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

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

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

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

The integral cost functionals we consider are of the form

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

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:

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

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

The spectral cost functionals we consider are of the form

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

where $\Phi : \mathbf{R}^{\mathbf{N}} \to \overline{\mathbf{R}}$ 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

$$\lambda_k^n \to \lambda_k \ \forall k \Longrightarrow \Phi(\lambda_n) \to \Phi(\lambda)$$
$$\Big(\text{resp. } \Phi(\lambda) \leq \liminf_n \Phi(\lambda_n)\Big).$$

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:

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

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

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

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

In particular the measure

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

is a capacitary measure and, taking $K = \Omega^c$, the space $H^1_\mu(\Omega)$ becomes in this case the usual Sobolev space $H^1_0(\Omega)$.

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* $u_n \to u$ *in* $L^2(\Omega)$ *we have*

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

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

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

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 $\varphi \in H_0^1(\Omega) \cap L_\mu^2(\Omega)$. The resolvent operator $R_\mu : L^2(\Omega) \to L^2(\Omega)$ 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:

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

Actually, it is enough to have $R_{\mu_n}(1) \to R_\mu(1)$. 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 $\mu_n \to \mu$ for the γ-convergence, the spectrum of the compact resolvent operator $\mathcal{R}_{\mu_n}$ converges to the spectrum of $\mathcal{R}_\mu$; then the eigenvalues of the Schrödinger operator $-\Delta + \mu_n$ defined on $H^1_0(\Omega)$ converge to the corresponding eigenvalues of the operator $-\Delta + \mu$.

The case of bounded constraints

Proposition *If* $V_n \to V$ *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

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

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

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

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

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

Note that in particular, we deduce the conditions of optimality

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

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

$$\min_{u \in H^1_0(\Omega)} \int_\Omega |\nabla u|^2 dx + \left(\int_\Omega |u|^{2p/(1+p)} dx\right)^{(1+p)/p} - \int_\Omega 2fu\,dx$$

which corresponds to the nonlinear PDE

$$-\Delta u + C_p |u|^{-2/(p+1)} u = f, \quad u \in H^1_0(\Omega)$$

where C_p is a constant depending on p.

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

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

where u solves the auxiliary problem

$$\min_{u \in H_0^1(\Omega)} \int_\Omega |\nabla u|^2 dx +$$

$$\frac{1}{\alpha}\int_\Omega u^2\Big(\int_\Omega \log(u^2)dx - \log(u^2)\Big)dx - \int_\Omega 2fudx.$$

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 $\Omega = \mathrm{R}^d$

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 $x_n \to \infty$, the sequence of translated potentials $V_n(x) = V(x + x_n)$ γ-converges to the capacitary measure

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

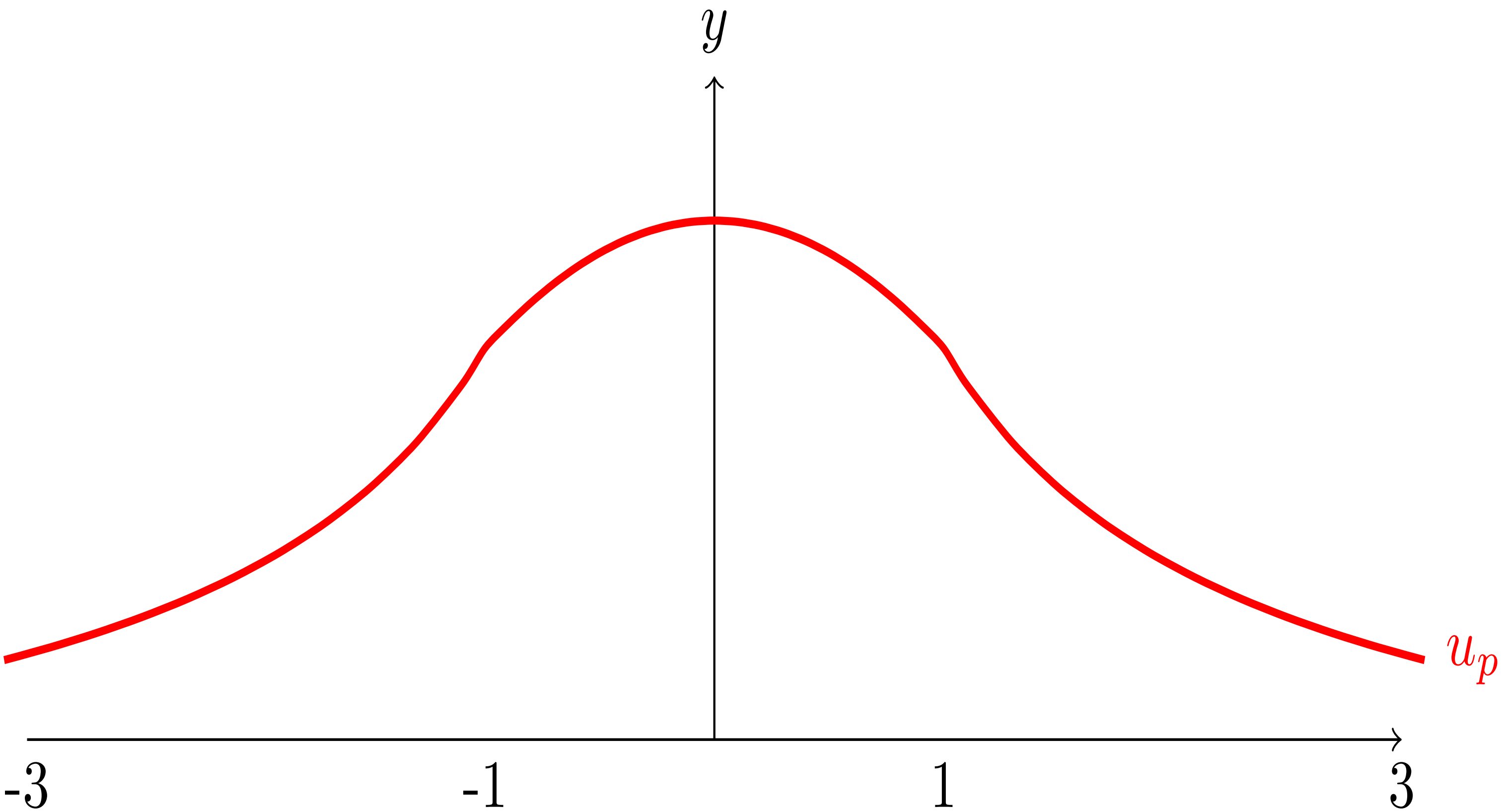
Thus increasing and translation invariant functionals are never γ-lower semicontinuous.

