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A PRIORI ERROR ANALYSIS OF LINEAR AND NONLINEAR PERIODIC SCHRÖDINGER EQUATIONS WITH ANALYTIC POTENTIALS

ERIC CANCÈS, GASPARD KEMLIN, AND ANTOINE LEVITT

Abstract. This paper is concerned with the numerical analysis of linear and nonlinear Schrödinger equations with analytic potentials. While the regularity of the potential (and the source term when there is one) automatically conveys to the solution in the linear cases, this is no longer true in general in the nonlinear case. We also study the rate of convergence of the planewave (Fourier) discretization method for computing numerical approximations of the solution.

1. Introduction

Kohn-Sham Density Functional Theory (KS-DFT) is currently the most popular model in quantum chemistry and materials science as it offers a good compromise between accuracy and computational efficiency. KS-DFT aims at computing, for a given configuration of the nuclei of the molecular system or material of interest, the electronic ground-state energy and density. From the latter, it is possible to compute the effective forces acting on the nuclei in this configuration, and thus to identify the (meta)stable equilibrium configurations of the system, or to simulate the dynamics of the molecular system in various thermodynamic conditions. In materials science applications, computations are commonly done in a periodic simulation cell, which can be either the unit cell of a crystal (for the special case of perfect crystals), or a supercell (for all the other cases: crystals with defects, disordered alloys, glassy materials, liquids...).

We denote by $\mathbb{L} = \mathbb{Z}\boldsymbol{a}_1 + \mathbb{Z}\boldsymbol{a}_2 + \mathbb{Z}\boldsymbol{a}_3$ the periodic lattice, where $(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)$ is a non-necessarily orthonormal basis of $\mathbb{R}^3$, and by $\Omega = [0,1)\boldsymbol{a}_1 + [0,1)\boldsymbol{a}_2 + [0,1)\boldsymbol{a}_3$ the simulation cell. Let us denote by

$$L^2_{\mathrm{per},\mathbb{L}} := \{u \in L^2_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{C}) \mid u \ \text{ is } \mathbb{L}\text{-periodic}\}$$

the Hilbert space of complex-valued $\mathbb{L}$-periodic locally square integrable functions on $\mathbb{R}^3$, endowed with its usual inner product. The KS-DFT equations read

$$H_\rho \varphi_i = \lambda_i \varphi_i, \quad (\varphi_i, \varphi_j)_{L^2_{\mathrm{per},\mathbb{L}}} = \delta_{ij}, \quad \rho(\boldsymbol{x}) = \sum_{i=1}^{N_\mathrm{p}} |\varphi_i(\boldsymbol{x})|^2, \tag{1}$$

where H_ρ is the Kohn-Sham Hamiltonian, a self-adjoint operator on $L^2_{\mathrm{per},\mathbb{L}}$ bounded below and with compact resolvent. The φ_i's are the Kohn-Sham orbitals, and the λ_i's their energies. Since H_ρ depends on ρ, which in turn depends on the eigenfunctions φ_i, $1 \leqslant i \leqslant N_\mathrm{p}$, (1) is a nonlinear eigenproblem. The parameter N_p represents physically the number of valence electron pairs per simulation cell and ρ the ground-state electronic density. We assume here, and this is the case for most physical systems, that $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_{N_\mathrm{p}}$ are the lowest N_p eigenvalues of H_ρ (*Aufbau* principle). The Kohn-Sham Hamiltonian with pseudopotentials reads

$$H_\rho = -\frac{1}{2}\Delta + V_\mathrm{nl} + V^{\mathrm{Hxc}}_{\mathrm{loc},\rho}$$

where V_nl is a finite-rank self-adjoint operator (the nonlocal part of the pseudopotential), and

$$V^{\mathrm{Hxc}}_{\mathrm{loc},\rho}(\boldsymbol{x}) = V_\mathrm{loc}(\boldsymbol{x}) + V_{\mathrm{H},\rho}(\boldsymbol{x}) + V_{\mathrm{xc},\rho}(\boldsymbol{x})$$

is a periodic real-valued function depending (nonlocally) on ρ. The function V_loc is the local component of the pseudopotential, the Hartree potential $V_{\mathrm{H},\rho}$ is the unique solution with zero mean to the periodic Poisson equation

$$-\Delta V_{\mathrm{H},\rho}(\boldsymbol{x}) = 4\pi\left(\rho(\boldsymbol{x}) - \frac{1}{|\Omega|}\int_\Omega \rho\right), \qquad \int_\Omega V_{\mathrm{H},\rho} = 0,$$

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and the function $V_{\mathrm{xc},\rho}$, called the exchange-correlation potential, depends on the chosen approximation of the exchange-correlation energy functional. In the simple Xα model [18], $V_{\mathrm{xc},\rho}(\boldsymbol{x}) = -C_{\mathrm{D}}\rho(\boldsymbol{x})^{1/3}$, where $C_{\mathrm{D}} > 0$ is the Dirac constant.

It is not mandatory to use pseudopotentials in KS-DFT calculations. Some softwares allow for all-electrons calculations in which the total pseudopotential operator $V_{\mathrm{nl}} + V_{\mathrm{loc}}$ is replaced with a local potential with Coulomb singularities at the positions of the nuclei. However, most calculations are done with pseudopotentials, or use the formally similar Projector Augmented Wave (PAW) method [5], for three reasons: (i) core electrons are barely affected by the chemical environment and can usually be considered to occupy "frozen states", (ii) in heavy atoms, core electrons must be dealt with relativistic quantum models which makes the simulation more expensive from a computational viewpoint, (iii) due to the Coulomb singularities, all-electron Kohn-Sham orbitals have cusps at the positions of the nuclei and are therefore only Lipschitz continuous, while the Kohn-Sham orbitals computed with pseudopotentials are much more regular and can be well approximated with Fourier spectral methods (usually called planewave discretization methods in the field).

Several methods for constructing pseudopotentials have been proposed in the literature, leading to local and nonlocal functions of different regularities. As expected, the rate of convergence of the planewave discretization method is directly linked to the regularities of these functions. The *a priori* error analysis of this problem was performed in [7] for pseudopotential with Sobolev regularity. It was proved in particular, for the simple Xα exchange-correlation functional, but also for the much more popular local density approximation (LDA) exchange-correlation functional, that if the local and nonlocal part of the pseudopotential are in the periodic Sobolev space of order $s > 3/2$, then the Kohn-Sham orbitals φ_i and the density ρ are in the periodic Sobolev space of order $s+2$, and (optimal) polynomial convergence rates were obtained in any Sobolev spaces of order r with $-s < r < s+2$. In addition, as for linear second-order elliptic eigenproblems, the error on the eigenvalues converges to zero as the square of the error on the eigenfunctions evaluated in H^1-norm. The analysis in [7] covers for example the case of Troullier-Martins pseudopotentials [19], for which $s = \frac{7}{2} - \epsilon$. On the other hand, these estimates are not sharp in the case of Goedecker-Teter-Hutter (GTH) pseudopotentials [10, 12], for which the local and nonlocal contributions are periodic sums of Gaussian-polynomial functions, and therefore have entire continuations to the whole complex plane. Such pseudopotentials are implemented in different DFT softwares, such as BigDFT [16], Quantum Espresso [9] or Abinit [11, 17], as well as DFTK, a recent electronic structure package in the Julia language [14].

