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

ERIC CANCES, GASPARD KEMLIN, AND ANTOINE LEVITT

ABSTRACT. This paper is concerned with the numerical analysis of linear and nonlinear Schrödinger equations with periodic analytic potentials. We prove that, for linear equations, when the potential is analytic in a strip of width  $A$  of the complex plane, the solution is analytic in the same strip, ensuring an exponential convergence of the plane-wave discretization of the equation with rate  $A$ . On the other hand, for nonlinear equations, we find that the solution may be analytic only in a strip of width smaller than  $A$ . This behavior is illustrated by two examples using a combination of numerical and analytical arguments.

## 1. INTRODUCTION

In this paper, we study models inspired by Kohn–Sham Density Functional Theory (KS-DFT). 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. It 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  $\mathbb{L} = \mathbb{Z}\mathbf{a}_1 + \mathbb{Z}\mathbf{a}_2 + \mathbb{Z}\mathbf{a}_3$  the periodic lattice, where  $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$  is a non-necessarily orthonormal basis of  $\mathbb{R}^3$ , and by  $\Omega = [0, 1)\mathbf{a}_1 + [0, 1)\mathbf{a}_2 + [0, 1)\mathbf{a}_3$  the simulation cell. Let us denote by

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

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

$$H_\rho \varphi_i = \lambda_i \varphi_i, \quad \langle \varphi_i, \varphi_j \rangle_{L^2_{\text{per},\mathbb{L}}} = \delta_{ij}, \quad \rho(\mathbf{x}) = 2 \sum_{i=1}^{N_p} |\varphi_i(\mathbf{x})|^2, \quad (1)$$

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

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

where  $V_{\text{nl}}$  is a finite-rank self-adjoint operator (the nonlocal part of the pseudopotential), and

$$V_{\text{loc},\rho}^{\text{Hxc}}(\mathbf{x}) = V_{\text{loc}}(\mathbf{x}) + V_{\text{H},\rho}(\mathbf{x}) + V_{\text{xc},\rho}(\mathbf{x})$$

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

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

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and the function  $V_{xc,\rho}$ , called the exchange-correlation potential, depends on the chosen approximation of the exchange-correlation energy functional. In the simple  $X\alpha$  model [22],  $V_{xc,\rho}(\mathbf{x}) = -C_D\rho(\mathbf{x})^{1/3}$ , where  $C_D > 0$  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  $V_{nl} + V_{loc}$  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 regularity. As expected, the rate of convergence of the planewave discretization method is directly linked to the regularity 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  $X\alpha$  exchange-correlation functional, but also for the much more popular local density approximation (LDA) exchange-correlation functional, that if the local and nonlocal parts of the pseudopotential are in the periodic Sobolev space of order  $s > 3/2$ , then the Kohn–Sham orbitals  $\varphi_i$  and the density  $\rho$  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 [23], for which  $s = \frac{7}{2} - \varepsilon$  for all  $\varepsilon > 0$ . 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 [19], Quantum Espresso [9] or Abinit [11, 21], as well as DFTEK, 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, 16, 18] 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 neighbourhood of  $\mathbb{R}^d$ , the size of this neighbourhood 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  $2\pi$ -periodic functions on the real line having analytic continuations to the strip  $\mathbb{R} + i(-A, A)$  of the complex plane. 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  $Hu = f$  is 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 present two examples for which we show, using a combination of numerical and analytical tools, that the analyticity strip of the solution may be much smaller than the one of the data. Finally, we consider in the Appendix 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  $L^2_{\text{per}}(\mathbb{R}, \mathbb{C})$  the space of locally square integrable complex-valued  $2\pi$ -periodic functions on  $\mathbb{R}$ , endowed with its natural inner product

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

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

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

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

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

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

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

where

$$w_A(k) := \cosh(2Ak) = \frac{1}{2}(e^{2Ak} + e^{-2Ak}),$$

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

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

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

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

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  $u : \Omega_A \rightarrow \mathbb{C}$  given by

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

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

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

We record for future use the

**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.* The proof is immediate from the analyticity of  $V$  in  $\Omega_B$ , which implies that  $\sup_{z, |\text{Im}(z)| \leq A} |V(z)| < \infty$ .  $\square$

## 3. THE LINEAR CASE

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

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

where  $V \in L_{\text{per}}^2(\mathbb{R}, \mathbb{R})$  and  $f \in L_{\text{per}}^2(\mathbb{R}, \mathbb{C})$  are given  $2\pi$ -periodic functions. We assume in this section that  $V \geq 1$ . It is then standard that (2) has a unique solution  $u$  satisfying the *a priori* bounds

$$\|u\|_{L_{\text{per}}^2} \leq \frac{\|f\|_{L_{\text{per}}^2}}{\alpha} \quad \text{and} \quad \|u\|_{H_{\text{per}}^1} \leq \|f\|_{H_{\text{per}}^{-1}}, \quad (3)$$

where  $\alpha := \lambda_1(-\Delta + V) \geq 1$  is the smallest eigenvalue of the self-adjoint operator  $H = -\Delta + V$  on  $L_{\text{per}}^2(\mathbb{R}, \mathbb{C})$ . By bootstrap arguments,  $u \in H_{\text{per}}^{s+2}(\mathbb{R}, \mathbb{C})$  whenever  $V$  and  $f$  are in  $H_{\text{per}}^s$ , for any  $s \geq 0$ . 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  $V \geq 1$  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*

$$\exists C > 0 \text{ independent of } f \text{ such that } \|u\|_A \leq C \|f\|_A. \quad (4)$$

