

Optimal potentials for Schrödinger operators

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We consider the **Schrödinger** operator $-\Delta + V(x)$ in a given bounded set Ω . The optimization problems we deal with are of the form

$$\min \{F(V) : V \in \mathcal{V}\},$$

where F is a suitable **cost functional** and \mathcal{V} is a suitable **admissible class**. We limit ourselves to the case $V \geq 0$.

The cost functionals we want to include in our framework are of the following types.

Integral functionals Given a right-hand side $f \in L^2(\Omega)$ we consider the solution u_V of the elliptic PDE

$$-\Delta u + V(x)u = f(x) \text{ in } \Omega, \quad u \in H_0^1(\Omega).$$

The **integral cost functionals** we consider are of the form

$$F(V) = \int_{\Omega} j(x, u_V(x), \nabla u_V(x)) dx$$

where j is a suitable integrand that we assume convex in the gradient variable and bounded from below as

$$j(x, s, z) \geq -a(x) - c|s|^2$$

with $a \in L^1(\Omega)$ and c smaller than the first eigenvalue of $-\Delta$ on $H_0^1(\Omega)$. In particular, the energy $\mathcal{E}_f(V)$ defined by

$$\mathcal{E}_f(V) = \inf_{u \in H_0^1(\Omega)} \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{2} V(x) u^2 - f(x) u \right) dx$$

belongs to this class since, integrating by parts its **Euler-Lagrange** equation, we have

$$\mathcal{E}_f(V) = -\frac{1}{2} \int_{\Omega} f(x) u_V dx$$

which corresponds to the integral functional above with

$$j(x, s, z) = -\frac{1}{2} f(x) s.$$

Spectral functionals For every admissible potential $V \geq 0$ we consider the spectrum $\lambda(V)$ of the **Schrödinger** operator $-\Delta + V(x)$ on $H_0^1(\Omega)$.

If Ω is bounded or has finite measure, or if the potential V satisfies some suitable integral properties, the operator $-\Delta + V(x)$ has a **compact resolvent** and so its spectrum $\lambda(V)$ is discrete:

$$\lambda(V) = (\lambda_1(V), \lambda_2(V), \dots),$$

where $\lambda_k(V)$ are the eigenvalues counted with their multiplicity.

The **spectral cost functionals** we consider are of the form

$$F(V) = \Phi(\lambda(V))$$

where $\Phi : \mathbf{R}^{\mathbf{N}} \rightarrow \overline{\mathbf{R}}$ is a given function. For instance, taking $\Phi(\lambda) = \lambda_k$ we obtain

$$F(V) = \lambda_k(V).$$

We say that Φ is continuous (resp. lsc) if

$$\lambda_k^n \rightarrow \lambda_k \quad \forall k \implies \Phi(\lambda_n) \rightarrow \Phi(\lambda) \\ \left(\text{resp. } \Phi(\lambda) \leq \liminf_n \Phi(\lambda_n) \right).$$

Optimization problems for changing sign potentials have been recently considered by **Carlen-Frank-Lieb** for the cost $F(V) = \lambda_1(V)$. They prove the inequality:

$$\lambda_1(V) \geq -c_{p,d} \left(\int_{\mathbf{R}^d} V_-^{p+\frac{d}{2}} dx \right)^{\frac{1}{p}}.$$

Our goal is to obtain similar inequalities for more general cost functionals and integral constraints on the potential; on the other hand, we limit ourselves to the case of **non-negative** potentials.

The γ -convergence

We denote by $\mathcal{M}_0^+(\Omega)$ the class of **capacitary measures** on Ω , i.e. the **Borel** (not necessarily finite) measures μ on Ω such that $\mu(E) = 0$ for any set $E \subset \Omega$ of capacity zero.

