Schrödinger equations with analytic potentials

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Functional setting

We define the space $\mathcal{H}_A$ of analytic functions for $A > 0$ by

$$\mathcal{H}_A := \left\{ u \in \mathrm{L}^2_\#(\mathbb{R}, \mathbb{C}) \;\middle|\; \sum_{k\in\mathbb{Z}} |\widehat{u}_k|^2 \, w_A(k) < \infty \right\},$$

equipped with the norm $\|u\|_A^2 := \sum_{k\in\mathbb{Z}} |\widehat{u}_k|^2 \, w_A(k)$, where $w_A(k) = \cosh(2Ak)$ and the $\widehat{u}_k$'s are the Fourier coefficients of u. There is a direct isometry between $\mathcal{H}_A$ and $\widetilde{\mathcal{H}}_A$ the space of functions that are analytic in a band of size A around the real axis in the complex plane:

$$\widetilde{\mathcal{H}}_A := \left\{ u \text{ analytic on } \mathbb{R} + \mathrm{i}(-A, A) \;\middle|\; \begin{array}{l} [-A, A] \ni y \mapsto u(\cdot + \mathrm{i}y) \in \mathrm{L}^2_\#(\mathbb{R}, \mathbb{C}) \text{ is continuous,} \\ \|u\|^2_{\widetilde{\mathcal{H}}_A} = \frac{1}{2}\int_0^{2\pi} |u(x+iA)|^2 + |u(x-iA)|^2 \, \mathrm{d}x < \infty \end{array} \right\}.$$

Proposition

For $B > 0$ and $V \in \mathcal{H}_B$, the multiplicative operator by V is bounded from $\mathcal{H}_A$ to $\mathcal{H}_A$ for any $0 < A < B$, with $\|V\|_{\mathcal{L}(\mathcal{H}_A)} \to \infty$ when $A \to B$.

Question

To which $\mathcal{H}_A$ the solutions of Schrödinger equations belong if the input data (potential, source terms, ...) are in some $\mathcal{H}_B$ for a given B?

Linear case

Theorem 1

Let $B > 0$ and $V \in \mathcal{H}_B$ be such that $V \geqslant 1$. Then, $\forall\, 0 < A < B$, if $f \in \mathcal{H}_A$, the unique solution u of $-\Delta u + Vu = f$ in $\mathrm{H}^2_\#(\mathbb{R}, \mathbb{C})$ also belongs to $\mathcal{H}_A$. Moreover, we have the following estimate

$$\forall\, \varepsilon > 0, \ \exists\, C_\varepsilon > 0, \ \|u\|_A \leqslant \varepsilon \|f\|_A + C_\varepsilon \|f\|_{\mathrm{L}^2_\#}.$$

Corollary: if V and f are entire, then so is u.

Sketch of proof: Let u be the unique solution to $-\Delta u + Vu = f$ (which we know to belong to $\mathrm{H}^2_\#(\mathbb{R}, \mathbb{C})$ by classical results). For $N > 0$, we decompose it into $u = u_1 + u_2$ where $u_1 \in X_N$ and $u_2 \in X_N^\perp$, where $X_N := \left\{ u \in \mathrm{L}^2_\#(\mathbb{R}, \mathbb{C}) \mid \widehat{u}_k = 0, \ \forall\, |k| > N \right\}$. Then,

- $u_1 \in \mathcal{H}_A$ as it has finite Fourier support;
- $u_2 \in \mathcal{H}_A$ for N large enough: the restriction of $-\Delta + V$ to $X_N^\perp$ is invertible and its inverse is in $\mathcal{L}(\mathcal{H}_A)$ if N is large enough.

Put things together to get that $u = u_1 + u_2 \in \mathcal{H}_A$ for N large enough. □

We can extend, in a similar way, this theorem to the linear eigenvalue problem.

Theorem 2

Let $B > 0$ and $V \in \mathcal{H}_B$. Then, $\forall\, 0 < A < B$, the solution $(u, \lambda) \in \mathrm{H}^2_\#(\mathbb{R}, \mathbb{C}) \times \mathbb{R}$ of the eigenvalue problem,

$$\begin{cases} -\Delta u + Vu = \lambda u, \\ \|u\|_{\mathrm{L}^2_\#(\mathbb{R},\mathbb{C})} = 1, \end{cases} \qquad (1)$$

is such that u also belongs to $\mathcal{H}_A$.

