v-Representability on Periodic Domains: a Sobolev Space Approach

Sarina Sutter, Markus Penz, Michael Ruggenthaler, Robert van Leeuwen, Klaas Giesbertz

December 03, 2024

Introduction

$$\boxed{\text{potentials}} \longleftrightarrow \boxed{\text{densities}}$$

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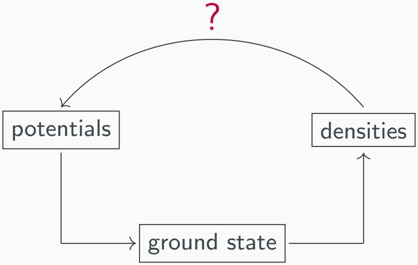

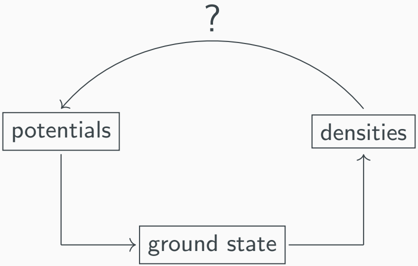

Known as v-reprensentability problem

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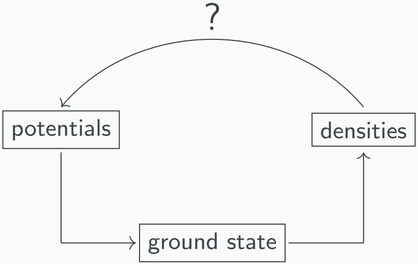

Known as *v*-reprensentability problem

In this talk: Define a setting where we are able to find a (large) set of densities which are (ensemble) *v*-representable.

Lieb's Setting

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Then, $\mathscr{I}_N \subset L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$ and if $v \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ then potential energy satisfies

$$\int \mathrm{d}x \rho(x) v(x) < \infty.$$

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The ground state energy is

$$E(v) := \inf\left\{\langle \psi, H_v \psi \rangle \mid \psi \in \mathscr{W}_N\right\}$$

where $\mathscr{W}_N := \{\psi \in Q(H_v) \mid \|\psi\|_2 = 1\}$.

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On $\mathscr{I}_N$ we define the functional $\tilde{F}(\rho) := \inf\left\{\langle \psi, H_0 \psi\rangle \mid \psi \to \rho, \psi \in \mathscr{W}_N\right\}$ and we get

$$E(v) = \inf_{\rho \in \mathscr{I}_N}\left\{\tilde{F}(\rho) + \langle \rho, v\rangle\right\}.$$

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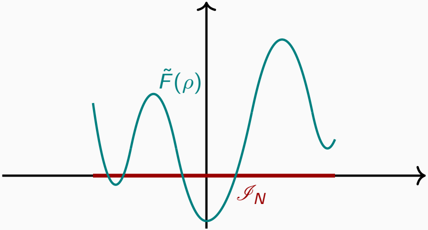

$\tilde{F}(\rho) \coloneqq \inf\left\{\langle\psi, H_0\psi\rangle \mid \psi \to \rho, \psi \in \mathscr{W}_N\right\}$ on $\mathscr{I}_N$

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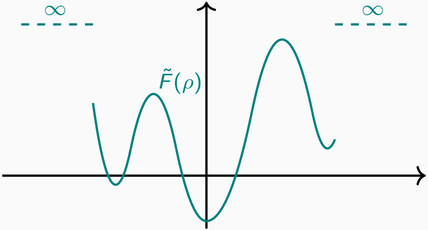

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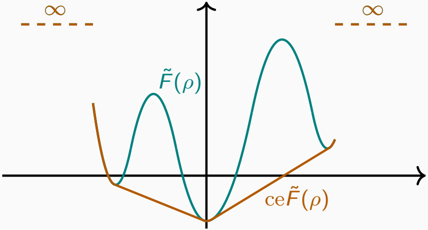

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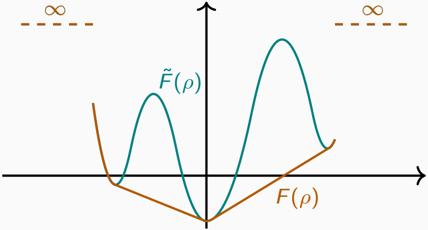

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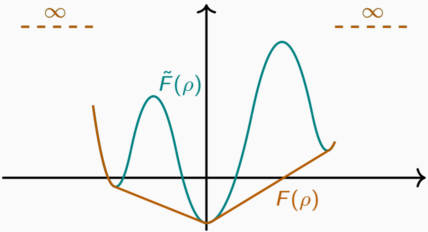