For any capacitary measure $\mu \in \mathcal{M}_0^+(\Omega)$, we define the **Sobolev** space

$$H_\mu^1 = \left\{ u \in H^1(\mathbf{R}^d) : \int_{\mathbf{R}^d} |u|^2 d\mu < +\infty \right\},$$

which is a **Hilbert** space when endowed with the norm $\|u\|_{1,\mu}$, where

$$\|u\|_{1,\mu}^2 = \int_{\mathbf{R}^d} |\nabla u|^2 dx + \int_{\mathbf{R}^d} u^2 dx + \int_{\mathbf{R}^d} u^2 d\mu.$$

If $u \notin H_{\mu}^1$, we set $\|u\|_{1,\mu} = +\infty$.

In particular the measure

$$\infty_K(E) = \begin{cases} 0 & \text{if } \text{cap}(E \cap K) = 0 \\ +\infty & \text{if } \text{cap}(E \cap K) > 0 \end{cases}$$

is a capacity measure and, taking $K = \Omega^c$, the space $H_{\mu}^1(\Omega)$ becomes in this case the usual **Sobolev** space $H_0^1(\Omega)$.

Definition We say that a sequence (μ_n) of capacitary measures γ -converges to the capacitary measure μ if the sequence of functionals $\|\cdot\|_{1,\mu_n}$ Γ -converges to the functional $\|\cdot\|_{1,\mu}$ in $L^2(\Omega)$, i.e. the following two conditions are satisfied:

- for every $u_n \rightarrow u$ in $L^2(\Omega)$ we have

$$\|u\|_{1,\mu}^2 \leq \liminf_{n \rightarrow \infty} \|u_n\|_{1,\mu_n}^2;$$

- for every $u \in L^2(\Omega)$, there exists $u_n \rightarrow u$ in $L^2(\Omega)$ such that

$$\|u\|_{1,\mu}^2 = \lim_{n \rightarrow \infty} \|u_n\|_{1,\mu_n}^2.$$

For every $\mu \in \mathcal{M}_0(\Omega)$ and $f \in L^2(\Omega)$ we may consider the PDE formally written as

$$\begin{cases} -\Delta u + \mu u = f \\ u \in H_0^1(\Omega) \end{cases}$$

whose precise meaning has to be given in the [weak form](#)

$$\int_{\Omega} \nabla u \nabla \varphi \, dx + \int_{\Omega} u \varphi \, d\mu = \int_{\Omega} f \varphi \, dx$$

for every $\varphi \in H_0^1(\Omega) \cap L^2_{\mu}(\Omega)$. The [resolvent operator](#) $R_{\mu} : L^2(\Omega) \rightarrow L^2(\Omega)$ associates to every $f \in L^2(D)$ the unique solution u of the PDE above.

Properties of the γ -convergence

- The γ -convergence is **equivalent** to:

$$R_{\mu_n}(f) \rightarrow R_{\mu}(f) \text{ for every } f \in L^2(D).$$

Actually, it is enough to have $R_{\mu_n}(1) \rightarrow R_{\mu}(1)$.
In this way, the distance

$$d_{\gamma}(\mu_1, \mu_2) = \|R_{\mu_1}(1) - R_{\mu_2}(1)\|_{L^2(\Omega)}$$

is equivalent to the γ -convergence.

- The space $\mathcal{M}_0(\Omega)$ endowed with the distance d_{γ} is a **compact metric space**.
- Identifying a domain A with the measure $\infty_{\Omega \setminus A}$, the class of all smooth domains $A \subset \Omega$ is **d_{γ} -dense** in $\mathcal{M}_0(\Omega)$.

- The measures of the form $V(x) dx$, with V smooth, are d_γ -dense in $\mathcal{M}_0(\Omega)$.
- If $\mu_n \rightarrow \mu$ for the γ -convergence, the spectrum of the compact resolvent operator \mathcal{R}_{μ_n} converges to the spectrum of \mathcal{R}_μ ; then the eigenvalues of the Schrödinger operator $-\Delta + \mu_n$ defined on $H_0^1(\Omega)$ converge to the corresponding eigenvalues of the operator $-\Delta + \mu$.

