Linear and nonlinear periodic Schrödinger equations with analytic potentials

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Motivation: Kohn–Sham DFT equations with pseudopotentials

- Popular model in quantum chemistry and materials science for its accuracy and computational efficiency.
- The goal is to solve the nonlinear eigenvalue problem

Kinetic and potential term

$$\begin{cases} (H_{\rho_\Phi}\phi_n)(\boldsymbol{x}) := \left(-\frac{1}{2}\Delta + V_{\mathrm{ext}}(\boldsymbol{x})\right)\phi_n(\boldsymbol{x}) + V_{\mathrm{Hxc}}[\rho_\Phi](\boldsymbol{x})\,\phi_n(\boldsymbol{x}) = \lambda_n\phi_n(\boldsymbol{x}), \quad \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_{N_{\mathrm{el}}}, \\ \int_\Omega \phi_n^*(\boldsymbol{x})\phi_m(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = \delta_{nm}, \\ \rho_\Phi(\boldsymbol{x}) = \sum_{n=1}^{N_{\mathrm{el}}} |\phi_n(\boldsymbol{x})|^2 . \end{cases}$$

Nonlinear term modeling the interaction of electrons together

Electronic density

- **Pseudopotentials:** replace the core electrons by a noninteracting equivalent potential to reduce computational time $\Rightarrow V_{\mathrm{ext}} = V_{\mathrm{pseudo}}$.

Pseudopotentials and regularity results

Cancès, Chakir, Maday[1]

For a specific class of V_{Hxc}, it was proved that if $V_{\mathrm{pseudo}} \in \mathrm{H}^s$ for $s > 3/2$, then ϕ_n and ρ are in H^{s+2} $\Rightarrow$ optimal polynomial convergence rates for planewave discretizations in any H^r with $-s < r < s+2$.
This applies to Troullier-Martins pseudopotentials[2], for which $s = \frac{7}{2} - \varepsilon$.

[1] E. Cancès, R. Chakir, and Y. Maday. Numerical analysis of the planewave discretization of some orbital-free and Kohn-Sham models. *ESAIM: Mathematical Modelling and Numerical Analysis*, 46(2):341388, 2012.
[2] N. Troullier and J. L. Martins. Efficient pseudopotentials for plane-wave calculations. *Physical Review B*, 43(3):19932006, 1991.
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What happens for other classes of pseudopotentials ? In particular, Goedecker-Teter-Hutter (GTH) pseudopotentials[3], which have entire continuations to the entire complex plane. The latter applies, but is nonoptimal.

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Objectives

Study the periodic Schrödinger operator $H := -\Delta + V$ when V is a periodic analytic potential, in the case of the linear elliptic equation $Hu = f$ and the eigenvalue problem $Hu = \lambda u$.

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[5] A. Friedman. On the Regularity of the Solutions of Non-Linear Elliptic and Parabolic Systems of Partial Differential Equations. *Indiana University Mathematics Journal*, 7(1):4359, 1958.

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- The size of this neighborhood is *a priori* unknown. In the periodic setting, it has a direct impact on the convergence of the planewave approximation.

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- The size of this neighborhood is *a priori* unknown. In the periodic setting, it has a direct impact on the convergence of the planewave approximation.

$\Rightarrow$ In this talk, we study this question in 1D.

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Some notations

- $\mathrm{L}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$: square-integrable 2π-periodic functions on $\mathbb{R}$, $(\cdot,\cdot)_{\mathrm{L}^2}$ its usual inner product;
- for $u \in \mathrm{L}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ we define its Fourier coefficients

$$\forall\, k \in \mathbb{Z}, \quad \widehat{u}_k := (e_k, u)_{\mathrm{L}^2_{\mathrm{per}}} = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} u(x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x, \quad \text{with } e_k(x) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}kx};$$

