ionization threshold

Corollary (Existence of minimizers for the generalized HF model)

Let $T \geq 0$. Assume that β satisfies **(A1)–(A3)**, *and* **(A4)** *if T is positive. Then there exists $q_{\max} > 0$ such that the nonlinear minimization problem has a minimizer for any $q \in [0, q_{\max}]$*

- Ionization threshold: How does $q_{\max}$ depend on T is an essentially open question

Non-zero temperature solutions of the gravitational Hartree system

Gonca L. Aki, Jean Dolbeault and Christof Sparber. *Thermal effects in gravitational Hartree systems.* To appear in Annales Henri Pincaré

The variational problem

We introduce the following Banach space of operators

$$\mathfrak{H} = \left\{ \rho : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \;:\; \rho^* = \rho \geq 0,\; \rho \in \mathfrak{S}_1,\; \sqrt{-\Delta}\,\rho\,\sqrt{-\Delta} \in \mathfrak{S}_1 \right\}$$

equipped with the norm

$$\|\rho\|_{\mathfrak{H}} = \operatorname{tr}\rho + \operatorname{tr}\left(\sqrt{-\Delta}\,\rho\,\sqrt{-\Delta}\right)$$

We are interested in a minimization problem under a mass constraint

$$i_{M,T} := \inf_{\rho \in \mathfrak{H}_M} \mathcal{F}_T[\rho]\,, \qquad \mathcal{F}_T[\rho] = \operatorname{tr}(-\Delta\rho) - \frac{1}{2}\operatorname{tr}(V_\rho\,\rho) + T\operatorname{tr}\beta(\rho)$$

on the set of the physical state

$$\mathfrak{H}_M := \{\rho \in \mathfrak{H} \;:\; \operatorname{tr}\rho = M\}$$

The free energy is well-defined and bounded from below

- Potential energy term: By the Hardy-Littlewood-Sobolev inequality and Sobolev's embedding

$$\mathcal{E}_{\rm pot}[\rho] = \frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{n_\rho(x)n_\rho(y)}{|x-y|}\,\mathrm{d}x\,\mathrm{d}y \le C\,\|n_\rho\|_{L^1}^{3/2}\,\mathrm{tr}(-\Delta\rho)^{1/2}$$

This yields

$$\mathcal{E}_H[\rho] \ge \mathrm{tr}(-\Delta\rho) - CM^{3/2}\ \mathrm{tr}(-\Delta\rho)^{1/2} \ge -\frac{1}{4}\,C^2M^3$$

- Entropy term: $\mathcal{S}[\rho] = -\,\mathrm{tr}\,\beta(\rho)$

(β1): $\beta \in C^1$ is convex
(β2): $\beta(0) = 0 \Longrightarrow 0 \le \beta(\rho) \le \beta(M)\rho$ for all $\rho \in \mathfrak{H}$
Then $\beta(\rho) \in \mathfrak{S}_1$, provided $\rho \in \mathfrak{S}_1$

Hence, $\mathcal{F}_T$ is well-defined and bounded on $\mathfrak{H}_M$

Sub-additivity of $i_{M,T}$ w.r.t. M

(*i*) *As a function of* M, $i_{M,T}$ *is sub-additive. In addition, for any* $M > 0$, $m \in (0, M)$ *and* $T > 0$, *we have*

$$i_{M,T} \leq i_{M-m,T} + i_{m,T}$$

Consider two states as "almost minimizers" $\rho \in \mathfrak{H}_{M-m}$ and $\sigma \in \mathfrak{H}_m$

$$\rho = \sum_{j=1}^{J} \lambda_j |\varphi_j\rangle\langle\varphi_j|, \quad \sigma = \sum_{j=1}^{J} \bar{\lambda}_j |\varphi_j\rangle\langle\varphi_j|$$

with smooth eigenfunctions $(\varphi_j)_{j=1}^J$ having compact support in a ball $B(0,R)$. Next translate one of the states so that they have disjoint supports, observe that $\rho + \sigma \in \mathfrak{H}_M$

(*ii*) *The function* $i_{M,T}$ *is a decreasing function of* M *and an increasing function of* T

Maximal temperature T^*

Let $T^*(M) := \sup\{ T > 0 \ : \ i_{M,T} < 0\}$.