The purpose of this paper is to investigate this case. While it has been known for a long time (see e.g. [3, 8, 15] and references therein for historical insight or [4, 13] for more recent developments) that the solutions to elliptic equations on $\mathbb{R}^d$ with real-analytic data have an analytic continuation in a complex neighborhood of $\mathbb{R}^d$, the size of this neighborhood is *a priori* unknown. In the periodic case we are considering, the latter directly impact the decay rate of the Fourier coefficients of the solution, hence the convergence rate of the planewave discretization method. For pedagogical reasons, we will work most of the time with one dimensional linear or nonlinear Schrödinger equations, because (i) it is easier to visualize analytic or entire continuations of functions originally defined on the real space $\mathbb{R}^d$ when $d = 1$, and (ii) exponential convergence rates of planewave discretization methods are easier to spot in 1D. However, most of our arguments extend to the multidimensional case. In Section 2, we introduce a hierarchy of spaces $(\mathcal{H}_A)_{A>0}$ of complex-valued 2π-periodic functions on the real line having analytic continuations to the strip $\mathbb{R} + i(-A, A)$. We then pick a real-valued function $V \in \mathcal{H}_B$ for some $B > 0$ and consider the one-dimensional Schrödinger operator $H = -\Delta + V$. A low *vs* high-frequency decomposition of the periodic L^2 space allows to prove that for all $0 < A < B$, the solution u to the linear equation $Hu = f$ lays in $\mathcal{H}_A$ whenever $f \in \mathcal{H}_A$ (see subsection 3.1), and that the eigenfunctions of H are in $\mathcal{H}_A$ (see subsection 3.2). We rely on this result to prove in subsection 3.3 that the planewave discretization method converges exponentially in this case. We turn in Section 4 to the nonlinear setting, where we expose a counter example for which we show that such results are not true anymore. Finally, we consider in Section 5 the multidimensional case, which is an immediate extension, and its application to Kohn-Sham models.

2. Spaces of analytic functions

Let us first introduce some notation. We denote by $L^2_{\mathrm{per}}(\mathbb{R}, \mathbb{C})$ the space of square integrable complex-valued 2π-periodic functions on $\mathbb{R}$, endowed with its natural inner product

$$(u, v)_{L^2_{\mathrm{per}}} := \int_0^{2\pi} \overline{u(x)}\, v(x)\, dx,$$

and by $\mathcal{S}'_{\rm per}(\mathbb{R},\mathbb{C})$ the space of tempered complex-valued 2π-periodic distributions on $\mathbb{R}$. For each $u \in \mathcal{S}'_{\rm per}(\mathbb{R},\mathbb{C})$, we denote by $(\widehat{u}_k)_{k\in\mathbb{Z}}$ the Fourier coefficients of u with the following normalization convention:

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

where $e_k(x) := \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}kx}$ is the $L^2_{\rm per}$-normalized Fourier mode with wavevector $k \in \mathbb{Z}$. Recall that the 2π-periodic Sobolev spaces are the Hilbert spaces $H^s_{\rm per}(\mathbb{R},\mathbb{C})$, $s \in \mathbb{R}$, defined by

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

We will also use the self-explanatory notation $C^k_{\rm per}(\mathbb{R},\mathbb{R})$, $C^k_{\rm per}(\mathbb{R},\mathbb{C})$, $L^p_{\rm per}(\mathbb{R},\mathbb{R})$, $L^p_{\rm per}(\mathbb{R},\mathbb{C})$ for $k \in \mathbb{N} \cup \{\infty\}$ and $1 \leqslant p \leqslant \infty$, all these spaces being endowed with their natural norms or topologies. We now introduce, for any $A > 0$, the space

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

endowed with the inner product

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

Note that $\mathcal{H}_A$ can be canonically identified with the space of analytic functions

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

where $\Omega_A := \mathbb{R} + \mathrm{i}(-A,A) \subset \mathbb{C}$ is the horizontal strip of width $2A$ of the complex plane centered on the real axis, endowed with the inner product

$$(u,v)_{\widetilde{\mathcal{H}}_A} = \frac{1}{2} \left((u(\cdot + \mathrm{i}A), v(\cdot + \mathrm{i}A))_{L^2_{\rm per}} + (u(\cdot - \mathrm{i}A), v(\cdot - \mathrm{i}A))_{L^2_{\rm per}} \right).$$

The canonical unitary mapping $\mathcal{H}_A$ onto $\widetilde{\mathcal{H}}_A$ is the analytic continuation: any function $u \in \mathcal{H}_A$ has a unique analytic continuation $u : \Omega_A \to \mathbb{C}$ given by

$$\forall\, z = x + \mathrm{i}y \in \Omega_A, \quad u(z) = \sum_{k\in\mathbb{Z}} \widehat{u}_k \, \frac{\mathrm{e}^{\mathrm{i}kz}}{\sqrt{2\pi}} = \sum_{k\in\mathbb{Z}} \widehat{u}_k \, \mathrm{e}^{-ky} \, e_k(x).$$

It can be easily seen that the Fourier coefficients of $u(\cdot \pm \mathrm{i}A)$ are the Fourier coefficients of u rescaled by a factor $\mathrm{e}^{\mp kA}$ and that the function $(-A,A) \ni y \mapsto u(\cdot + \mathrm{i}y) = \sum_{k\in\mathbb{Z}} \widehat{u}_k \, \mathrm{e}^{-ky} \, e_k(\cdot) \in L^2_{\rm per}(\mathbb{R},\mathbb{C})$ has a unique continuation to $[-A,A]$. Therefore,

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

Proposition 1. *Let $B > 0$. Then, for all $0 < A < B$, the multiplication by a function $V_B \in \mathcal{H}_B$ defines a bounded operator on $\mathcal{H}_A$.*

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

$$\begin{aligned} \|V\|^2_{\mathcal{L}(\mathcal{H}_A)} &= \sup_{u \in \mathcal{H}_A \setminus \{0\}} \frac{\|Vu\|^2_A}{\|u\|^2_A} = \sup_{u \in \mathcal{H}_A \setminus \{0\}} \frac{\|V(\cdot + \mathrm{i}A) u(\cdot + \mathrm{i}A)\|^2_{L^2_{\rm per}} + \|V(\cdot - \mathrm{i}A) u(\cdot - \mathrm{i}A)\|^2_{L^2_{\rm per}}}{\|u(\cdot + \mathrm{i}A)\|^2_{L^2_{\rm per}} + \|u(\cdot - \mathrm{i}A)\|^2_{L^2_{\rm per}}} \\ &\leqslant 2 \max \left\{ \|V(\cdot + \mathrm{i}A)\|^2_{L^\infty_{\rm per}}, \|V(\cdot - \mathrm{i}A)\|^2_{L^\infty_{\rm per}} \right\}. \end{aligned}$$

As the right hand-side is finite for all $0 < A < B$, the proposition follows. $\square$

3. The linear case

3.1. **The linear elliptic problem.** We consider in a first stage the one-dimensional linear elliptic problem

$$\text{seek } u \in H^2_{\text{per}}(\mathbb{R},\mathbb{C}) \quad \text{such that} \quad -\Delta u + Vu = f \text{ on } \mathbb{R}, \tag{2}$$

where $V \in L^2_{\text{per}}(\mathbb{R},\mathbb{R})$ and $f \in L^2_{\text{per}}(\mathbb{R},\mathbb{C})$ are given 2π-periodic functions. For simplicity, we assume in this section that $V \geqslant 1$, a sufficient condition for the operator $-\Delta + V$ to be invertible. It is well-known that (2) has a unique solution u satisfying the *a priori* bounds

$$\|u\|_{L^2_{\text{per}}} \leqslant \frac{\|f\|_{L^2_{\text{per}}}}{\alpha} \quad \text{and} \quad \|u\|_{H^1_{\text{per}}} \leqslant \|f\|_{H^{-1}_{\text{per}}}, \tag{3}$$

where $\alpha := \lambda_1(-\Delta + V) \geqslant 1$ is the smallest eigenvalue of the self-adjoint operator $H = -\Delta + V$ on $L^2_{\text{per}}(\mathbb{R},\mathbb{C})$. By elementary bootstrap arguments, $u \in H^{s+2}_{\text{per}}(\mathbb{R},\mathbb{C})$ whenever V and f are in H^s_{per}, for any $s \geqslant 0$. The following result deals with the case of real-analytic potentials V and right-hand sides f.