• for the problem

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

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 $\mathbf{R}^d$.



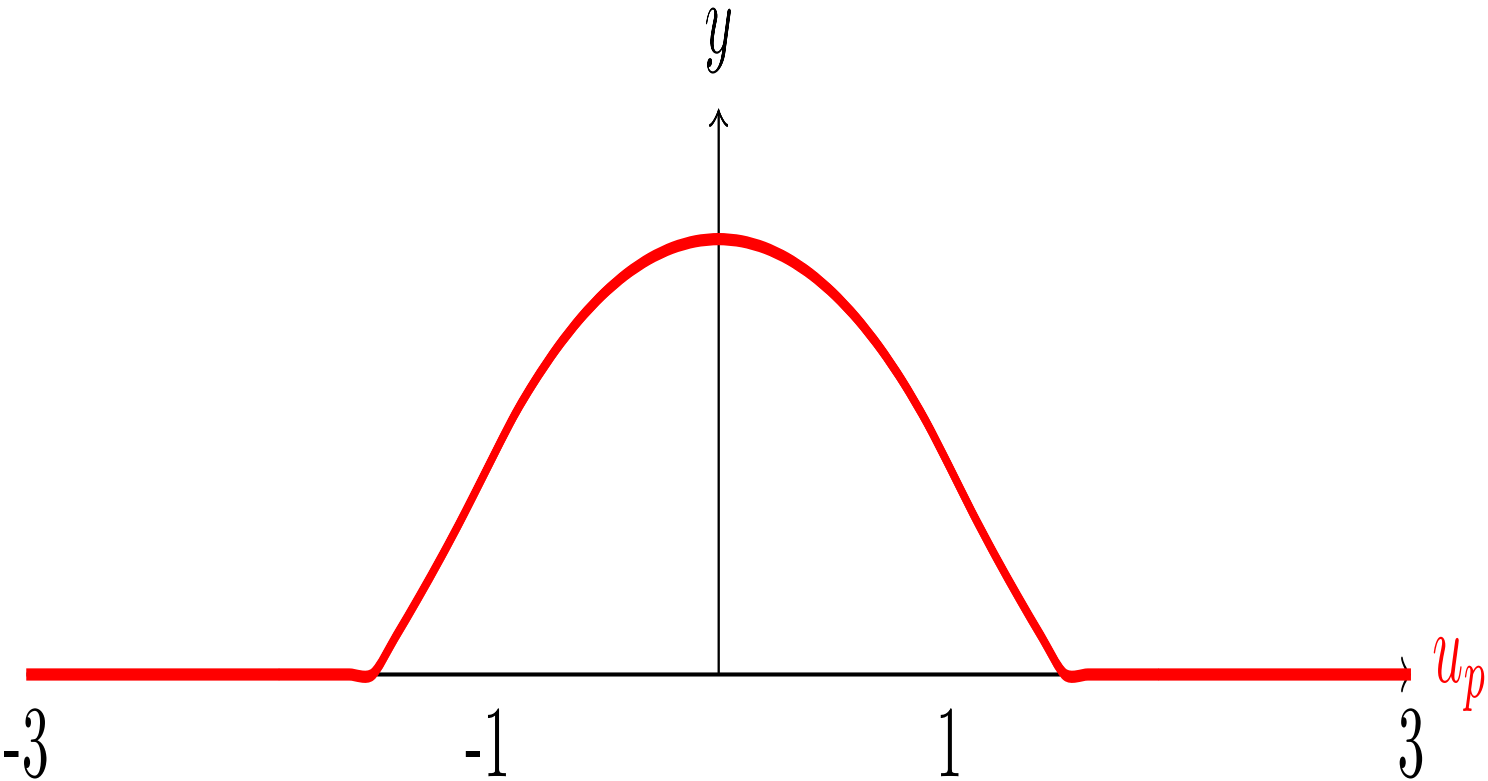
The solution u_p and $f = \chi_{B(0,1)}$ does not have a compact support.

- for the problem

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

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

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

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.