Corollary: if V is entire, then so is u.

Convergence of planewave approximations

Let $(u, \lambda) \in \mathrm{H}^2_\#(\mathbb{R}, \mathbb{C}) \times \mathbb{R}$ be the solution to the linear eigenvalue problem (1) and (u_N, λ_N) be the variational approximation of (u, λ) in $X_N \times \mathbb{R}$. From [1], we know that if $V \in \mathrm{H}^s_\#(\mathbb{R}, \mathbb{C})$ with $s > 1/2$, then there exists $C > 0$, such that

$$\forall\, N > 0, \quad \|u - u_N\|_{\mathrm{H}^1_\#} \leqslant C/N^{s+1}.$$

Here, if $V \in \mathcal{H}_B$ for $B > 0$ ($\Rightarrow V \in \mathrm{H}^s_\#$ for any s) and a consequence of Theorem 2 is that $\forall\, 0 < A < B$, $u \in \mathcal{H}_A$ and there exists $C > 0$, such that $C \to \infty$ when $A \to B$ and

$$\forall\, N > 0, \quad \|u - u_N\|_{\mathrm{H}^1_\#} \leqslant C \exp(-AN).$$

[1] E. Cancès, R. Chakir, and Y. Maday.
Numerical Analysis of Nonlinear Eigenvalue Problems.
Journal of Scientific Computing, 45(1):90–117, 2010.

Nonlinear case: a counter example

In the nonlinear case, such results are not true anymore and we propose the following counter example. Let $f := \mu \sin$ for $\mu > 0$ and u be the solution to the nonlinear Gross-Pitaevskii equation with source term, for some $\varepsilon \geqslant 0$:

$$-\varepsilon \Delta u_\varepsilon + u_\varepsilon + u_\varepsilon^3 = f. \qquad (2)$$

$\underline{\varepsilon = 0}$: The real solution can be obtained with the the Cardan formula, with discriminant $R(x) := -(4 + 27f(x)^2) < 0$ for $x \in [0, 2\pi]$. However, its analytic continuation $\widetilde{u}_0$ has a branching point for $z \in \mathbb{C}$ such that $R(z) = 0$, *i.e.* $z = \pm \mathrm{i}B$ where $f(\mathrm{i}B) = \sqrt{4/27}\mathrm{i}$: $\widetilde{u}_0$ is not entire.

$\underline{\varepsilon > 0}$: We show that u is not in entire even if f is. Let $\psi_\varepsilon(y) := \mathrm{Im}\,(\widetilde{u}_\varepsilon(\mathrm{i}y))$. It solves the ODE:

$$\begin{cases} \varepsilon \ddot{\psi}_\varepsilon + \psi_\varepsilon - \psi_\varepsilon^3 = \mu \sinh, \\ \psi_\varepsilon(0) = 0, \quad \dot{\psi}_\varepsilon(0) = u'_\varepsilon(0). \end{cases} \qquad (3)$$

As soon as ψ_ε reaches $1 + \eta$ for some $\eta > 0$ (which can be justified with combined numerical and convexity arguments), we can use comparison theorems for systems of ODE to prove that ψ_ε is bounded from below by the solution to the ODE

$$\begin{cases} \dot{\xi}_{\varepsilon,\eta} = \frac{1}{2\sqrt{\varepsilon/2}}(\xi^2_{\varepsilon,\eta} - 1), \\ \xi_{\varepsilon,\eta}(y_\eta) = 1 + \eta, \end{cases}$$

whose solution is defined only up to $Y_{\varepsilon,\eta} = \sqrt{\frac{\varepsilon}{2}} \log\left(1 + \frac{2}{\eta}\right) + y_\eta$. As ψ_ε is bounded from below by $\xi_{\varepsilon,\eta}$, it is defined only up to $Y_\varepsilon \leqslant Y_{\varepsilon,\eta}$ and thus $\widetilde{u}_\varepsilon$ is not entire.