- the periodic Sobolev space of order s:

$$\mathrm{H}^s_{\mathrm{per}}(\mathbb{R},\mathbb{C}) := \left\{ u \in \mathrm{L}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C}) \;\middle|\; \sum_{k\in\mathbb{Z}} (1+|k|^2)^s \left|\widehat{u}_k\right|^2 < \infty \right\}, \quad (u,v)_{\mathrm{H}^s_{\mathrm{per}}} := \sum_{k\in\mathbb{Z}} (1+|k|^2)^s \, \overline{\widehat{u}_k}\, \widehat{v}_k.$$

Spaces of analytic functions

Definition

For $A > 0$ define the space

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

endowed with the inner product

$$(u, v)_A := \sum_{k\in\mathbb{Z}} w_A(k)\, \overline{\widehat{u}_k}\, \widehat{v}_k.$$

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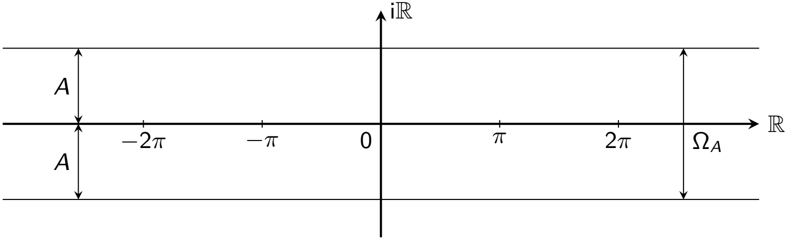
$\mathcal{H}_A$ can be canonically identified with

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

where $\Omega_A := \mathbb{R} + \mathrm{i}(-A,A) \subset \mathbb{C}$, $(u,v)_{\widetilde{\mathcal{H}}_A} = \frac{1}{2}\left((u(\cdot+\mathrm{i}A), v(\cdot+\mathrm{i}A))_{\mathrm{L}^2_{\mathrm{per}}} + (u(\cdot-\mathrm{i}A), v(\cdot-\mathrm{i}A))_{\mathrm{L}^2_{\mathrm{per}}} \right)$.



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Proof:

$$\begin{aligned}
\|u\|^2_{\widetilde{\mathcal{H}}_A} &= \frac{1}{2}\left(\|u(\cdot+\mathrm{i}A)\|^2_{\mathrm{L}^2_{\mathrm{per}}} + \|u(\cdot-\mathrm{i}A)\|^2_{\mathrm{L}^2_{\mathrm{per}}} \right) \\
&= \frac{1}{2}\left(\sum_{k\in\mathbb{Z}} \left|\widehat{u}_k\,\mathrm{e}^{-kA}\right|^2 + \sum_{k\in\mathbb{Z}} \left|\widehat{u}_k\,\mathrm{e}^{+kA}\right|^2 \right) \\
&= \sum_{k\in\mathbb{Z}} w_A(k)\,|\widehat{u}_k|^2 = \|u\|^2_A.
\end{aligned}$$

□

Analytic potentials

Proposition

Let $B > 0$. Then, for all $0 < A < B$, the multiplication by a function $V \in \mathcal{H}_B$ defines a bounded operator on $\mathcal{H}_A$.

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Let $B > 0$. Then, for all $0 < A < B$, the multiplication by a function $V \in \mathcal{H}_B$ defines a bounded operator on $\mathcal{H}_A$.

Proof: Let $V \in \mathcal{H}_B$. It holds, for all $0 < A < B$,

$$\|V\|^2_{\mathcal{L}(\mathcal{H}_A)} = \sup_{u \in \mathcal{H}_A \setminus \{0\}} \frac{\|Vu\|_A^2}{\|u\|_A^2} = \sup_{u \in \mathcal{H}_A \setminus \{0\}} \frac{\|V(\cdot + \mathrm{i}A)u(\cdot + \mathrm{i}A)\|^2_{\mathrm{L}^2_{\mathrm{per}}} + \|V(\cdot - \mathrm{i}A)u(\cdot - \mathrm{i}A)\|^2_{\mathrm{L}^2_{\mathrm{per}}}}{\|u(\cdot + \mathrm{i}A)\|^2_{\mathrm{L}^2_{\mathrm{per}}} + \|u(\cdot - \mathrm{i}A)\|^2_{\mathrm{L}^2_{\mathrm{per}}}}$$

$$\leqslant 2 \max \left\{ \|V(\cdot + \mathrm{i}A)\|^2_{\mathrm{L}^\infty_{\mathrm{per}}}, \|V(\cdot - \mathrm{i}A)\|^2_{\mathrm{L}^\infty_{\mathrm{per}}} \right\} < +\infty.$$