The case of bounded constraints

Proposition *If $V_n \rightarrow V$ weakly in $L^1(\Omega)$ the capacitary measures $V_n dx$ γ -converge to $V dx$.*

As a consequence, all the optimization problems of the form

$$\min\{F(V) : V \in \mathcal{V}\}$$

with F γ -l.s.c (very weak assumption) and \mathcal{V} closed convex and bounded in $L^p(\Omega)$ with $p > 1$, admit a solution.

Example If $p > 1$ the problem

$$\max \left\{ \mathcal{E}_f(V) : V \geq 0, \int_{\Omega} V^p dx \leq 1 \right\}$$

has the unique solution

$$V_p = \left(\int_{\Omega} |u_p|^{2p/(p-1)} dx \right)^{-1/p} |u_p|^{2/(p-1)},$$

where u_p is the minimizer on $H_0^1(\Omega)$ of

$$\frac{1}{2} \int_{\Omega} |\nabla u|^2 dx + \frac{1}{2} \left(\int_{\Omega} |u|^{2p/(p-1)} dx \right)^{\frac{p-1}{p}} - \int_{\Omega} f u dx$$

corresponding to the nonlinear PDE

$$-\Delta u + C|u|^{2/(p-1)}u = f.$$

Similar results for $\lambda_1(V)$ (see also [Henrot Birkhäuser 2006]).

If $p < 1$ the problem

$$\max \left\{ \mathcal{E}_f(V) : V \geq 0, \int_{\Omega} V^p dx \leq 1 \right\}$$

has **no solution**. Indeed, take for instance $f = 1$; it is not difficult to construct a sequence V_n such that

$$\int_{\Omega} V_n^p dx \leq 1 \quad \text{and} \quad \mathcal{E}_f(V_n) \rightarrow 0.$$

The conclusion follows since no potential V can provide zero energy.

An interesting case is when $p = 1$.

The solution of

$$\max \left\{ \mathcal{E}_f(V) : V \geq 0, \int_{\Omega} V \, dx \leq 1 \right\}$$

is **in principle a measure**. However, it is possible to prove that for every $f \in L^2(\Omega)$, denoting by w the solution of the **auxiliary problem**

$$\min_{u \in H_0^1(\Omega)} \left\{ \frac{1}{2} \int_{\Omega} |\nabla u|^2 \, dx + \frac{1}{2} \|u\|_{L^\infty(\Omega)}^2 - \int_{\Omega} u f \, dx \right\},$$

and setting $M = \|w\|_{L^\infty(\Omega)}$, $\omega_+ = \{w = M\}$,
 $\omega_- = \{w = -M\}$,

we have

$$V_{opt} = \frac{f}{M} (\mathbf{1}_{\omega_+} - \mathbf{1}_{\omega_-}).$$

Note that in particular, we deduce the conditions of optimality

- $f \geq 0$ on ω_+ ,
- $f \leq 0$ on ω_- ,
- $\int_{\omega_+} f \, dx - \int_{\omega_-} f \, dx = M.$

The case of unbounded constraints

We consider now problems of the form

$$\min \left\{ F(V) : V \geq 0, \int_{\Omega} \Psi(V) dx \leq 1 \right\}$$

with admissible classes of potentials **unbounded** in every L^p . For example:

- $\Psi(s) = s^{-p}$, for any $p > 0$;
- $\Psi(s) = e^{-\alpha s}$, for any $\alpha > 0$.

Theorem Let Ω be bounded, F **increasing** and γ -lower semicontinuous, Ψ strictly decreasing with $\Psi^{-1}(s^p)$ convex for some $p > 1$. Then there exists a solution.