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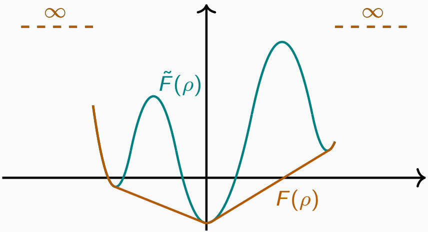
$$F_{\mathrm{DM}}(\rho) \coloneqq \begin{cases} \inf\{\mathrm{Tr}[\Gamma H_0] \mid \Gamma \to \rho\} & \text{if } \rho \in \mathscr{I}_N \\ \infty & \text{otherwise.} \end{cases}$$



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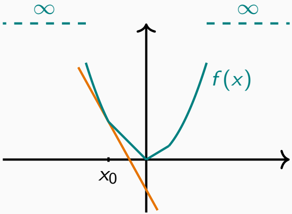

F locally bounded implies non-empty subdifferential.

$\Rightarrow$ Densities where F is locally bounded are (ensemble) v-representable.

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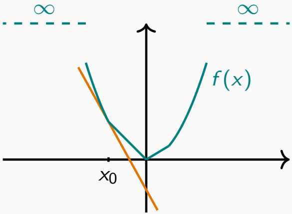

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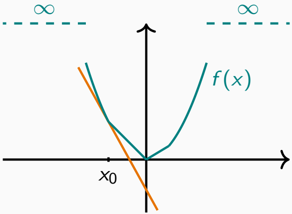

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Problem: The interior of the domain of F is empty.

Empty interior

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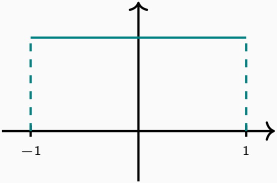

Element in $\mathscr{I}_N \Rightarrow F < \infty$

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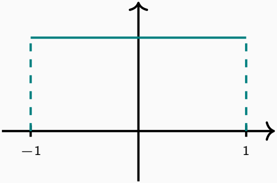

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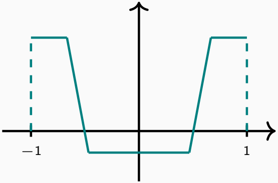

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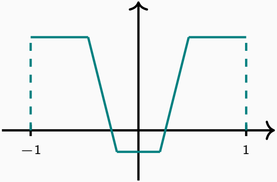

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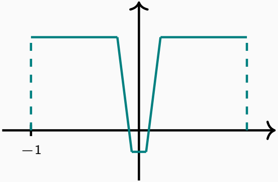

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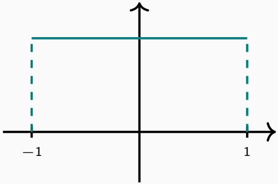

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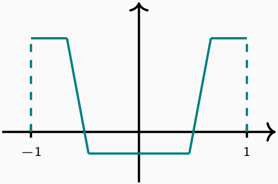

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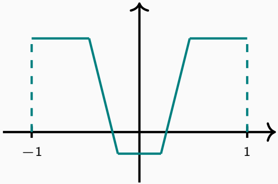

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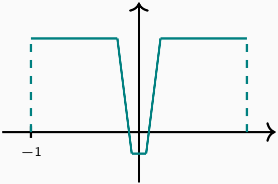

Element not in $\mathscr{I}_N \Rightarrow F = \infty$

$\Rightarrow$ Include derivative in the norm.

$\Rightarrow$ Use H^1 norm: $\|f\|_{1,2}^2 = \|f\|_2^2 + \|\nabla f\|_2^2$.

Sobolev Setting

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Recall the set of physical densities $\mathscr{I}_N := \left\{\rho \mid \sqrt{\rho} \in H^1(\mathbb{T}), \rho \geq 0, \int \rho = N\right\}$.
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Potential energy is finite if $v \in H^{-1}(\mathbb{T})$. That is, $v = f + \nabla g$ with $f, g \in L^2(\mathbb{T})$ and it is paired with ρ by

$$\langle v, \rho \rangle = \int \mathrm{d}x f(x)\rho(x) - \int \mathrm{d}x g(x)\nabla\rho(x).$$