(*iii*) *For any* $M > 0$, $T^*(M) > 0$ *is positive, maybe even infinite. As a function of* M *it is increasing and satisfies*

$$T^*(M) \geq \max_{0 \leq m \leq M} \frac{m^3}{\beta(m)} \ |i_{1,0}|$$

If $T < T^*$, *we have* $i_{M,T} < 0$

- $i_{M,0} = M^3 \ i_{1,0}$ by the homogeneity of zero-temp. minimal energy
- By sub-additivity $i_{M,T} \leq n \ i_{M/n,T} \leq n\beta\left(\frac{M}{n}\right) T - \frac{M^3}{n^2} \ |i_{1,0}|$

(*iv*) *As a consequence,* $T^*(M) = +\infty$ *for any* $M > 0$, *if*

$$\lim_{s \to 0_+} \frac{\beta(s)}{s^3} = 0$$

Euler-Lagrange equations and Lagrange multiplier

Theorem (Euler-Lagrange equations)

Let $M > 0$, $T \in (0, T^*(M)]$ and assume that $(\beta 1)$–$(\beta 2)$ hold. Consider a density matrix operator $\rho \in \mathfrak{H}_M$ which minimizes $\mathcal{F}_T$. Then ρ satisfies the self-consistent equation

$$\rho = (\beta')^{-1}\left(\tfrac{1}{T}\,(\mu - H_\rho)\right)$$

where $\mu \leq 0$ denotes the Lagrange multiplier associated to the mass constraint. Explicitly, it is given by

$$\mu = \frac{1}{M}\left(\operatorname{tr}\left(H_\rho + T\,\beta'(\rho)\right)\rho\right)$$

An equivalent formulation: countably many nonlinear eigenvalue problem

The decomposition yields the following stationary problem:

$$\begin{cases} \Delta\psi_j + V\psi_j + \mu_j\,\psi_j = 0, \quad j \in \mathbb{N} \\ -\Delta V = 4\pi \displaystyle\sum_{j\in\mathbb{N}} \lambda_j |\psi_j|^2 \end{cases}$$

where $(\mu_j)_{k\in\mathbb{N}} \in \mathbb{R}_-$ denote the energy eigenvalues of the Hamiltonian

$$H_\rho = -\Delta - V_\rho \quad \text{where} \quad V_\rho = n_\rho * \frac{1}{|\cdot|}$$

Here the energy eigenvalues are given in terms of the occupation probabilities

$$\mu_j = \mu - T\beta'(\lambda_j) \quad \text{provided } \mu_j \le \mu$$

The Lagrange multiplier is negative

Assume that

($\beta 3$) $p(M) := \sup_{m\in(0,M)} \frac{m\,\beta'(m)}{\beta(m)} \le 3.$

Lemma (negativity of μ)

Let $M>0$ and $T<T^*(M)$. Assume that $\rho\in\mathfrak{H}_M$ is a minimizer of $\mathcal{F}_T$ and let μ be the corresponding Lagrange multiplier. If $p(M)\le 3$, then $M\,\mu \le p(M)\, i_{M,T} < 0$

The proof follows from the observations:

$$i_{M,T} = \mathrm{tr}\left(-\Delta\,\rho - \tfrac{1}{2}\,V_\rho\,\rho + T\,\beta(\rho)\right)$$
$$M\,\mu = \mathrm{tr}\left(-\Delta\,\rho - V_\rho\,\rho + T\,\beta'(\rho)\,\rho\right)$$

and by the fact that $\mathrm{tr}(V_\rho\rho) = 4\,\mathrm{tr}(-\Delta\rho)$

A priori estimates for minimizers

- A decay property of the spatial density:

Let $\rho \in \mathfrak{H}_M$ be a minimizer for $\mathcal{F}_T$. There exists a constant $C > 0$ such that for all $R > 0$ sufficiently large:

$$\int_{|x|>R} n_\rho(x)\,\mathrm{d}x \le \frac{C}{R^2}$$

- *Binding inequality* or strict sub-additivity inequality:

Let $M^{(1)} > 0$ and $M^{(2)} > 0$. If there are minimizers for $i_{M^{(1)},T}$ and $i_{M^{(2)},T}$, then

$$i_{M^{(1)}+M^{(2)},T} < i_{M^{(1)},T} + i_{M^{(2)},T}$$

Existence of minimizers below T^*

Theorem (Existence of minimizers)

Assume that (β1)–(β3) hold. Let $M > 0$ and consider $T^* = T^*(M)$ as the maximal temperature. For all $T < T^*$, there exists an operator

$$\rho \quad \text{in} \quad \mathfrak{H}_M \qquad \text{such that} \quad \mathcal{F}_T[\rho] = i_{M,T}$$

Moreover, every minimizing sequence $(\rho_n)_{n\in\mathbb{N}}$ for $i_{M,T}$ is relatively compact in $\mathfrak{H}$ up to translations

The proof relies on the concentration-compactness method once it is known that $i_{M,T} < 0$:

- Vanishing: can be ruled out by the fact that $n_\rho \in L^{7/5}$
- Dichotomy: splitting behaviour: $i_{M,T} = i_{M^{(1)},T} + i_{M-M^{(1)},T}$ contradicts the binding inequality $i_{M^{(1)}+M^{(2)},T} < i_{M^{(1)},T} + i_{M^{(2)},T}$
- Compactness