Examples If $\Psi(s) = s^{-p}$ with $p > 0$, the optimal potential for the energy \mathcal{E}_f is

$$V_{opt} = \left(\int_{\Omega} |u|^{2p/(p+1)} dx \right)^{1/p} |u|^{-2/(p+1)}$$

where u solves the **auxiliary problem**

$$\min_{u \in H_0^1(\Omega)} \int_{\Omega} |\nabla u|^2 dx + \left(\int_{\Omega} |u|^{2p/(1+p)} dx \right)^{(1+p)/p} - \int_{\Omega} 2f u dx$$

which corresponds to the **nonlinear PDE**

$$-\Delta u + C_p |u|^{-2/(p+1)} u = f, \quad u \in H_0^1(\Omega)$$

where C_p is a constant depending on p .

Similarly, if $\Psi(s) = e^{-\alpha s}$, we have

$$V_{opt} = \frac{1}{\alpha} \left(\log \left(\int_{\Omega} u^2 dx \right) - \log(u^2) \right)$$

where u solves the **auxiliary problem**

$$\min_{u \in H_0^1(\Omega)} \int_{\Omega} |\nabla u|^2 dx + \frac{1}{\alpha} \int_{\Omega} u^2 \left(\int_{\Omega} \log(u^2) dx - \log(u^2) \right) dx - \int_{\Omega} 2f u dx.$$

which corresponds to the **nonlinear PDE**

$$-\Delta u + C_{\alpha} u - \frac{1}{\alpha} u \log(u^2) = f, \quad u \in H_0^1(\Omega)$$

where C_{α} is a constant depending on α .

PROBLEMS WITH $\Omega = \mathbf{R}^d$

When $\Omega = \mathbf{R}^d$ most of the cost functionals **are not** γ -lower semicontinuous; for example, if $V(x)$ is any potential, with $V = +\infty$ outside a compact set, then, for every $x_n \rightarrow \infty$, the sequence of translated potentials $V_n(x) = V(x + x_n)$ γ -converges to the capacitary measure

$$I_\emptyset(E) = \begin{cases} 0 & \text{if } \text{cap}(E) = 0 \\ +\infty & \text{if } \text{cap}(E) > 0. \end{cases}$$