□

The linear Schrödinger equation with source term

For $V \in \mathrm{L}^2_{\mathrm{per}}(\mathbb{R},\mathbb{R})$, $V \geqslant 1$ and $f \in \mathrm{L}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$, we know that the problem

(1) Seek $u \in \mathrm{H}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ such that $-\Delta u + Vu = f$ on $\mathbb{R}$

has a unique solution u satisfying $\|u\|_{\mathrm{L}^2_{\mathrm{per}}} \leqslant \dfrac{\|f\|_{\mathrm{L}^2_{\mathrm{per}}}}{\alpha}$ and $\|u\|_{\mathrm{H}^1_{\mathrm{per}}} \leqslant \|f\|_{\mathrm{H}^{-1}_{\mathrm{per}}}$, where $\alpha = \lambda_1(-\Delta + V) \geqslant 1$.

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Theorem

Let $B > 0$ and $V \in \mathcal{H}_B$ be real-valued and such that $V \geqslant 1$ on $\mathbb{R}$. Then, for all $0 < A < B$ and $f \in \mathcal{H}_A$, the unique solution u of (1) is in $\mathcal{H}_A$. Moreover, we have the following estimate

$$\exists\ C > 0 \text{ independent of } f \text{ such that } \|u\|_A \leqslant C\,\|f\|_A .$$

As a consequence, if V and f are entire, then so is u.

Proof: Let $u \in \mathrm{H}^2_\#(\mathbb{R}, \mathbb{C})$ be the unique solution to $-\Delta u + Vu = f$. 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

$$X_N := \mathrm{Span}\{e_k,\ |k| \leqslant N\}.$$

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Then, write the equations satisfied by $u_{1,2}$ by projecting $-\Delta u + Vu = f$ onto X_N and $X_N^{\perp}$:

- $u_1 \in \mathcal{H}_A$ 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. □

The linear eigenvalue problem

We study the $\mathcal{H}_A$ regularity of the solutions to

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

The linear eigenvalue problem

We study the $\mathcal{H}_A$ regularity of the solutions to

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

Theorem

Let $B > 0$, $V \in \mathcal{H}_B$ be real-valued, and $(u, \lambda) \in \mathrm{H}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C}) \times \mathbb{R}$ a normalized eigenmode of $H = -\Delta + V$, with isolated eigenvalue (i.e. a solution to (2)).
Then, u is in $\mathcal{H}_A$ for all $0 < A < B$. As a consequence, if V is entire, then so is u.

Proof: very similar to $Hu = f$. □

Consequences on the convergence of planewave discretization

We study the convergence of planewave approximation of the linear eigenvalue problem (2).

Planewave approximation: variational approximation in the finite dimensional space

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$$\begin{cases} \text{Seek } (u_N, \lambda_N) \in X_N \times \mathbb{R} \text{ such that } \|u_N\|_{\mathrm{L}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})} = 1 \text{ and} \\ \forall\ v_N \in X_N, \quad \int_0^{2\pi} \overline{\nabla u_N} \cdot \nabla v_N + \int_0^{2\pi} V \overline{u_N} v_N = \lambda_N \int_0^{2\pi} \overline{u_N} v_N, \end{cases}$$