Theorem 1. *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 (2) is in $\mathcal{H}_A$. Moreover, we have the following estimate*

$$\exists\, C > 0 \text{ independent of } f \text{ such that } \|u\|_A \leqslant C\,\|f\|_A\,. \tag{4}$$

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

Proof. For $N > 0$, we consider the decomposition $L^2_{\text{per}}(\mathbb{R},\mathbb{C}) = X_N \oplus X_N^\perp$ where

$$X_N := \text{Span}(e_k,\ |k| \leqslant N) = \left\{u \in L^2_{\text{per}}(\mathbb{R},\mathbb{C}) \mid \widehat{u}_k = 0,\ \forall\ |k| > N\right\}. \tag{5}$$

Let Π_N be the orthogonal projector on X_N and $\Pi_N^\perp := 1 - \Pi_N$ the orthogonal projector on $X_N^\perp$. Note that the restriction of Π_N to the Sobolev space $H^s_{\text{per}}(\mathbb{R},\mathbb{C})$, $s > 0$, is also the orthogonal projector on X_N for the H^s_{per} inner product, and that the same property holds for the Hilbert spaces $\mathcal{H}_A$.

For a fixed N, we decompose u as $u = u_1 + u_2$ with $u_1 \in X_N$ and $u_2 \in X_N^\perp$. As u_1 has compact Fourier support, it obviously belongs to $\mathcal{H}_A$ and we have the estimate

$$\|u_1\|_A \leqslant \|u\|_{L^2_{\text{per}}} \sqrt{w_A(N)} \leqslant \frac{\|f\|_{L^2_{\text{per}}}}{\alpha} \sqrt{w_A(N)}. \tag{6}$$

Let us show that, for N large enough, u_2 also belongs to $\mathcal{H}_A$. Projecting $-\Delta u + Vu = f$ onto $X_N^\perp$, we get

$$T_{22}u_2 + V_{22}u_2 = f_2 - V_{21}u_1, \tag{7}$$

where T_{22} is the restriction to the invariant subspace $\mathcal{H}_A \cap X_N^\perp$ of the self-adjoint operator $-\Delta$ on $L^2_{\text{per}}(\mathbb{R},\mathbb{C})$, $V_{22} := \Pi_N^\perp V \Pi_N^\perp \in \mathcal{L}(\mathcal{H}_A \cap X_N^\perp)$, $V_{21} := \Pi_N^\perp V \Pi_N \in \mathcal{L}(\mathcal{H}_A \cap X_N, \mathcal{H}_A \cap X_N^\perp)$ and $f_2 := \Pi_N^\perp f \in \mathcal{H}_A \cap X_N^\perp$. The operator T_{22} is bounded from below by N^2 and is therefore invertible with inverse T_{22}^{-1} bounded by N^{-2} in $\mathcal{L}(\mathcal{H}_A \cap X_N^\perp)$. As $f_2, V_{21}u_1 \in \mathcal{H}_A \cap X_N^\perp$, we can therefore rewrite (7) as

$$(1 + T_{22}^{-1}V_{22})u_2 = T_{22}^{-1}(f_2 - V_{21}u_1). \tag{8}$$

Since $\|T_{22}^{-1}\|_{\mathcal{L}(\mathcal{H}_A \cap X_N^\perp)} \leqslant N^{-2}$ and $\|V_{22}\|_{\mathcal{L}(\mathcal{H}_A \cap X_N^\perp)} \leqslant \|V\|_{\mathcal{L}(\mathcal{H}_A)}$, the operator $(1 + T_{22}^{-1}V_{22}) \in \mathcal{L}(\mathcal{H}_A \cap X_N^\perp)$ is invertible for N large enough and it holds

$$u_2 = (1 + T_{22}^{-1}V_{22})^{-1}T_{22}^{-1}(f_2 - V_{21}u_1) = \left(\sum_{n=0}^{+\infty}(-1)^n(T_{22}^{-1}V_{22})^n\right)T_{22}^{-1}(f_2 - V_{21}u_1). \tag{9}$$

Putting things together with Neumann series, we get

$$\begin{aligned} \|u_2\|_A &\leqslant \frac{\|f_2\|_A + \|V_{21}u_1\|_A}{N^2 - \|V\|_{\mathcal{L}(\mathcal{H}_A)}} \leqslant \frac{\|f\|_A + \|V\|_{\mathcal{L}(\mathcal{H}_A)}\,\|u_1\|_A}{N^2 - \|V\|_{\mathcal{L}(\mathcal{H}_A)}} \\ &\leqslant \frac{\|f\|_A}{N^2 - \|V\|_{\mathcal{L}(\mathcal{H}_A)}} + \|V\|_{\mathcal{L}(\mathcal{H}_A)} \frac{\|f\|_{L^2_{\text{per}}}}{\alpha} \frac{\sqrt{w_A(N)}}{N^2 - \|V\|_{\mathcal{L}(\mathcal{H}_A)}}, \end{aligned} \tag{10}$$

Finally, combining (6) and (10) with $\|u\|_A \leqslant \|u_1\|_A + \|u_2\|_A$ yields the bound on $\|u\|_A$. □

Remark 1. If we require in addition that $V(\cdot \pm \mathrm{i}B)$ is not only in $L^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ but also in $L^\infty_{\mathrm{per}}(\mathbb{R},\mathbb{C})$, then the exact same argument as in the proof of Proposition 1 yields

$$\|V\|_{\mathcal{L}(\mathcal{H}_B)} \leqslant 2\max\left\{\|V(\cdot+\mathrm{i}B)\|_{L^\infty_{\mathrm{per}}}, \|V(\cdot-\mathrm{i}B)\|_{L^\infty_{\mathrm{per}}}\right\},$$

so that $f \in \mathcal{H}_B$ then implies $u \in \mathcal{H}_B$.

3.2. **The linear eigenvalue problem.** We now focus on the linear eigenvalue problem,

$$\begin{cases} -\Delta u + Vu = \lambda u, \\ \|u\|_{L^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})} = 1, \end{cases} \tag{11}$$

where $V \in \mathcal{H}_B$ for some $B > 0$. Using the same technique as for the proof of Theorem 1, we get the following result.

Theorem 2. *Let $B > 0$, $V \in \mathcal{H}_B$ be real-valued, and $(u,\lambda) \in H^2_{\mathrm{per}}(\mathbb{R},\mathbb{C}) \times \mathbb{R}$ a normalized eigenmode of $H = -\Delta + V$, with isolated eigenvalue (i.e. a solution to (11)). Then, u is in $\mathcal{H}_A$ for all $0 < A < B$. Moreover, we have the following estimate*

$$\|u\|_A \leqslant \left(1 + \|V\|_{\mathcal{L}(\mathcal{H}_A)}\right)\sqrt{w_A\left(\sqrt{\|V\|_{\mathcal{L}(\mathcal{H}_A)} + \lambda + 1}\right)}.$$

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

Proof. Although the proof of Theorem 2 follows basically the same lines as the one of Theorem 1, we provide it for the sake of completeness.