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

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

$$X_N := \text{Span}(e_k, |k| \leq N) = \{u \in L_{\text{per}}^2(\mathbb{R}, \mathbb{C}) \mid \widehat{u}_k = 0, \forall |k| > N\}. \quad (5)$$

Let  $\Pi_N$  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  $\Pi_N$  to the Sobolev space  $H_{\text{per}}^s(\mathbb{R}, \mathbb{C})$ ,  $s > 0$ , is also the orthogonal projector on  $X_N$  for the  $H_{\text{per}}^s$  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

$$\|u_1\|_A \leq \|u\|_{L_{\text{per}}^2} \sqrt{w_A(N)} \leq \frac{\|f\|_{L_{\text{per}}^2}}{\alpha} \sqrt{w_A(N)}. \quad (6)$$

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

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

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

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

Since  $\|T_{22}^{-1}\|_{\mathcal{L}(\mathcal{H}_A \cap X_N^\perp)} \leq N^{-2}$  and  $\|V_{22}\|_{\mathcal{L}(\mathcal{H}_A \cap X_N^\perp)} \leq \|V\|_{\mathcal{L}(\mathcal{H}_A)}$ , we can choose  $N$  large enough so that the operator  $(1 + T_{22}^{-1}V_{22})$  is invertible on  $\mathcal{H}_A \cap X_N^\perp$ . It then holds

$$u_2 = (1 + T_{22}^{-1}V_{22})^{-1}T_{22}^{-1}(f_2 - V_{21}u_1) \quad (9)$$

and the result follows from  $\|V_{21}\|_{\mathcal{L}(\mathcal{H}_A)} \leq \|V\|_{\mathcal{L}(\mathcal{H}_A)}$  and the bound (6) on  $u_1$ .  $\square$

Note that the same result also holds if we only require that  $V(\cdot \pm iA) \in L_{\text{per}}^\infty(\mathbb{R}, \mathbb{C})$ .

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

$$-\Delta u + Vu = \lambda u, \quad \|u\|_{L_{\text{per}}^2(\mathbb{R}, \mathbb{C})} = 1, \quad (10)$$

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

**Theorem 2.** *Let  $B > 0$ ,  $V \in \mathcal{H}_B$  be real-valued, and  $(u, \lambda) \in H_{\text{per}}^2(\mathbb{R}, \mathbb{C}) \times \mathbb{R}$  be a normalized eigenmode of  $H = -\Delta + V$ , with isolated eigenvalue (i.e. a solution to (10)). Then,  $u$  is in  $\mathcal{H}_A$  for all  $0 < A < B$ . As a consequence, if  $V$  is entire, then so is  $u$ .*

*Proof.* The proof proceeds along the same lines as that of [Theorem 1](#). Let  $(u, \lambda) \in H_{\text{per}}^2(\mathbb{R}, \mathbb{C}) \times \mathbb{R}$  be a solution to [\(10\)](#). 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

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

Therefore, choosing  $N$  large enough, we have

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

from which we deduce that  $u_2 \in \mathcal{H}_A$  and the result follows.  $\square$

**3.3. Planewave approximation of the linear Schrödinger equation.** Using  $X_N = \text{Span}(e_k, |k| \leq N) \subset H_{\text{per}}^1(\mathbb{R}, \mathbb{C})$  as a variational approximation space for [\(10\)](#), we obtain the finite-dimensional problem

$$\begin{cases} \text{seek } (u_N, \lambda_N) \in X_N \times \mathbb{R} \text{ such that } \|u_N\|_{L_{\text{per}}^2(\mathbb{R}, \mathbb{C})} = 1 \text{ and} \\ \forall v_N \in X_N, \quad \int_0^{2\pi} \overline{\nabla u_N} \cdot \nabla v_N + \int_0^{2\pi} V \overline{u_N} v_N = \lambda_N \int_0^{2\pi} \overline{u_N} v_N, \end{cases} \quad (11)$$

which is equivalent to seeking the eigenpairs of the Hermitian matrix  $H_N$  with entries

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

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,  $i \in \mathbb{N}^*$  and  $0 < A < B$ . Let  $\lambda_i$  be the  $i^{\text{th}}$  lowest eigenvalue of the self-adjoint operator  $H = -\Delta + V$  on  $L_{\text{per}}^2(\mathbb{R}, \mathbb{C})$  counting multiplicities, and  $\mathcal{E}_i = \text{Ker}(H - \lambda_i)$  the corresponding eigenspace. For  $N$  large enough, we denote by  $\lambda_{i,N}$  the  $i^{\text{th}}$  lowest eigenvalue of [\(11\)](#), and by  $u_{i,N}$  an associated normalized eigenvector. Then, there is a constant  $C_{i,A} \in \mathbb{R}_+$  such that, for  $N$  large enough,*

$$d_{H_{\text{per}}^1}(u_{i,N}, \mathcal{E}_i) \leq C_{i,A} \exp(-AN) \quad \text{and} \quad 0 \leq \lambda_{i,N} - \lambda_i \leq C_{i,A} \exp(-2AN).$$