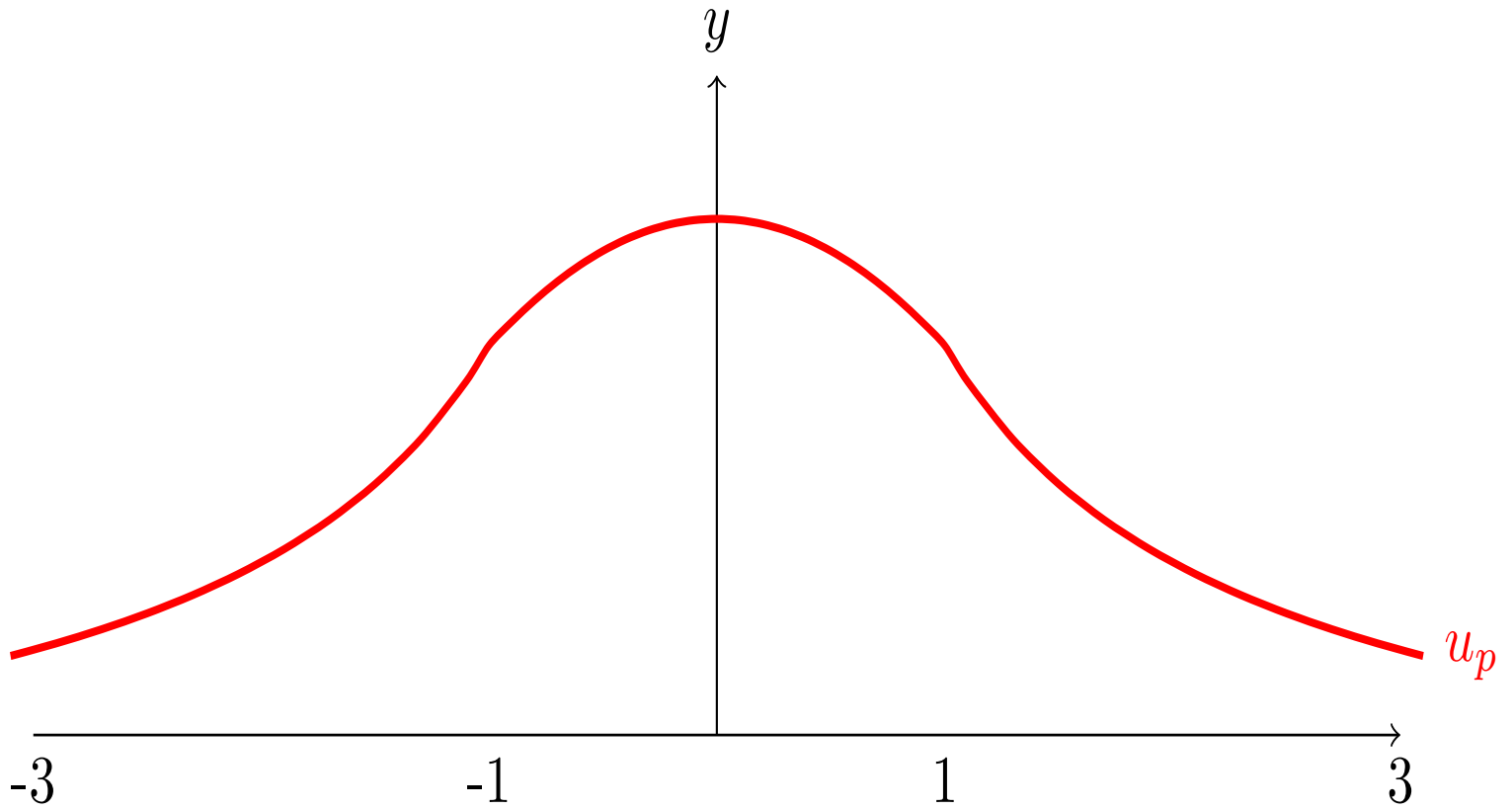
Thus increasing and translation invariant functionals **are never** γ -lower semicontinuous.

- for the problem

$$\max \left\{ F(V) : V \geq 0, \int_{\mathbf{R}^d} V^p dx \leq 1 \right\}$$

most of the results obtained in the case Ω bounded can be repeated.

In the cases $F = \mathcal{E}_f$ and $F = \lambda_1$ in general the optimal potentials **are not** compactly supported, even if f is compactly supported. For instance, taking $f = 1_{B_1}$ the optimal potential V_{opt} is **radially decreasing** and supported in the whole \mathbf{R}^d .