Let $(u,\lambda) \in H^2_{\mathrm{per}}(\mathbb{R},\mathbb{C}) \times \mathbb{R}$ be a solution to (11). Using the same notation as in the proof of Theorem 1, we decompose u as $u = u_1 + u_2$ with $u_1 \in X_N$ and $u_2 \in X_N^\perp$, and observe that for N large enough,

$$u_2 = -(1 + T_{22}^{-1}(V_{22} - \lambda))^{-1} T_{22}^{-1} V_{21} u_1,$$

with

$$\left\|T_{22}^{-1}(V_{22} - \lambda)\right\|_{\mathcal{L}(\mathcal{H}_A \cap X_N^\perp)} \leqslant \frac{\|V\|_{\mathcal{L}(\mathcal{H}_A)} + |\lambda|}{N^2}.$$

Therefore, choosing $N_\lambda = \sqrt{\|V\|_{\mathcal{L}(\mathcal{H}_A)} + |\lambda| + 1}$, we have

$$\left\|(1 + T_{22}^{-1}(V_{22} - \lambda))^{-1} T_{22}^{-1}\right\|_{\mathcal{L}(\mathcal{H}_A \cap X_{N_\lambda}^\perp)} < 1,$$

which yields

$$\|u_2\|_A \leqslant \|V\|_{\mathcal{L}(\mathcal{H}_A)} \sqrt{w_A(N_\lambda)}.$$

Combining this with $\|u_1\|_A \leqslant \sqrt{w_A(N_\lambda)}$ yields the desired estimate. □

3.3. **Planewave approximation of the linear Schrödinger equation.** Using $X_N = \mathrm{Span}(e_k,\ |k| \leqslant N) \subset H^1_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ as a variational approximation space for (11), we obtain the finite-dimensional problem

$$\begin{cases} \text{seek } (u_N, \lambda_N) \in X_N \times \mathbb{R} \text{ such that } \|u_N\|_{L^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})} = 1 \text{ and} \\ \forall\ v_N \in X_N, \quad \displaystyle\int_0^{2\pi} \overline{\nabla u_N} \cdot \nabla v_N + \int_0^{2\pi} V \overline{u_N} v_N = \lambda_N \int_0^{2\pi} \overline{u_N} v_N, \end{cases} \tag{12}$$

which is equivalent to seeking the eigenpairs of the Hermitian matrix $H_N \in \mathbb{C}^{\mathcal{N}\times\mathcal{N}}_{\mathrm{herm}}$, where $\mathcal{N} = 2\lfloor N \rfloor + 1$, with entries

$$[H_N]_{kk'} := |k|^2 \delta_{kk'} + \widehat{V}_{k-k'}, \quad k,k' \in \mathbb{Z},\ |k| \leqslant N,\ |k'| \leqslant N.$$

The following theorem states that if $V \in \mathcal{H}_B$ for some $B > 0$, the planewave discretization method has an exponential convergence rate. Note that a similar result holds for the planewave approximation of the linear problem $-\Delta u + Vu = f$, whenever $f \in \mathcal{H}_A$.

Theorem 3. *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 $L^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ 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 (12), and by $u_{j,N}$ an associated normalized eigenvector. Then, there exists a constant $c_{j,A} \in \mathbb{R}_+$ such that*

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

Proof. First, note that $-\Delta + V$ has compact resolvent so that its eigenvalues λ_j are isolated. Let $0 < A < B$ and $A' = \frac{A+B}{2}$. We have

$$\forall\, v \in \mathcal{H}_{A'}, \quad \|v - \Pi_N v\|_{H^1_{\mathrm{per}}} \leqslant c_{A,B}\|v\|_{A'}\mathrm{e}^{-AN} \quad \text{with} \quad c_{A,B} := \left(\max_{k\in\mathbb{Z}} \frac{(1+|k|^2)\mathrm{e}^{2A|k|}}{w_{A'}(k)}\right)^{1/2} < \infty.$$

The operator H is self-adjoint on $L^2_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ with form domain $H^1_{\mathrm{per}}(\mathbb{R},\mathbb{C})$ and it follows from Theorem 2 that all the eigenfunctions of the operator H are in $\mathcal{H}_{A'}$. The result follows from classical arguments on the variational approximations of the eigenmodes of bounded below self-adjoint operators with compact resolvent (see e.g. [1, Theorems 8.1 and 8.2]). □

4. The nonlinear case: a counter-example

Still in the perspective of studying nonlinear elliptic problems with analytic data, we now consider the nonlinear periodic elliptic equation with cubic nonlinearity

$$-\varepsilon\Delta u_\varepsilon + u_\varepsilon + u_\varepsilon^3 = f \quad \text{in } H^1_{\mathrm{per}}(\mathbb{R},\mathbb{R}), \tag{13}$$

where $\varepsilon > 0$, and $f : \mathbb{R} \to \mathbb{R}$ is a real-analytic 2π-periodic function admitting an entire continuation, still denoted by f, to the complex plane. We will show that, in this particular case, the same kind of results are not true anymore and we provide an estimation of the width of the horizontal analyticity strip of the solution, which is finite even though the source term f is.

The singular limit $\varepsilon = 0$ gives rise to the algebraic equation $u_0(x) + u_0(x)^3 = f(x)$, which has a unique real solution for each $x \in \mathbb{R}$. The latter can be computed by Cardano's formula: the discriminant of the cubic equation is

$$R(x) = -\left(4 + 27f^2(x)\right) < 0,$$

so that

$$u_0(x) = \sqrt[3]{\frac{1}{2}\left(f(x) + \sqrt{\frac{-R(x)}{27}}\right)} + \sqrt[3]{\frac{1}{2}\left(f(x) - \sqrt{\frac{-R(x)}{27}}\right)}, \tag{14}$$

the other two roots being complex conjugates with nonzero imaginary parts.

In the rest of this section, we will use the function $f : x \mapsto \mu\sin(x)$, for a fixed $\mu > 0$. The analytic continuation of the function u_0 originally defined on $\mathbb{R}$ satisfies

$$u_0(z) + u_0^3(z) = f(z), \tag{15}$$

with $\sqrt{\cdot}$ and $\sqrt[3]{\cdot}$ (used in (14)) the continuations of the square root and cubic root functions with branch cut respectively $\mathbb{R}_-$ and $\mathrm{i}\mathbb{R}$. The maximal horizontal strip of the complex plane on which the function $u_0(z)$ is analytic is $\mathbb{R} + \mathrm{i}(-B_0, B_0)$ where $B_0 = \operatorname{arcsinh}\left(\mu^{-1}\sqrt{4/27}\right) > 0$ is such that the discriminant cancels for $z = \pm\mathrm{i}B_0$. More precisely, the function $u_0(z)$ has branching points on the imaginary axis at $z_\pm = \pm\mathrm{i}B_0$. It holds $u_0(z_\pm) = \pm\mathrm{i}/\sqrt{3}$, $f(z_\pm) = \pm\mathrm{i}\sqrt{4/27}$, and $R(z_\pm) = 0$. The complex number $u_0(z_\pm)$ is the threefold degenerate root of the cubic equation

$$Z^3 + Z - f(z_\pm) = (Z - u_0(z_\pm))^3 = 0,$$

and we have

$$\left|\frac{\mathrm{d}u_0}{\mathrm{d}t}(tz_\pm)\right| = \left|\frac{\frac{\mathrm{d}f}{\mathrm{d}t}(tz_\pm)}{1 + 3(\frac{\mathrm{d}u_0}{\mathrm{d}t}(tz_\pm))^2}\right| \to \infty \quad \text{when } \mathbb{R} \ni t \to 1_-.$$

In particular, although the source term f has an entire continuation, the solution u_0 of (15) does not.

When $\varepsilon > 0$, we can approximate numerically the solution to (13) with the planewave approximation introduced before. The plots in Figure 2 suggest that increasing ε increases the width B_ε of the horizontal analyticity strip of $u_\varepsilon(z)$, but does not make it entire.