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

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

The operator  $H$  is self-adjoint on  $L_{\text{per}}^2(\mathbb{R}, \mathbb{C})$  with form domain  $H_{\text{per}}^1(\mathbb{R}, \mathbb{C})$  and we infer from [Theorem 2](#) that all the eigenfunctions of the operator  $H$  are in  $\mathcal{H}_{A'}$ . [Theorem 3](#) then follows from classical arguments on the variational approximations of the eigenmodes of bounded below self-adjoint operators with compact resolvent (see e.g. [\[1, Theorems 8.1 and 8.2\]](#)).  $\square$

#### 4. THE NONLINEAR CASE

In the nonlinear case, the analyticity strip of the solution can be much smaller than the one of the data. First, we report numerical simulations on a nonlinear periodic Gross–Pitaevskii eigenvalue problem with a cubic nonlinearity and a potential admitting an entire continuation, illustrating the fact that the eigenfunction belongs to  $\mathcal{H}_A$  for some  $A > 0$ , but does not seem to be entire. Next, we study a nonlinear Schrödinger equation with entire potential and source term and cubic nonlinearity. We show that the solution is not entire and we provide an upper bound of the width of the horizontal analyticity strip of the solution.

**4.1. Analyticity on a strip.** We consider here the nonlinear eigenvalue problem

$$-\Delta u + Vu + u^3 = \lambda u, \quad \|u\|_{L^2_{\text{per}}(\mathbb{R}, \mathbb{C})} = 1, \quad (12)$$

where  $V \in \mathcal{H}_B$  for any  $B > 0$  is real-valued. Similarly to the linear case, we consider the planewave variational approximation: using again  $X_N = \text{Span}(e_k, |k| \leq N)$ , we obtain the finite-dimensional problem

$$\begin{cases} \text{seek } (u_N, \lambda_N) \in X_N \times \mathbb{R} \text{ such that } \|u_N\|_{L^2_{\text{per}}(\mathbb{R}, \mathbb{C})} = 1 \text{ and} \\ \forall v_N \in X_N, \quad \int_0^{2\pi} \overline{\nabla u_N} \cdot \nabla v_N + \int_0^{2\pi} V \overline{u_N} v_N + \int_0^{2\pi} |u_N|^2 \overline{u_N} v_N = \lambda_N \int_0^{2\pi} \overline{u_N} v_N. \end{cases} \quad (13)$$

Then, the following theorem holds, which is a simple corollary of known results on the analyticity of elliptic partial differential equations. Note that this result only yields the existence of a finite strip of analyticity in the complex plane. However, even if the data is entire, there is *a priori* no reason for the solution to be entire too, as shown by the counter-examples that follow.

**Theorem 4.** *Let  $V$  real-valued be in  $\mathcal{H}_B$  for any  $B > 0$  and  $(u, \lambda) \in H^2_{\text{per}}(\mathbb{R}, \mathbb{R}) \times \mathbb{R}$  be the ground-state of (12), uniquely defined under the assumption that  $u > 0$ . Then, there exists  $A > 0$  such that  $u \in \mathcal{H}_A$ . Moreover, if  $(u_N, \lambda_N)$  is the variational approximation of  $(u, \lambda)$  in  $X_N \times \mathbb{R}$ , then*

$$\exists C_A > 0, \quad \|u - u_N\|_{H^1_{\text{per}}} \leq C_A \exp(-AN).$$

*Proof.* Existence and uniqueness of  $u$  is a classical result, proved for instance in [6, Appendix]. In addition, as  $V \in H^s_{\text{per}}(\mathbb{R}, \mathbb{R})$  for any  $s > 0$ , we know from [6, Theorem 2] and by an immediate bootstrap argument that  $u$  also belongs to  $H^s_{\text{per}}(\mathbb{R}, \mathbb{R})$  for any  $s > 0$ . Therefore,  $u \in C^\infty_{\text{per}}(\mathbb{R}, \mathbb{R})$ .

Knowing that  $u \in C^\infty_{\text{per}}(\mathbb{R}, \mathbb{R})$ , standard results on the analyticity of solutions to nonlinear elliptic equations yield that  $u$  is analytic on a neighbourhood of every point  $x_0$  of the periodicity cell  $[0, 2\pi]$ , see for instance [4, Theorem 1.1] or [8, 15, 16]. By a compactness argument, we therefore have that  $u$  is analytic on a strip of size  $A > 0$  around the real axis, for some  $A > 0$ .

We now consider the variational approximation  $(u_N, \lambda_N)$  of  $(u, \lambda)$  in  $X_N \times \mathbb{R}$ . We know from [6, Theorem 1] that there exists  $C > 0$  such that

$$\|u - u_N\|_{H^1_{\text{per}}} \leq C \|u - \Pi_N u\|_{H^1_{\text{per}}}.$$

The result then follows similarly to the proof of Theorem 3.  $\square$

**Remark 1.** In order to establish the convergence rate of the eigenvalues of the ground-state of (12), one can follow the proof of [6, Theorem 2]. Using in particular equations (50) and (53) from this reference, with the negative Sobolev norms replaced by the dual norms of  $\mathcal{H}_A$ , one can obtain that there exists  $C_A > 0$  such that  $|\lambda - \lambda_N| \leq C_A \exp(-2AN)$ .

**4.2. Counter-examples.** We analyze in this section two counter-examples based on the nonlinear Gross–Pitaevskii equation with entire potentials and source terms, for which the solutions are not entire. We present numerical tests performed with the DFTK software [14], which uses a plane-wave basis and an iterative nonlinear solver. The numerical observations can be reproduced with Julia scripts available at [https://github.com/gkemlin/analytic\\_potentials](https://github.com/gkemlin/analytic_potentials).