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Theorem

Let $B > 0$, $V \in \mathcal{H}_B$ be real-valued, $j \in \mathbb{N}^*$ and $0 < A < B$. Let λ_j the lowest j^{th} eigenvalue of the self-adjoint operator $H = -\Delta + V$ on $\mathrm{L}^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ counting multiplicities, and $\mathcal{E}_j = \mathrm{Ker}(H - \lambda_j)$ the corresponding eigenspace. For N large enough, we denote by $\lambda_{j,N}$ the lowest j^{th} eigenvalue of (3), and by $u_{j,N}$ an associated normalized eigenvector. Then, there exists a constant $c_{j,A} \in \mathbb{R}_+$ such that

$$\forall\ N > 0 \text{ s.t. } 2\lfloor N \rfloor + 1 \geqslant j, \quad d_{\mathrm{H}^1_{\mathrm{per}}}(u_{j,N}, \mathcal{E}_j) \leqslant c_{j,A} \exp(-AN) \quad \text{and} \quad 0 \leqslant \lambda_{j,N} - \lambda_j \leqslant c_{j,A} \exp(-2AN).$$

The nonlinear case: a counter-example

Consider the Gross-Pitaevskii-type equation, for f with an entire analytic continuation:

$$-\varepsilon\Delta u_\varepsilon + u_\varepsilon + u_\varepsilon^3 = f := \mu \sin\,. \tag{4}$$

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Let $\psi_\varepsilon(y) := \mathrm{Im}\,(u_\varepsilon(\mathrm{i}y))$. It solves the ODE:

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

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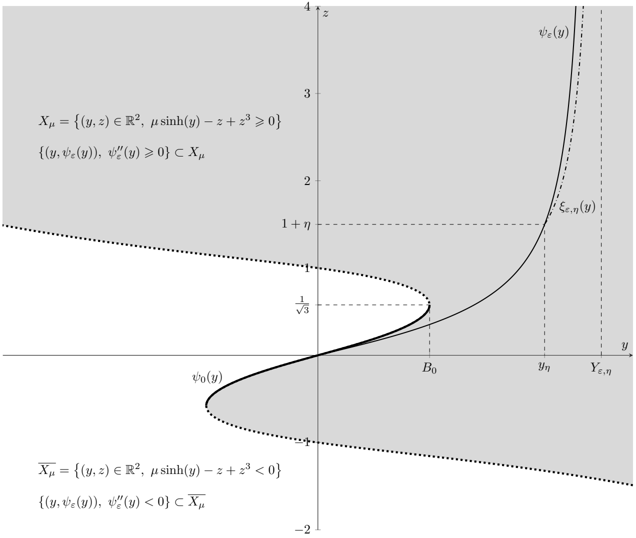
As soon as ψ_ε reaches $1+\eta$ for some $\eta > 0$ (which can be justified with combined numerical and convexity arguments), we can use comparison theorems for systems of ODE to prove that ψ_ε is bounded from below by the solution to the ODE

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

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 u_ε is not entire.

$\varepsilon = 0.1,\ \mu = 0.5,\ \eta = 0.5$



Take-home messages

- Analyticity of the input data (source term, potentials) automatically conveys to the solution in the linear case. In particular, if the data is entire, so is the solution.
- This has direct consequence on the convergence of planewave approximation: the rate is exponential. In particular, for entire data, the numerical approximation converges faster than any exponential.
  $\Rightarrow$ justifies the use of GTH pseudopotentials (*e.g.* in DFTK, see Michael F. Herbst's talk)

Take-home messages

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- This has direct consequence on the convergence of planewave approximation: the rate is exponential. In particular, for entire data, the numerical approximation converges faster than any exponential.
  $\Rightarrow$ justifies the use of GTH pseudopotentials (*e.g.* in DFTK, see Michael F. Herbst's talk)
- In the nonlinear case, such results are not true anymore and determining the analyticity band size must be dealt with case by case.
  $\Rightarrow$ in the periodic setting, planewave approximation with GTH pseudopotentials still converges exponentially

Pre-print available at `https://hal.inria.fr/hal-03692851v2`.

Joint work with

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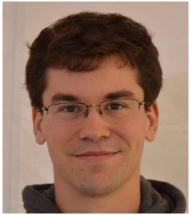

Merci !