In this particular case, we can obtain an upper bound of the value of B_ε. Let $\varphi_\varepsilon(y) := u_\varepsilon(\mathrm{i}y)$. We also have $f(\mathrm{i}y) = \mu\sin(\mathrm{i}y) = \mathrm{i}\mu\sinh(y)$. Since u_ε is analytic at $z = 0$, φ_ε satisfies the second-order ODE:

$$\begin{cases} \varepsilon\varphi_\varepsilon''(y) + \varphi_\varepsilon(y) + \varphi_\varepsilon^3(y) = \mathrm{i}\mu\sinh, \\ \varphi_\varepsilon(0) = u_\varepsilon(0) = 0, \quad \varphi_\varepsilon'(0) = \mathrm{i}u_\varepsilon'(0), \end{cases}$$

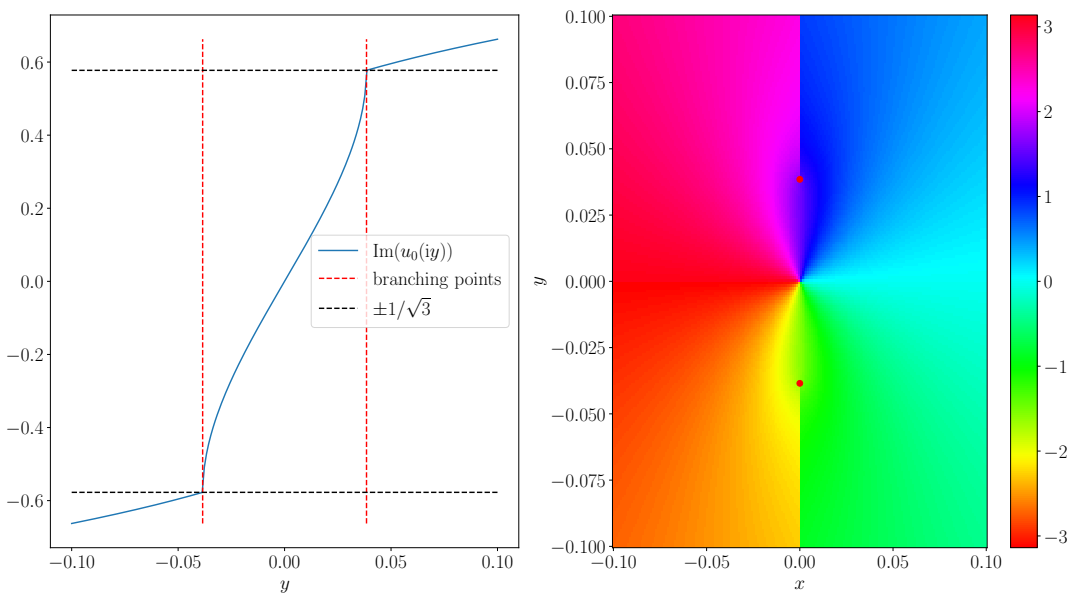

FIGURE 1 – Analytic continuation of u_0 for $\mu = 10$, for which $B_0 \approx 0.0385$. (Right) Phase of $z \mapsto u_0(z)$. A branching point, in red, appears at the expected position. (Left) Imaginary part of $y \mapsto u_0(\mathrm{i}y)$. A discontinuity also appears at the expected position.

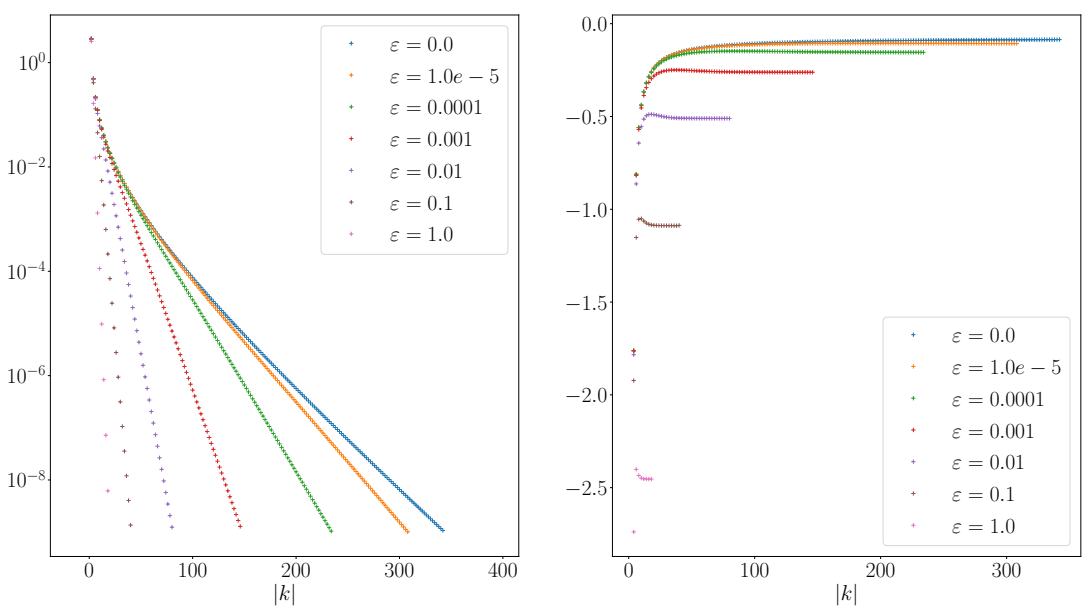

FIGURE 2 – (Left) Fourier coefficients of u_ε. (Right) Logarithm of the ratio of two successive nonzero Fourier coefficients.

where $u_\varepsilon'(0) \in \mathbb{R}$ since u_ϵ is real-valued on $\mathbb{R}$. Decomposing φ_ε in its real part θ_ε and imaginary part ψ_ε (i.e. $\varphi_\varepsilon = \theta_\varepsilon + \mathrm{i}\psi_\varepsilon$), we see that θ_ε and ψ_ε satisfy the coupled system of ODEs

$$\begin{cases} \varepsilon\theta_\varepsilon'' + \theta_\varepsilon + \theta_\varepsilon^3 - 3\theta_\varepsilon\psi_\varepsilon^2 = 0, \\ \theta_\varepsilon(0) = 0, \quad \theta_\varepsilon'(0) = 0, \end{cases} \qquad \begin{cases} \varepsilon\psi_\varepsilon'' + \psi_\varepsilon - \psi_\varepsilon^3 + 3\theta_\varepsilon^2\psi_\varepsilon = \mu\sinh, \\ \psi_\varepsilon(0) = 0, \quad \psi_\varepsilon'(0) = u_\varepsilon'(0). \end{cases}$$

This implies that $\theta_\varepsilon = 0$, ψ_ε is odd, and u_ε remains remains purely imaginary along the imaginary axis. We now focus on the ODE satisfied by ψ_ε on $\mathbb{R}_+$, which can be rewritten as a first-order ODE on $\Psi_\varepsilon(y) := \begin{bmatrix} \psi_\varepsilon(y) \\ \psi_\varepsilon'(y) \end{bmatrix} \in \mathbb{R}^2$

$$\Psi_\varepsilon'(y) = \begin{bmatrix} \Psi_{\varepsilon,2}(y) \\ \varepsilon^{-1}\left(\mu\sinh(y) - \Psi_{\varepsilon,1}(y) + \Psi_{\varepsilon,1}^3(y)\right) \end{bmatrix}, \qquad \Psi_\varepsilon(0) := \begin{bmatrix} 0 \\ u_\varepsilon'(0) \end{bmatrix}. \tag{16}$$

If we can prove that Ψ_ε blows up at a finite $0 < Y_\varepsilon < \infty$, then this will imply that the width B_ε of the horizontal analyticity strip of u_ε satisfies $B_\varepsilon \leqslant Y_\varepsilon < \infty$.

In order to estimate Y_ε, we need comparison theorems for systems of ODEs. We use the following simplified version of more general results on systems of differential inequalities [21, 22]. In the sequel the inequality $a \geqslant b$ for two vectors $a, b \in \mathbb{R}^d$ means that $a_i \geqslant b_i$ for all $1 \leqslant i \leqslant d$.