**4.2.1. A nonlinear Gross–Pitaevskii eigenvalue problem.** We study in this section the following nonlinear eigenvalue problem:

$$\begin{cases} -\varepsilon \Delta u_\varepsilon + \gamma \cos(x) u_\varepsilon + u_\varepsilon^3 = \lambda_\varepsilon u_\varepsilon & \text{in } H^1_{\text{per}}(\mathbb{R}, \mathbb{R}), \\ \|u_\varepsilon\|_{L^2_{\text{per}}} = 1, \quad u_\varepsilon > 0, \end{cases} \quad (14)$$

with entire data. In view of the results we obtained in the linear case, we could expect the solution  $u_\varepsilon$  to (14) (which we know to exist) to be entire. However, our numerical experiments suggest on the contrary that  $u_\varepsilon$  is analytic only on a band of finite size.

The singular limit  $\varepsilon \rightarrow 0$  yields the algebraic equation  $\gamma \cos(x) u_0(x) + u_0(x)^3 = \lambda_0 u_0(x)$ . If we assume that  $u_0$  does not vanish on the unit cell  $[0, 2\pi]$ , we can divide by  $u_0(x)$  and then integrate over  $[0, 2\pi]$ : using the normalization condition, we obtain  $\lambda_0 = 1/2\pi$ . This yields

$$u_0(x) = \sqrt{\frac{1}{2\pi} - \gamma \cos(x)}, \quad (15)$$



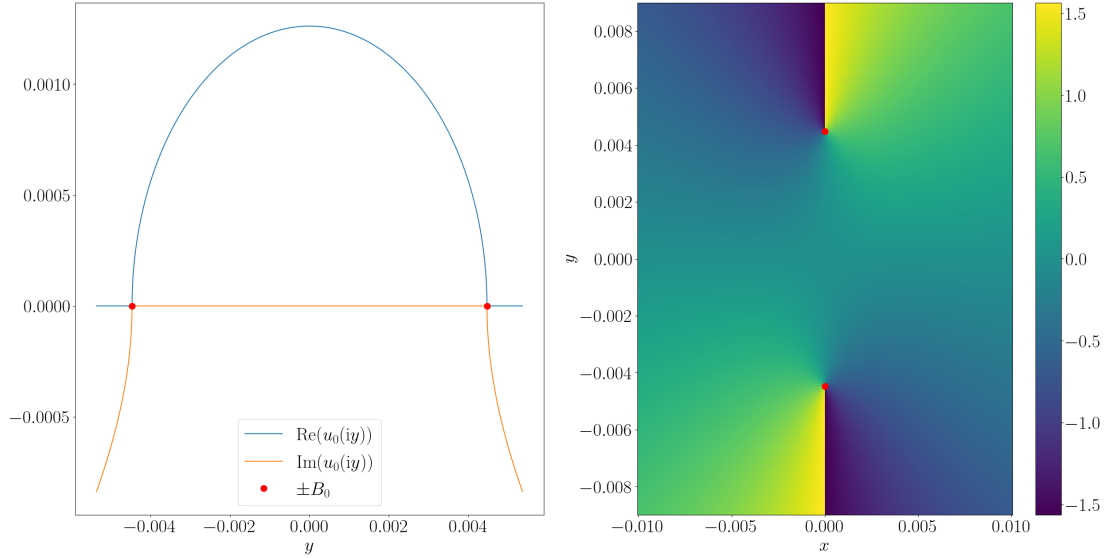
which is indeed bounded away from zero as soon as  $\beta_0 := 1/(2\pi\gamma) > 1$ , which we take in the following. The analytic continuation of  $u_0$ , still denoted by  $u_0$ , satisfies

$$\gamma \cos(z)u_0(z) + u_0(z)^3 = \frac{1}{2\pi}u_0(z),$$

with  $\sqrt{\cdot}$  in (15) being the continuation of the square root with branch cut  $\mathbb{R}_-$ . The maximal horizontal strip of the complex plane on which  $u_0$  is analytic is  $\mathbb{R} + i(-B_0, B_0)$ , where  $B_0$  is such that  $\cos(\pm iB_0) = \beta_0$ , that is to say  $B_0 = \log\left(\beta_0 + \sqrt{\beta_0^2 - 1}\right)$ . More precisely, the function  $z \mapsto u_0(z)$  admits two branching points at  $z_{\pm} = \pm iB_0$ , for which  $u_0(z_{\pm}) = 0$  and

$$\left| \frac{du_0}{dt}(tz_{\pm}) \right| = \left| \frac{\gamma \sin(tz_{\pm})}{2\sqrt{\frac{1}{2\pi} - \gamma \cos(tz_{\pm})}} \right| \rightarrow \infty \quad \text{when } \mathbb{R} \ni t \rightarrow 1_-,$$

see Figure 1.



**FIGURE 1** – [Nonlinear eigenvalue problem] Analytic continuation of  $u_0$  for  $\beta_0 = 1.00001$ , for which  $B_0 \approx 0.0045$ . (Left) Imaginary and real parts of  $y \mapsto u_0(iy)$ . A discontinuity of the derivative appears at the expected positions. (Right) Phase of  $z \mapsto u_0(z)$  where  $z = x + iy$ . Branching points, in red, appear at the expected positions.