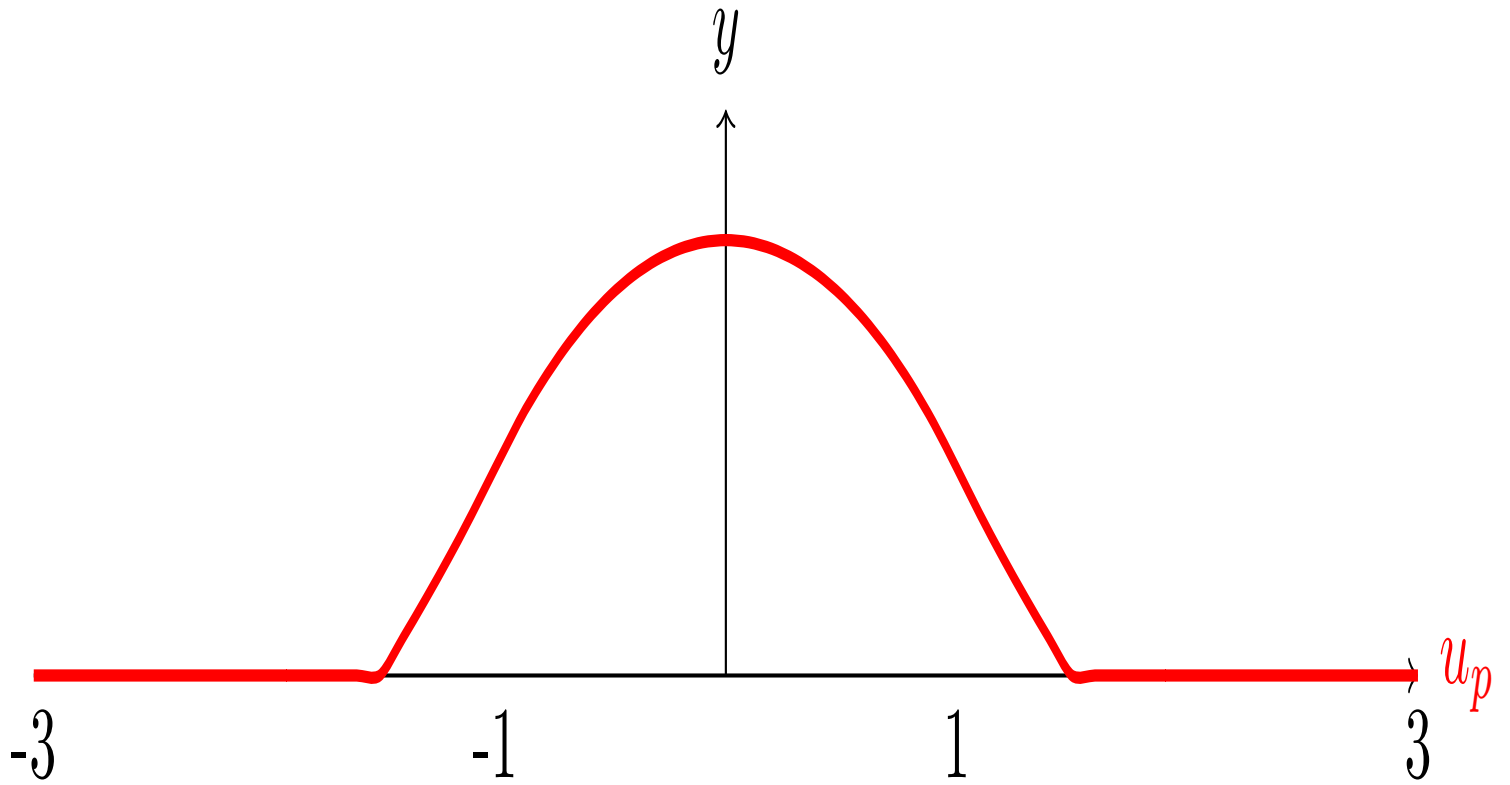
The solution u_p and $f = \chi_{B(0,1)}$ does not have a compact support.

- for the problem

$$\min \left\{ F(V) : V \geq 0, \int_{\mathbf{R}^d} V^{-p} dx \leq 1 \right\}$$

we **do not** have a general existence theorem but only proofs in some **special cases**, as the Dirichlet Energy \mathcal{E}_f (or the first eigenvalue of the Dirichlet Laplacian).

In these cases, if f is compactly supported, we have that $1/V_{opt}$ is compactly supported, that is $V_{opt} = +\infty$ out of a compact set (hence the Dirichlet condition is imposed out of a compact set to the related PDE).



The solution u_p and $f = \chi_{B(0,1)}$ has a compact support.

If we limit ourselves to the **spectral optimization problems**

$$\min \left\{ \lambda_k(V) : V \geq 0, \int_{\mathbf{R}^d} V^{-p} dx \leq 1 \right\}$$

the problems are:

Problem 1. for every k an optimal potential V_k exists;

Problem 2. for every k the optimal potential V_k above is such that $1/V_k$ is compactly supported.

In [Bucur-B.-Velichkov] (paper in preparation) we are able to show that the two problems above have a positive answer.

For the moment the proof cannot be adapted to other kinds of cost functionals $F(V)$, as for instance integral functionals or spectral functionals.