Theorem 4. *(See e.g. [21, p. 112]). Let $d \geqslant 1$ and $G : \mathbb{R}^d \to \mathbb{R}^d$ be locally Lipschitz and quasimonotone in the sense that for all $X, Z \in \mathbb{R}^d$,*

$$(Z_i = X_i \text{ and } Z_j \geqslant X_j \text{ for } j \neq i) \quad \Rightarrow \quad (G(X) \leqslant G(Z)).$$

Let $0 \leqslant y_0 < y_{\mathrm{M}} \leqslant +\infty$ and $\Phi \in C^1([y_0, y_{\mathrm{M}}), \mathbb{R}^d)$ and $\Psi \in C^1([y_0, y_{\mathrm{M}}), \mathbb{R}^d)$ satisfying respectively the ODE

$$\Phi'(y) = G(\Phi(y)), \qquad \Phi(y_0) \in \mathbb{R}^d,$$

and the differential inequality

$$\Psi'(y) \geqslant G(\Psi(y)), \qquad \Psi(y_0) = \Phi(y_0).$$

Then we have

$$\forall\ y \in [y_0, y_{\mathrm{M}}), \quad \Psi(y) \geqslant \Phi(y).$$

To apply this result to (16), we introduce the function $G_\varepsilon : \mathbb{R}^2 \to \mathbb{R}^2$ defined by

$$\forall\ X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \in \mathbb{R}^2, \quad G_\varepsilon(X) = \begin{bmatrix} X_2 \\ \varepsilon^{-1}(-X_1 + X_1^3) \end{bmatrix},$$

and the maximal solution Φ_ε to

$$\Phi_\varepsilon'(y) = G_\varepsilon(\Phi_\varepsilon(y)), \qquad \Phi_\varepsilon(0) = \begin{bmatrix} 0 \\ u_\varepsilon'(0) \end{bmatrix}. \tag{17}$$

As $\sinh(y) \geqslant 0$ for all $y \geqslant 0$, we have

$$\Psi_\varepsilon'(y) \geqslant G_\varepsilon(\Psi_\varepsilon(y)), \qquad \Psi_\varepsilon(0) = \Phi_\varepsilon(0).$$

However, Theorem 4 cannot be directly applied as the quasimonotonicity assumption is not satisfied everywhere in $\mathbb{R}^2$: $G_{\varepsilon,i}(X_1, X_2)$ is nondecreasing in X_2 for $i = 1$ but it is not in X_1 for $i = 2$. It is only the case if X_1 is in the domain where $x \mapsto x^3 - x$ is nondecreasing. Thus, in order to be able to apply the comparison theorem, we have to show that $\psi_\varepsilon = (\Psi_\varepsilon)_1$ is in this domain at some y_0 and stays in it for all $y \geqslant y_0$.

To this end, we introduce the set

$$X_\mu = \left\{(y, \upsilon) \in \mathbb{R}^2,\ \mu\sinh(y) - \upsilon + \upsilon^3 \geqslant 0\right\}.$$

This set is such that, if $(y, \psi_\varepsilon(y))$ lies strictly in X_μ, then ψ_ε is locally strictly convex. For $y < B_0$, ψ_ε might oscillate on both sides of the boundary of X_μ [20]. We investigated numerically the behavior of this function for the set of parameters used in Figure 3 ($\varepsilon = 0.1$, $\mu = 0.5$), and observed that $0 < \psi_\varepsilon(B_0) < \frac{1}{\sqrt{3}}$ and $\psi_\varepsilon'(B_0) > 0$. This numerical observation can be trusted as the ODE satisfied by ψ_ε' the interval $[0, B_0]$ for $\varepsilon = 0.1$ and $\mu = 0.5$ is not stiff. It is therefore easy to solve it numerically with high accuracy with *a posteriori* error estimates guaranteeing that $\psi_\varepsilon(B_0)$ is indeed strictly between 0 and $\frac{1}{\sqrt{3}}$, and $\psi_\varepsilon'(B_0)$ is positive. Therefore, given the shape of the set X_μ (see Figure 3), ψ_ε is strictly convex on $[B_0, Y_\varepsilon)$. It is thus always above its tangent at $y = B_0$, whose slope is $\psi_\varepsilon'(B_0) > 0$. Therefore, for any $\eta > 0$, there is $y_\eta \geqslant B_0$ such that $\psi_\varepsilon(y_\eta) = 1 + \eta$ and $\psi_\varepsilon(y) \geqslant 1 + \eta > 1$ for any

$y \geqslant y_\eta$. We are now ready to compute an upper bound of Y_ε with the use of Theorem 4, that can be applied as the quasimonotonicity assumption is now satisfied in the domain of interest. To this end, we rewrite (17) as

$$\Phi_\varepsilon'(y) = G_\varepsilon(\Phi_\varepsilon(y)), \qquad \Phi_\varepsilon(y_\eta) = \begin{bmatrix} 1+\eta \\ \psi_\varepsilon'(y_\eta) \end{bmatrix}. \tag{18}$$

Theorem 4 then yields:

$$\forall\ y \geqslant y_\eta,\ \Psi_\varepsilon(y) \geqslant \Phi_\varepsilon(y).$$

This leads us to study of the ODE

$$\begin{cases} \varepsilon\phi_\varepsilon'' = -\phi_\varepsilon + \phi_\varepsilon^3 \\ \phi_\varepsilon(y_\eta) = 1+\eta,\ \phi_\varepsilon'(y_\eta) = \psi_\varepsilon'(y_\eta) > 0. \end{cases}$$

We have

$$\frac{\varepsilon}{2}\frac{\mathrm{d}}{\mathrm{d}y}\left(\phi_\varepsilon'\right)^2 = \frac{\mathrm{d}}{\mathrm{d}y}\left(-\frac{1}{2}\phi_\varepsilon^2 + \frac{1}{4}\phi_\varepsilon^4\right),$$

from which we deduce

$$\frac{\varepsilon}{2}(\phi_\varepsilon')^2 = \frac{1}{4}\phi_\varepsilon^4 - \frac{1}{2}\phi_\varepsilon^2 + C(\eta),$$

with

$$\begin{aligned} C(\eta) &= -\frac{1}{4}(1+\eta)^4 + \frac{1}{2}(1+\eta)^2 + \frac{\varepsilon}{2}(\psi_\varepsilon'(y_\eta))^2 \\ &\geqslant -\frac{1}{4}(1+\eta)^4 + \frac{1}{2}(1+\eta)^2 + \frac{\varepsilon}{2}(\psi_\varepsilon'(y_0))^2, \end{aligned}$$

where $C(\eta)$ is computed from the initial conditions at $y = y_\eta$ and $B_0 < y_0 < y_\eta$ is such that $\psi_\varepsilon(y_0) = 1$. Note that $\eta \mapsto -\frac{1}{4}(1+\eta)^4 + \frac{1}{2}(1+\eta)^2 + \frac{\varepsilon}{2}(\psi_\varepsilon'(y_0))^2$ is decreasing on $\mathbb{R}_*^+$ and takes the value $\frac{1}{4} + \frac{\varepsilon}{2}(\psi_\varepsilon'(y_0))^2 > \frac{1}{4}$ at $\eta = 0$. Thus, for $\eta > 0$ small enough, $C(\eta) \geqslant \frac{1}{4}$ and we have

$$\frac{\varepsilon}{2}(\phi_\varepsilon')^2 \geqslant \frac{1}{4}\phi_\varepsilon^4 - \frac{1}{2}\phi_\varepsilon^2 + \frac{1}{4} = \frac{1}{4}\left(\phi_\varepsilon^2 - 1\right)^2,$$

hence

$$\phi_\varepsilon' \geqslant \frac{1}{\sqrt{2\varepsilon}}\left(\phi_\varepsilon^2 - 1\right) \quad \text{on } [y_\eta, Y_\epsilon).$$