When  $\varepsilon > 0$ , we can approximate numerically the solution of (14) using the planewave approximation presented before, see Figure 2. Although it is not possible to rule out a transition to a different asymptotic regime in the limit of extremely small values of  $\varepsilon$  or very large values of  $k$  because of finite numerical accuracy, our numerical results are compatible with the decay of the Fourier coefficients of  $u_\varepsilon$  as  $1/(|k|^{3/2} \sqrt{\cosh(2B_0k)})$ . This leads to the conclusion that the solution  $u_\varepsilon$  is analytic on a band strip of size close to  $B_0$ , which is in contradiction with the results from the linear case. In the next section, we study a similar nonlinear elliptic equation where we reach similar conclusions and where, in addition, we can provide an upper bound of the width of the horizontal strip on which the solutions are analytic.

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

$$-\varepsilon \Delta u_\varepsilon + u_\varepsilon + u_\varepsilon^3 = f \quad \text{in } H_{\text{per}}^1(\mathbb{R}, \mathbb{R}), \quad (16)$$

where  $\varepsilon > 0$ , and  $f : \mathbb{R} \rightarrow \mathbb{R}$  is a real-analytic  $2\pi$ -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 we showed for the



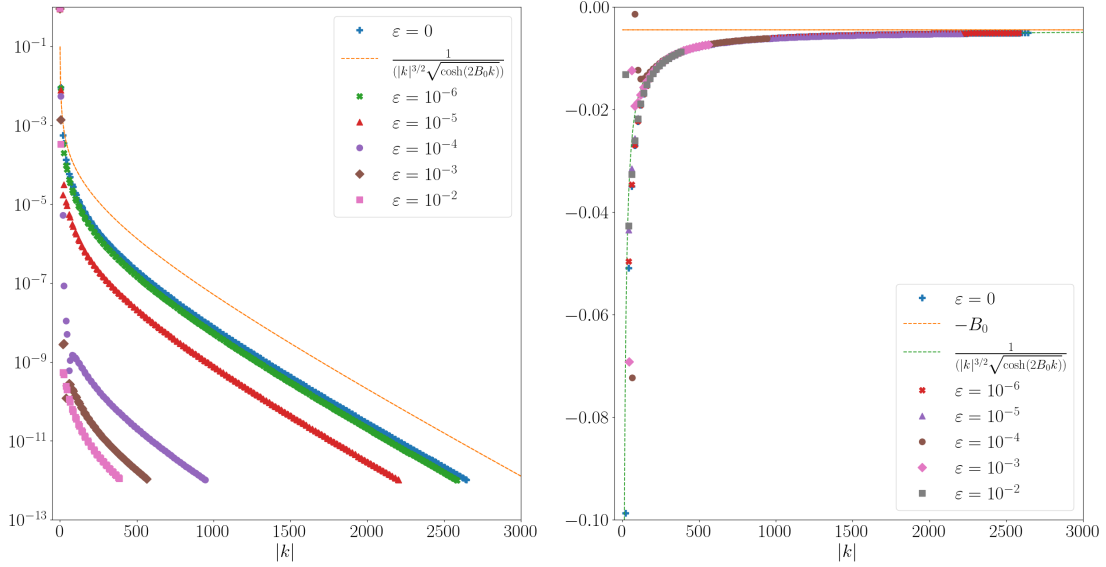


FIGURE 2 – [Nonlinear eigenvalue problem] (Left) Fourier coefficients of  $u_\varepsilon$ : they seem to decrease like  $1/(|k|^\alpha \sqrt{\cosh(2B_0 k)})$  with  $\alpha = 3/2$ , the prefactor  $2B_0$  in the cosh being confirmed by the plot on the right. (Right) Logarithm of the ratio of two successive nonzero Fourier coefficients.

linear case are not true any more 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 entire.

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

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

so that

$$u_0(x) = \sqrt[3]{\frac{1}{2} \left( f(x) + \sqrt{\frac{-R(x)}{27}} \right)} + \sqrt[3]{\frac{1}{2} \left( f(x) - \sqrt{\frac{-R(x)}{27}} \right)}, \quad (17)$$

the other two roots being complex conjugates with nonzero imaginary parts. The function  $u_0$  can be analytically continued from the real axis upwards in the complex plane as long as  $R(z)$  does not touch zero; it has branching points (with an exploding first derivative) at the points where  $R(z) = 0$ . In the rest of this section, we will use the function  $f(x) = \mu \sin(x)$ , for a fixed  $\mu > 0$ . The analytic continuation of  $u_0$  has branching points at  $2\pi\mathbb{Z} \pm iB_0$ , with

$$B_0 = \operatorname{arcsinh} \sqrt{\frac{4}{27\mu^2}} > 0.$$

In particular, although the source term  $f$  has an entire continuation, the solution  $u_0$  given by (17) does not.

When  $\varepsilon > 0$ , we can approximate numerically the solution to (16) with the planewave approximation introduced before. The plots in Figure 4 suggest that increasing  $\varepsilon$  increases the width  $B_\varepsilon$  of the horizontal analyticity strip of  $u_\varepsilon(z)$ , but does not make it entire.