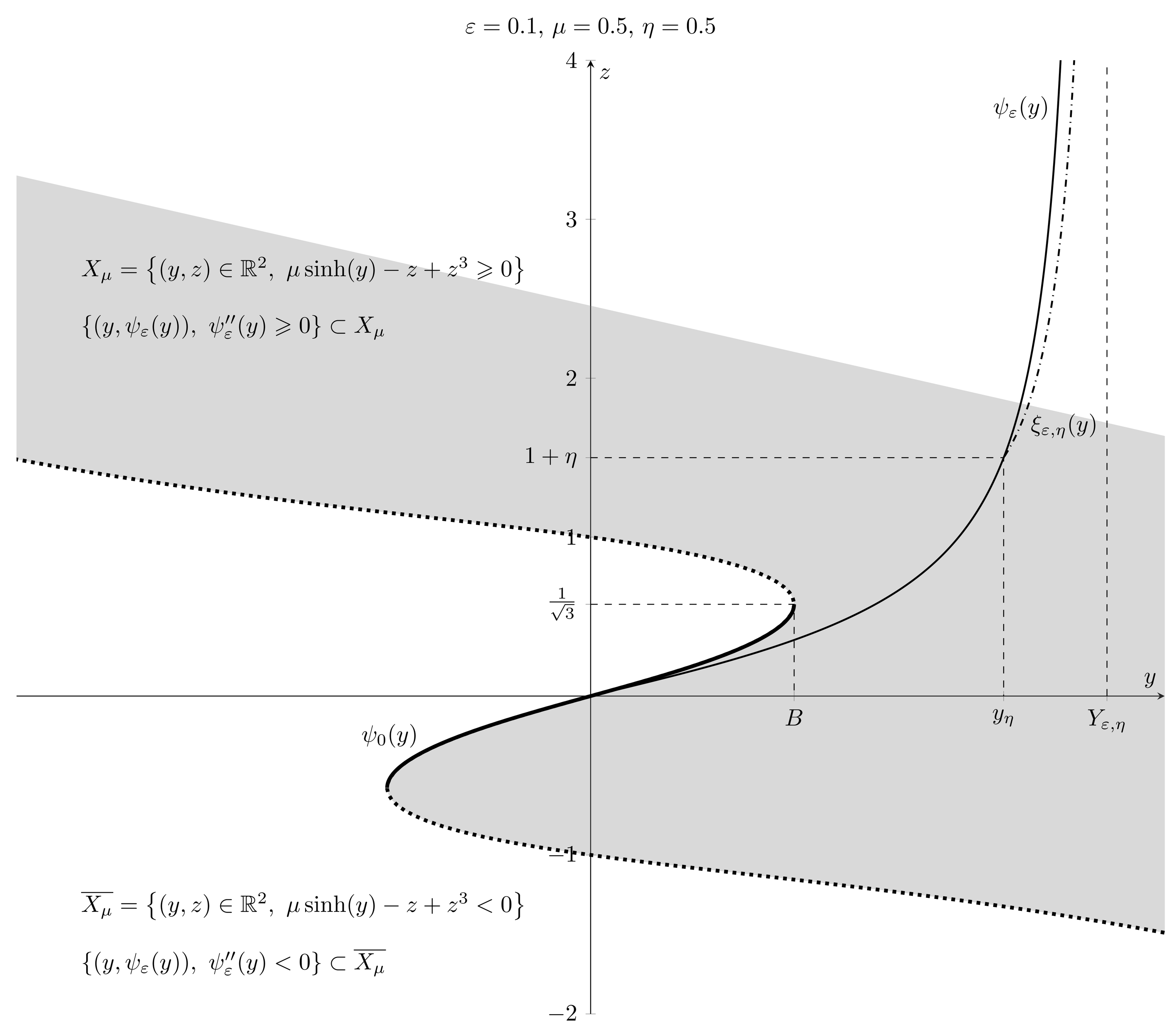

Figure 1: The analytic continuation of the solution to (2) is analytic only on a band of finite size around the real axis, even if f is analytic.