Finally, we consider the ODE

$$\xi_{\varepsilon,\eta}' = \frac{1}{\sqrt{2\varepsilon}}(\xi_{\varepsilon,\eta}^2 - 1), \qquad \xi_{\varepsilon,\eta}(y_\eta) = 1+\eta,$$

whose solution is

$$\xi_{\varepsilon,\eta}(y) = \frac{1 + \frac{2}{\eta} + \exp\left(\frac{y-y_\eta}{\sqrt{\varepsilon/2}}\right)}{1 + \frac{2}{\eta} - \exp\left(\frac{y-y_\eta}{\sqrt{\varepsilon/2}}\right)},$$

which is defined only up to $Y_{\varepsilon,\eta} := \sqrt{\frac{\varepsilon}{2}}\log\left(1 + \frac{2}{\eta}\right) + y_\eta$. Applying again Theorem 4, we have that $\phi_\varepsilon(y) \geqslant \xi_{\varepsilon,\eta}(y)$ for any $y \geqslant y_\eta$ such that both functions are still finite. Putting everything together, we obtain that ψ_ε is only defined up to some Y_ε with $B_0 < Y_\varepsilon \leqslant Y_{\varepsilon,\eta}$ and that

$$\forall\ y \in [y_\eta, Y_\varepsilon), \quad \psi_\varepsilon(y) \geqslant \xi_{\varepsilon,\eta}(y). \tag{19}$$

These results are illustrated on Figure 3, where we plotted the lower bound $\xi_{\varepsilon,\eta}$ for $\varepsilon = 0.1$ and $\eta = 0.5$.

We can deduce from these investigations that u_ε is only analytic on a horizontal strip of finite width of the complex plane although the source term f is an entire function: our results in the linear case are therefore no longer valid in general in the nonlinear case.

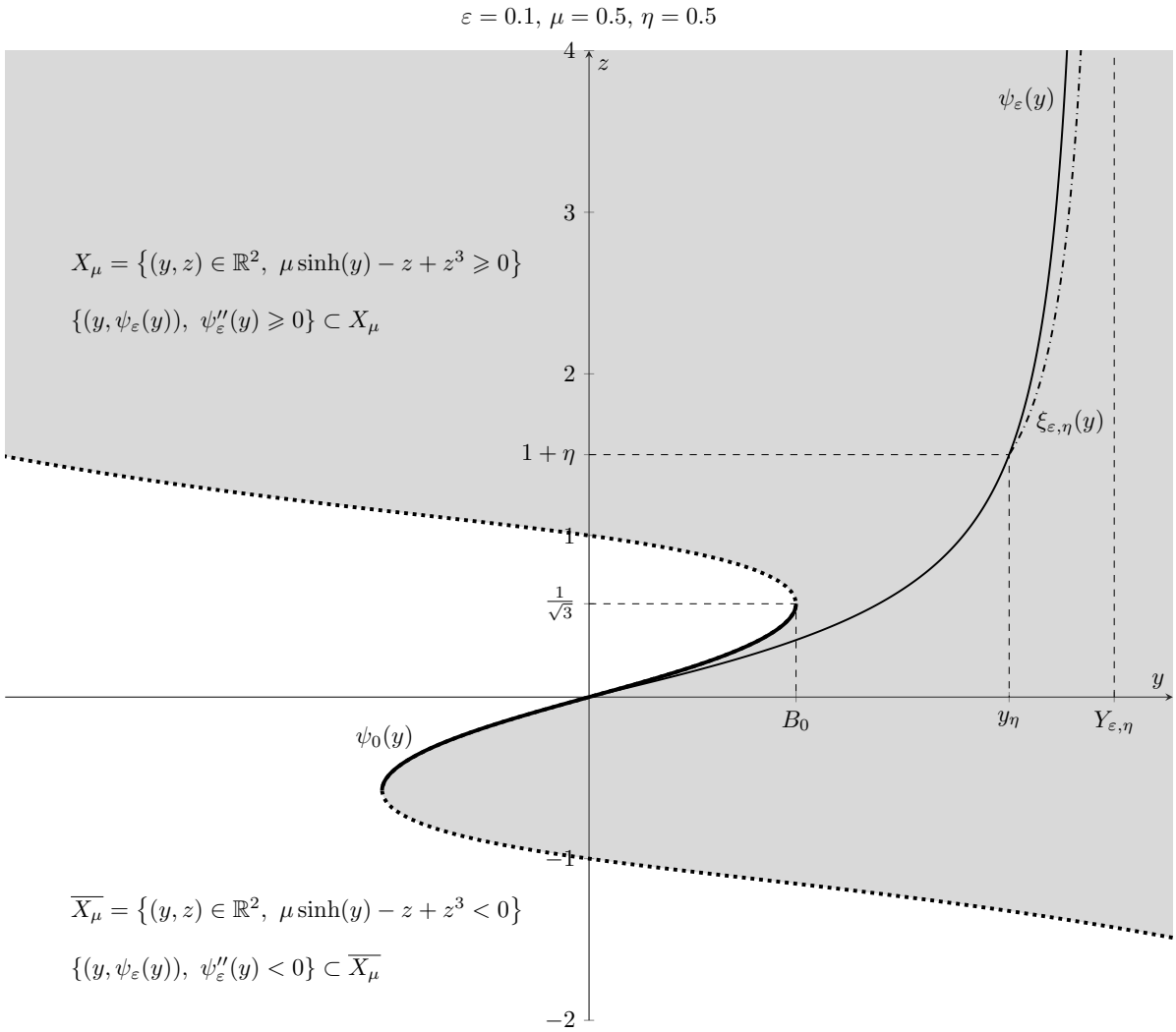

FIGURE 3 – Description of X_μ for $\mu = 0.5$, along with the plot of ψ_ε and the lowerbound $\xi_{\varepsilon,\eta}$ for $\varepsilon = 0.1$, $\eta = 0.5$. While $y < B_0$, ψ_ε can possibly oscillate around ψ_0, but as soon as $y \geqslant B_0$, ψ_ε is strictly convex and has no other choice than to explode in finite time $Y_\varepsilon \leqslant Y_{\varepsilon,\eta}$, where $Y_{\varepsilon,\eta}$ is the explosion time of the lower bound $\xi_{\varepsilon,\eta}$.

5. Extension to the multidimensional case with application to Kohn-Sham models.

The goal of this section is to extend the previous results to the multidimensional case and apply them to the linear version of the Kohn-Sham equations (1). To this end, consider a Bravais lattice $\mathbb{L} = \mathbb{Z}\boldsymbol{a}_1 + \cdots + \mathbb{Z}\boldsymbol{a}_d$ where $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_d$ are linearly independent vectors of $\mathbb{R}^d$ ($d = 3$ for KS-DFT). We denote by $\Omega = [0,1)\boldsymbol{a}_1 + \cdots + [0,1)\boldsymbol{a}_d$ a unit cell, by $\mathbb{L}^*$ the reciprocal lattice, by $e_{\boldsymbol{G}}(\boldsymbol{x}) = |\Omega|^{-1/2}\mathrm{e}^{\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{x}}$ the Fourier mode with wavevector $\boldsymbol{G} \in \mathbb{L}^*$, and by

$$H^s_{\mathrm{per},\mathbb{L}} := \left\{ u = \sum_{\boldsymbol{G}\in\mathbb{L}^*} \widehat{u}_{\boldsymbol{G}} e_{\boldsymbol{G}} \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}) \;\middle|\; \sum_{\boldsymbol{G}\in\mathbb{L}^*} (1+|\boldsymbol{G}|^2)^s |\widehat{u}_{\boldsymbol{G}}|^2 < \infty \right\}$$