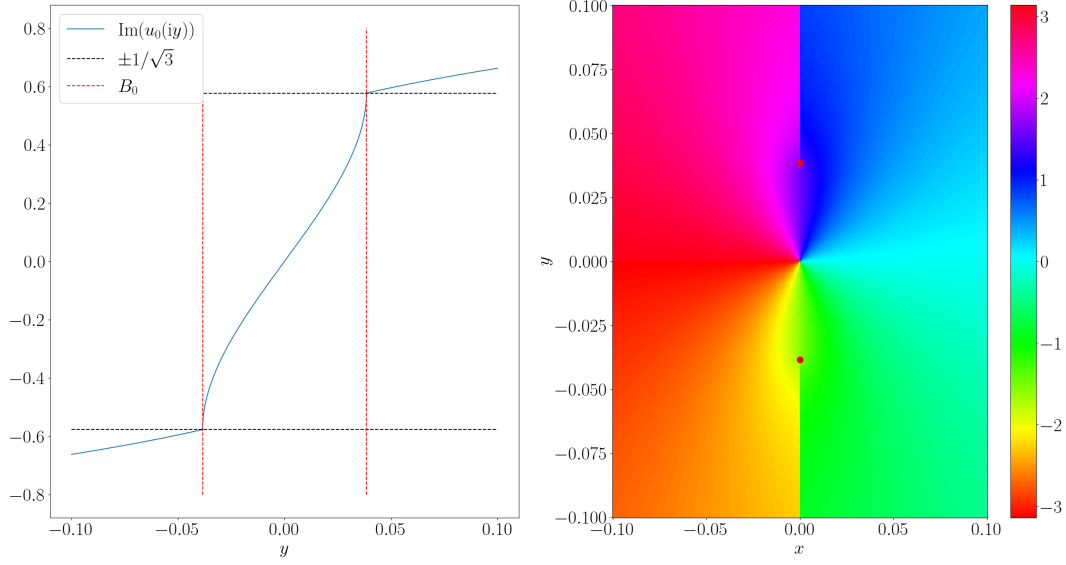


FIGURE 3 – [Nonlinear elliptic equation] Analytic continuation of  $u_0$  for  $\mu = 10$ , for which  $B_0 \approx 0.0385$ . (Left) Imaginary part of  $y \mapsto u_0(iy)$ . Discontinuities also appear at the expected positions  $\pm B_0$ . (Right) Phase of  $z \mapsto u_0(z)$  where  $z = x + iy$ . Branching points, in red, appear at the expected positions  $\pm B_0$ .

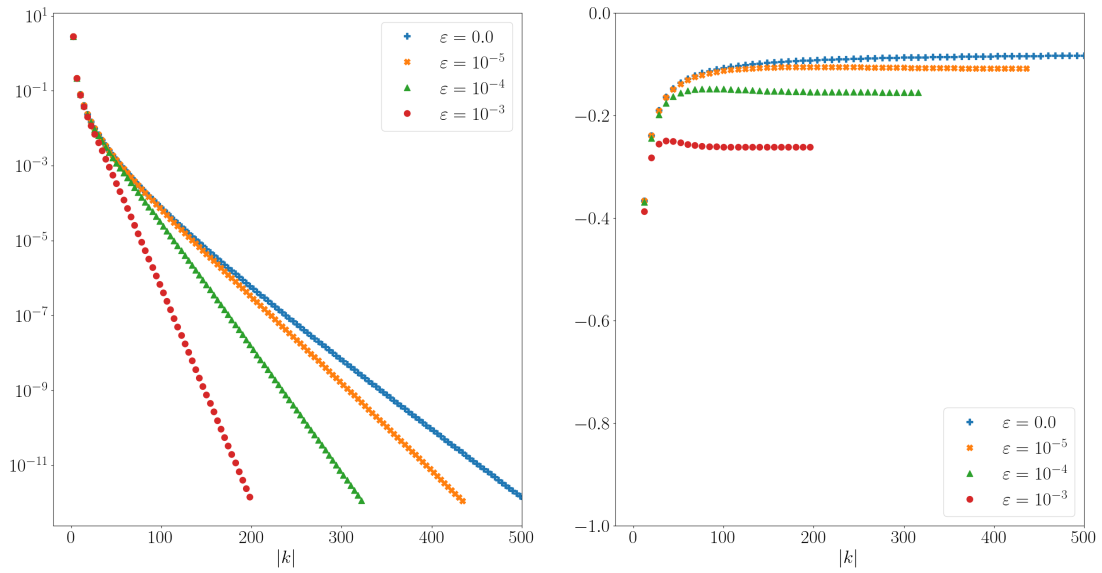


FIGURE 4 – [Nonlinear elliptic equation] (Left) Fourier coefficients of  $u_\epsilon$ . (Right) Logarithm of the ratio of two successive nonzero Fourier coefficients.

In this particular case, we are able to obtain an upper bound of the value of  $B_\varepsilon$  by an ODE technique. Let  $\varphi_\varepsilon(y) := u_\varepsilon(iy)$  be the value of the solution along the imaginary axis. Using the Cauchy–Riemann equations, we see that  $\varphi_\varepsilon$  satisfies the following second-order ODE:

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

with  $u_\varepsilon'(0) \in \mathbb{R}$ . Decomposing  $\varphi_\varepsilon$  in its real part  $\theta_\varepsilon$  and imaginary part  $\psi_\varepsilon$ , we see that  $\theta_\varepsilon$  satisfies the equation

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

and therefore vanishes. As a consequence,  $u_\varepsilon$  is purely imaginary along the imaginary axis (as could have been anticipated by the symmetries  $u_\varepsilon(-z) = -u_\varepsilon(z)$ ,  $u_\varepsilon(\bar{z}) = \overline{u_\varepsilon(z)}$ ). We are then left with studying the imaginary part  $\psi_\varepsilon$ , which satisfies the ODE

$$\begin{cases} \varepsilon\psi_\varepsilon'' + \psi_\varepsilon - \psi_\varepsilon^3 = \mu \sinh, \\ \psi_\varepsilon(0) = 0, \quad \psi_\varepsilon'(0) = u_\varepsilon'(0). \end{cases} \quad (18)$$