Orbital stability

A direct consequence of this variational approach is orbital stability: Consider the set of minimizers $\mathfrak{M}_M \subset \mathfrak{H}_M$ and denote

$$\mathrm{dist}_{\mathfrak{M}_M}(\rho(t),\rho) = \inf_{\rho \in \mathfrak{M}_M} \|\rho(t) - \rho\|$$

Here $\rho(t)$ solves the corresponding time-dependent system

$$i\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [H_{\rho(t)}, \rho(t)]\,, \quad \rho(0) = \rho_{\mathrm{in}}$$

where $H_\rho := -\Delta - n_\rho * \frac{1}{|\cdot|}$

Corollary (Orbital stability)

For given $M > 0$ let $T < T^*(M)$. Then for any $\varepsilon > 0$, there exists $\delta > 0$ such that, for all $\rho_{\mathrm{in}} \in \mathfrak{H}_M$ and $\rho \in \mathfrak{M}_M$ with $\mathrm{dist}_{\mathfrak{M}_M}(\rho_{\mathrm{in}},\rho) \leq \delta$ it holds:

$$\sup_{t \in \mathbb{R}_+} \mathrm{dist}_{\mathfrak{M}_M}(\rho(t),\rho) \leq \varepsilon$$

Pure states, mixed states and critical temperature

Let $\rho_0 = M|\psi_0\rangle\langle\psi_0|$ be the (appropriately scaled) minimizer for $T = 0$. Then the corresponding Hamiltonian operator

$$H_0 := -\Delta - |\psi_0|^2 * \frac{1}{|\cdot|}$$

admits countably many (negative) eigenvalues [2]

$$(\mu_j^0)_{j\in\mathbb{N}} \qquad \text{with} \quad \mu_j^0 \nearrow 0$$

Claim:

A critical temperature $T_c \in (0, T^*)$ exists, and depends on the entropy function β such that, for $T < T_c$ minimizers $\rho \in \mathfrak{M}_M$ are only pure states

[2] E. H. Lieb'77

Positivity of the critical temperature for all $M > 0$

$$T_c(M) := \max\{T > 0 : \; i_{M,T} = i_{M,0} + \tau\beta(M) \;\; \forall \tau \in (0, T]\}$$

Assume that (β1)–(β3) hold. Then $T_c(M)$ is positive for any $M > 0$

To see this, take $T_n \to 0$ and consider a sequence of minimizers $\rho^{(n)}$
Since $\rho^{(n)}$ is also a minimizing sequence for $\mathcal{F}_{T=0}$, we know

$$\mu_j^{(n)} \stackrel{n\to\infty}{\longrightarrow} \mu_j^0 \leq 0$$

We assume by contradiction that $\liminf_{n\to\infty} \lambda_1^{(n)} = \epsilon > 0$
Then the Euler-Lagrange equation implies $\mu^{(n)} > \mu_1^{(n)}$, yields a contradiction:

$$M = \lambda_0^{(0)} \geq \lim_{n\to\infty} \lambda_0^{(n)} \geq \lim_{n\to\infty} (\beta')^{-1} \left((\mu_1^0 - \mu_0^{(n)})/T_n \right) = +\infty$$

Hence $\exists\, [0, T_c]$ with $T_c > 0$ s.t. $\mu^{(n)} < \mu_1^{(n)}$ for any $T_n \in [0, T_c]$. Thus $\rho^{(n)}$ is of rank one

Characterization of the critical temperature T_c

Corollary

Assume that (β1)–(β3) hold. There is a pure state minimizer of mass M if and only if $T \in [0, T_c]$

For any $M > 0$ the critical temperature satisfies

$$T_c = \frac{\mu_1^0 - \mu_0^0}{\beta'(M)}$$

where $\mu_0^0 < \mu_1^0$ are the two lowest eigenvalues of H_0

Step 1: Prove $T_c \leq (\mu_1^0 - \mu_0^0)/\beta'(M)$ by using $\mu(T) = \mu_0^0 + T\beta'(M)$ for pure states ($T \leq T_c$)

Step 2: ($T > T_c$)Prove the equality (approaching to T_c from above) by using

$$M\mu^{(n)} = \sum_{j\in\mathbb{N}} \lambda_j^{(n)} \left(\mu_j^{(n)} + T^{(n)}\beta'(\lambda_j^{(n)})\right)$$

Remarks on the maximal temperature

- A case in which $T^* = \infty$:

$T^*(M) = +\infty$ for any $M > 0$, if

$$\lim_{s \to 0_+} \frac{\beta(s)}{s^3} = 0$$

- A case in which T^* is finite:

If $p \in (1, 7/5)$ given in the entropy generating function $\beta(s) = s^p$, then the maximal temperature, $T^*(M)$ is finite

- Limit case:

Assume $T^* < +\infty$. Then, $\lim_{T \to T^*_-} i_{M,T} = 0$ and $\lim_{T \to T^*_-} \mu(T) = 0$

- Open: If $p \in (7/5, 3)$ then T^* is finite ?

Thank you for your attention !