the $\mathbb{L}$-periodic Sobolev spaces endowed with their usual inner products. All the arguments in Sections 3.1-3.3 can be extended to the multidimensional case by introducing the Hilbert spaces

$$\mathcal{H}_{A,\mathbb{L}} := \left\{ u \in L^2_{\mathrm{per},\mathbb{L}} \;\middle|\; \sum_{\boldsymbol{G}\in\mathbb{L}} w_{A,\mathbb{L}}(\boldsymbol{G})\, |\widehat{u}_{\boldsymbol{G}}|^2 < \infty \right\}, \quad (u,v)_{A,\mathbb{L}} := \sum_{\boldsymbol{G}\in\mathbb{L}^*} w_{A,\mathbb{L}}(\boldsymbol{G}) \overline{\widehat{u}_{\boldsymbol{G}}} \widehat{v}_{\boldsymbol{G}},$$

where $w_{A,\mathbb{L}}(\boldsymbol{G}) = \sum_{n=1}^{d} w_A((2\pi)^{-1}\boldsymbol{G}\cdot\boldsymbol{a}_n)$. Note that the notation $w_{A,\mathbb{L}}$ is slightly misleading as the $w_{A,\mathbb{L}}$'s actually depend on the chosen basis $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_d$ of the lattice $\mathbb{L}$. Each $u \in \mathcal{H}_{A,\mathbb{L}}$ can be extended to an analytic function $u(z_1, \ldots, z_d)$ of d complex variables defined on a neighborhood on $\mathbb{R}^d$, and it holds

$$\sum_{\boldsymbol{G}\in\mathbb{L}^*} w_{A,\mathbb{L}}(\boldsymbol{G})\, |\widehat{u}_{\boldsymbol{G}}|^2 = \frac{1}{2}\sum_{n=1}^{d} \int_\Omega \left|u(\boldsymbol{x} + \mathrm{i}(2\pi)^{-1}A\boldsymbol{a}_n)\right|^2 + \left|u(\boldsymbol{x} - \mathrm{i}(2\pi)^{-1}A\boldsymbol{a}_n)\right|^2 \mathrm{d}\boldsymbol{x}.$$

The extension of Proposition 1 follows with the operator norm, for any $0 < A < B$,

$$\forall\, V \in \mathcal{H}_{B,\mathbb{L}}, \quad \|V\|_{\mathcal{L}(\mathcal{H}_{A,\mathbb{L}})} = \max_{1\leqslant n\leqslant d} \left\|V(\cdot + \mathrm{i}(2\pi)^{-1}A\boldsymbol{a}_n)\right\|_{L^\infty_{\mathrm{per}}}.$$

The approximation space $X_{N,\mathbb{L}}$ is then defined as

$$X_{N,\mathbb{L}} := \mathrm{Span}(e_{\boldsymbol{G}},\ \boldsymbol{G} \in \mathbb{L}^*,\ |\boldsymbol{G}| \leqslant N),$$

and the inverse $T^{-1}_{22,\mathbb{L}}$ of the restriction $T_{22,\mathbb{L}}$ of the operator $-\Delta$ on $L^2_{\mathrm{per},\mathbb{L}}$ to the invariant subspace $X^\perp_{N,\mathbb{L}} = \mathrm{Span}(e_{\boldsymbol{G}},\ \boldsymbol{G} \in \mathbb{L}^*,\ |\boldsymbol{G}| > N)$ satisfies

$$\|\, T_{22,\mathbb{L}}\|_{\mathcal{L}(X^\perp_{N,\mathbb{L}})} = \|\, T_{22,\mathbb{L}}\|_{\mathcal{L}(\mathcal{H}_{A,\mathbb{L}}\cap X^\perp_{N,\mathbb{L}})} \leqslant N^{-2}.$$

The proofs of Theorem 1, Theorem 2 and Theorem 3 can thus be straightforwardly adapted to the multidimensional case.

Lastly, if $V \in \mathcal{H}_{B,\mathbb{L}}$ for some $B > 0$, the Schrödinger operator $H = -\Delta + V$ *considered this time as a Schrödinger operator on* $L^2(\mathbb{R}^d, \mathbb{C})$ *with an* $\mathbb{L}$*-periodic potential*, can be decomposed by the Bloch transform and its Bloch fibers are the self-adjoint operators on $L^2_{\mathrm{per},\mathbb{L}}$ with domain $H^2_{\mathrm{per},\mathbb{L}}$ and form domain $H^1_{\mathrm{per},\mathbb{L}}$ defined as $H_{\boldsymbol{k}} = (-\mathrm{i}\nabla + \boldsymbol{k})^2 + V$. The following result is concerned with the Bloch eigenmodes of the H.

Theorem 5. *Let $B > 0$ and $V \in \mathcal{H}_{B,\mathbb{L}}$. For each $\boldsymbol{k} \in \mathbb{R}^d$, the eigenfunctions of the Bloch fibers $H_{\boldsymbol{k}} = (-\mathrm{i}\nabla + \boldsymbol{k})^2 + V$ of the periodic Schrödinger operator $H = -\Delta + V$ are in $\mathcal{H}_{A,\mathbb{L}}$ for any $0 < A < B$. Let $\lambda_{1,\boldsymbol{k}} \leqslant \lambda_{2,\boldsymbol{k}} \leqslant \cdots$ be the eigenvalues of $H_{\boldsymbol{k}}$ counted with multiplicities and ranked in non-decreasing order, and $\lambda_{1,\boldsymbol{k},N} \leqslant \lambda_{2,\boldsymbol{k},N} \leqslant \cdots \leqslant \lambda_{d_{\mathbb{L},N},\boldsymbol{k},N}$ the eigenvalues of the variational approximation of $H_{\boldsymbol{k}}$ in the $d_{\mathbb{L},N}$-dimensional space*

$$X_{\mathbb{L},\boldsymbol{k},N} := \mathrm{Span}(e_{\boldsymbol{G}},\ \boldsymbol{G} \in \mathbb{L}^*,\ |\boldsymbol{G} + \boldsymbol{k}| \leqslant N).$$

Then, for each $0 < A < B$ and $n \in \mathbb{N}^*$, there exists a constant $C \in \mathbb{R}_+$ such that

$$0 \leqslant \max_{\boldsymbol{k}\in\Omega^*} (\lambda_{n,\boldsymbol{k},N} - \lambda_{n,\boldsymbol{k}}) \leqslant C\mathrm{e}^{-2AN}, \tag{20}$$

where Ω^* is the first Brillouin zone (i.e. the Voronoi cell of the lattice $\mathbb{L}$ of $\mathbb{R}^d$ containing the origin).

Proof. It suffices to replace in the proofs of Theorem 2 and Theorem 3 X_N with $X_{\mathbb{L},\boldsymbol{k},N}$ and T_{22} with the restriction $T_{22,\mathbb{L},\boldsymbol{k}}$ of the operator $(-\mathrm{i}\nabla + \boldsymbol{k})^2$ to the invariant space $X^\perp_{\mathbb{L},\boldsymbol{k},N}$. The latter is invertible and such that $\|T^{-1}_{22,\mathbb{L},\boldsymbol{k}}\|_{\mathcal{L}(X^\perp_{\mathbb{L},\boldsymbol{k},N})} \leqslant N^{-2}$ and $\|T^{-1}_{22,\mathbb{L},\boldsymbol{k}}\|_{\mathcal{L}(\mathcal{H}_{A,\mathbb{L}}\cap X^\perp_{\mathbb{L},\boldsymbol{k},N})} \leqslant N^{-2}$. ∎

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