If we can prove that  $\psi_\varepsilon$  becomes non-analytic at a finite  $0 < Y_\varepsilon < \infty$ , this will imply that the width  $B_\varepsilon$  of the horizontal analyticity strip of  $u_\varepsilon$  satisfies  $B_\varepsilon \leq Y_\varepsilon < \infty$  and is therefore finite even though the data in (16) is entire. To this end, we prove in the Appendix B the following lemma, which gives a sufficient condition for the non-analyticity of  $\psi_\varepsilon$  in finite time.

**Lemma 1.** *Let  $Y_\varepsilon \in \mathbb{R}_+ \cup \{\infty\}$  be the maximum time of definition of  $\psi_\varepsilon$ . If, for some  $\eta > 0$  small enough, there exists  $y_\eta \geq B_0$  such that  $\psi_\varepsilon(y_\eta) = 1 + \eta > 1$  and  $\psi_\varepsilon'(y_\eta) > 0$ , then  $Y_\varepsilon < \infty$  and  $\psi_\varepsilon(y) \rightarrow \infty$  when  $y \rightarrow Y_\varepsilon$ .*

To prove that the sufficient condition from Lemma 1 is satisfied, we introduce the set

$$X_\mu = \{(y, v) \in \mathbb{R}^2, \mu \sinh(y) - v + v^3 \geq 0\}.$$

This set is such that, if  $(y, \psi_\varepsilon(y))$  lies strictly inside  $X_\mu$ , then  $\psi_\varepsilon$  is locally strictly convex. For  $y < B_0$ ,  $\psi_\varepsilon$  might oscillate on both sides of the boundary of  $X_\mu$  [24]. We investigated numerically the behavior of this function for the set of parameters used in Figure 5 ( $\varepsilon = 0.1$ ,  $\mu = 0.5$ ), 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  $\psi_\varepsilon'$  on 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,  $\psi_\varepsilon$  is locally strictly convex at  $y = B_0$ . Given the shape of  $X_\mu$  (see Figure 5 in appendix),  $\psi_\varepsilon$  lies, for any  $B_0 < y < Y_\varepsilon$ , above its tangent at  $y = B_0$ , whose slope is  $\psi_\varepsilon'(B_0) > 0$ . Strict convexity allows one to conclude that for any  $\eta > 0$ , there exists  $y_\eta > B_0$  such that

$$\begin{cases} \psi_\varepsilon(y_\eta) = 1 + \eta > 1, \\ \psi_\varepsilon'(y_\eta) > \psi_\varepsilon'(B_0) > 0. \end{cases}$$

Any  $\eta > 0$  is therefore suitable to apply Lemma 1 and conclude that  $\psi_\varepsilon$  blows up in finite time  $Y_\varepsilon$ . We can deduce from these investigations that  $u_\varepsilon$  is analytic only 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.

#### ACKNOWLEDGEMENTS

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#### APPENDIX A. 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  $\mathbb{L} = \mathbb{Z}\mathbf{a}_1 + \dots + \mathbb{Z}\mathbf{a}_d$  where  $\mathbf{a}_1, \dots, \mathbf{a}_d$  are linearly independent vectors of  $\mathbb{R}^d$  ( $d = 3$  for KS-DFT). Up to an affine change of variables (which

preserves analyticity), we can take without loss of generality  $\mathbb{L} = 2\pi\mathbb{Z}^d$ . We denote by  $\Omega = [0, 2\pi]^d$  a unit cell, by  $\mathbb{L}^* = \mathbb{Z}^d$  the reciprocal lattice, by  $e_{\mathbf{G}}(\mathbf{x}) = |\Omega|^{-1/2}e^{i\mathbf{G}\cdot\mathbf{x}}$  the Fourier mode with wavevector  $\mathbf{G} \in \mathbb{L}^*$ , and by

$$H_{\text{per},\mathbb{L}}^s := \left\{ u = \sum_{\mathbf{G} \in \mathbb{L}^*} \widehat{u}_{\mathbf{G}} e_{\mathbf{G}} \left| \sum_{\mathbf{G} \in \mathbb{L}^*} (1 + |\mathbf{G}|^2)^s |\widehat{u}_{\mathbf{G}}|^2 < \infty \right. \right\}$$

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

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

where  $w_{A,\mathbb{L}}(\mathbf{G}) = \sum_{n=1}^d w_A(G_n)$ . Each  $u \in \mathcal{H}_{A,\mathbb{L}}$  can be extended to an analytic function  $u(z_1, \dots, z_d)$  of  $d$  complex variables defined on a neighbourhood on  $\mathbb{R}^d$ , and it holds

$$\sum_{\mathbf{G} \in \mathbb{L}^*} w_{A,\mathbb{L}}(\mathbf{G}) |\widehat{u}_{\mathbf{G}}|^2 = \frac{1}{2} \sum_{j=1}^d \int_{\Omega} |u(\mathbf{x} + ie_j)|^2 + |u(\mathbf{x} - ie_j)|^2 d\mathbf{x}$$

with  $e_1, \dots, e_d$  the canonical basis vectors. The approximation space  $X_{N,\mathbb{L}}$  is then defined as