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Example: δ-function $\delta = f + \nabla g$ with $f(x) = 1$ and $g(x) = -x$,

$$\begin{aligned} \delta(\rho) &= \int_0^1 \rho(x)\mathrm{d}x + \int_0^1 x\nabla\rho(x)\mathrm{d}x \\ &= \int_0^1 \rho(x)\mathrm{d}x - \int_0^1 \rho(x)\mathrm{d}x + x\rho(x)\Big|_0^1 = \rho(1). \end{aligned}$$

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There exists two constants C_1, C_2 such that if $\rho \in \mathscr{I}_N$ then

$$\|\nabla \sqrt{\rho}\|_2^2 \leq F(\rho) \leq C_1 + C_2 \|\nabla \sqrt{\rho}\|_2^2.$$

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For $\rho \in \mathcal{P}_\eta := \{\rho \in \mathscr{I}_N \mid \rho > \eta > 0\}$ we have the bound

$$\|\nabla\sqrt{\rho}\|_2^2 = \left\|\frac{\nabla\rho}{2\sqrt{\rho}}\right\|_2^2 \leq \frac{1}{4\eta}\|\nabla\rho\|_2^2 \leq \frac{1}{4\eta}\|\rho\|_{H^1}^2.$$

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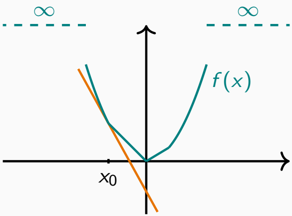
The set $\mathcal{P}_\eta$ is open due to $H^1(\mathbb{T}) \hookrightarrow C^0(\mathbb{T})$.
$\Rightarrow$ F is locally bounded at $\rho \in \mathcal{P}_\eta$.



Connection to Schrödinger Equation

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Problem: Is F related to the internal energy?

If $-v \in \underline{\partial} F(\rho)$, then

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We can show that $F(\rho) = F_{\mathrm{DM}}(\rho)$. Then,

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Problem: Is the Hamiltonian H_v with potential v self-adjoint?

KLMN Theorem

Let A be a positive self-adjoint operator on a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ with form domain $Q(A)$. Let B be a symmetric quadratic form on $Q(A)$ such that there exists $0 \leq a < 1$ and $b \in \mathbb{R}$ with

$$|\langle \psi, B\psi \rangle_{\mathcal{H}}| \leq a \langle \psi, A\psi \rangle_{\mathcal{H}} + b \langle \psi, \psi \rangle_{\mathcal{H}}$$

for all ψ in $Q(A)$. Then the operator $A + B$ is self-adjoint with domain $Q(A)$ and is bounded from below by $-b$.

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Remark: We need to assume that the interaction satisfies the KLMN condition.

Connection to Schrödinger Equation

Theorem

Assume that the interaction W is weakly continuous. Then the minimum of the energy functional $\mathcal{E}(\psi) := \langle \psi, H_v \psi \rangle$ is attained. Moreover, let ψ_0 be the minimizer. Assume that $|\langle \psi_0, W\phi \rangle|$ is finite for all $\phi \in [C^\infty(\mathbb{T}) \otimes \mathbb{C}^2]^{\wedge N}$. Then ψ_0 satisfies

$$\Big(\sum_j -\frac{1}{2}\Delta_j + v(x_j) + W \Big)\psi_0 = E_0 \psi_0$$

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Remark: An interaction of the form $W = \sum_{i<j} w(x_i - x_j)$ with $w \in L^1([-1,1]])$ and a distributional interaction of the form $W = \sum_{i<j} \nabla_{x_i} g(x_i - x_j)$ with $g \in L^2([-1,1])$ satisfy all condition on W.

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$F_{\mathrm{DM}}(\rho) = \min_{\Gamma \to \rho} \mathrm{Tr}[\Gamma H_0]$	$F^{\beta}_{\mathrm{DM}}(\rho) = \inf_{\Gamma \to \rho} \mathrm{Tr}\{\Gamma(H_0 + \beta^{-1} \log(\Gamma))\}$
$\partial F_{\mathrm{DM}}(\rho) \neq \emptyset$ for $\rho > 0$	$\partial F^{\beta}_{\mathrm{DM}}(\rho) \neq \emptyset$ for $\rho > 0$
	v-rep. densities satisfy $\rho > 0$.
	$\partial F^{\beta}_{\mathrm{DM}}(\rho)$ is single-valued.

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Ground state of a Hamiltonian H_v exists and satisfies the Schrödinger equation in a distributional sense.

For elevated temperature and fixed number of particles, we have a full characterization of H^{-1} v-representable densities and F^{β}_{DM} is Gâteaux differentiable at densities $\rho > 0$.