$$X_{N,\mathbb{L}} := \text{Span}(e_{\mathbf{G}}, \mathbf{G} \in \mathbb{L}^*, |\mathbf{G}| \leq N),$$

and the inverse  $T_{22,\mathbb{L}}^{-1}$  of the restriction  $T_{22,\mathbb{L}}$  of the operator  $-\Delta$  on  $L_{\text{per},\mathbb{L}}^2$  to the invariant subspace  $X_{N,\mathbb{L}}^\perp = \text{Span}(e_{\mathbf{G}}, \mathbf{G} \in \mathbb{L}^*, |\mathbf{G}| > N)$  satisfies

$$\|T_{22,\mathbb{L}}^{-1}\|_{\mathcal{L}(X_{N,\mathbb{L}}^\perp)} = \|T_{22,\mathbb{L}}^{-1}\|_{\mathcal{L}(\mathcal{H}_{A,\mathbb{L}} \cap X_{N,\mathbb{L}}^\perp)} \leq N^{-2}.$$

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 [\[20, Section XIII.16\]](#) and its Bloch fibers are the self-adjoint operators on  $L_{\text{per},\mathbb{L}}^2$  with domain  $H_{\text{per},\mathbb{L}}^2$  and form domain  $H_{\text{per},\mathbb{L}}^1$  defined as  $H_{\mathbf{k}} = (-i\nabla + \mathbf{k})^2 + V$ . The following result is concerned with the Bloch eigenmodes of the  $H_{\mathbf{k}}$ 's.

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

$$X_{\mathbb{L},\mathbf{k},N} := \text{Span}(e_{\mathbf{G}}, \mathbf{G} \in \mathbb{L}^*, |\mathbf{G} + \mathbf{k}| \leq N).$$

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

$$0 \leq \max_{\mathbf{k} \in \Omega^*} (\lambda_{i,\mathbf{k},N} - \lambda_{i,\mathbf{k}}) \leq C_{i,A} e^{-2AN}, \quad (19)$$

where  $\Omega^*$  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  $X_{\mathbb{L},\mathbf{k},N}$  and  $T_{22}$  with the restriction  $T_{22,\mathbb{L},\mathbf{k}}$  of the operator  $(-i\nabla + \mathbf{k})^2$  to the invariant space  $X_{\mathbb{L},\mathbf{k},N}^\perp$ . The latter is invertible and such that  $\|T_{22,\mathbb{L},\mathbf{k}}^{-1}\|_{\mathcal{L}(X_{\mathbb{L},\mathbf{k},N}^\perp)} \leq N^{-2}$  and  $\|T_{22,\mathbb{L},\mathbf{k}}^{-1}\|_{\mathcal{L}(\mathcal{H}_{A,\mathbb{L}} \cap X_{\mathbb{L},\mathbf{k},N}^\perp)} \leq N^{-2}$ . The result then follows similarly.  $\square$

**Remark 2.** As a conclusion, let us mention that, under appropriate assumptions, we can extend these results to the KS-DFT equations [\(1\)](#) with GTH pseudopotentials in the case where an analytic parametrization of the exchange-correlation functional is used. This is relevant for instance when studying condensed-phase systems, for which the periodic setting is well suited, and where the commonly used approximations of  $V_{\text{xc},\rho}$  are analytic on the

positive density values that are of interest in such cases [17]. Then we can rewrite (1) as a system of elliptic PDEs:

$$\begin{cases} \left( -\frac{1}{2}\Delta + V_{\text{nl}} + V_{\text{loc}} + V_{\text{H},\rho} + V_{\text{xc},\rho} \right) \varphi_i - \lambda_i \varphi_i = 0, & (\varphi_i, \varphi_j)_{L^2_{\text{per},\mathbb{L}}} = \delta_{ij}, \\ \rho(\mathbf{x}) = \sum_{i=1}^{N_p} |\varphi_i(\mathbf{x})|^2, \\ -\Delta V_{\text{H},\rho}(\mathbf{x}) = 4\pi \left( \rho(\mathbf{x}) - \frac{1}{|\Omega|} \int_{\Omega} \rho \right), & \int_{\Omega} V_{\text{H},\rho} = 0, \end{cases}$$

We can then use known results for elliptic systems of PDEs [15, 16] to conclude, in a way similar to what we proved in Theorem 4, that the orbitals  $\varphi_i$  belong to  $\mathcal{H}_{A,\mathbb{L}}$  for some  $A > 0$ . In particular, this leads to the exponential convergence of planewave approximations, justifying the use of GTH pseudopotentials.

#### APPENDIX B. PROOF OF LEMMA 1

We start by rewriting (18) as a first-order ODE on  $\Psi_\varepsilon(y) := \begin{bmatrix} \psi_\varepsilon(y) \\ \psi'_\varepsilon(y) \end{bmatrix} \in \mathbb{R}^2$ , starting at  $y_\eta \geq B_0$ :

$$\Psi'_\varepsilon(y) = \begin{bmatrix} \Psi_{\varepsilon,2}(y) \\ \varepsilon^{-1} (\mu \sinh(y) - \Psi_{\varepsilon,1}(y) + \Psi_{\varepsilon,1}^3(y)) \end{bmatrix}, \quad \Psi_\varepsilon(y_\eta) := \begin{bmatrix} \psi_\varepsilon(y_\eta) \\ \psi'_\varepsilon(y_\eta) \end{bmatrix} = \begin{bmatrix} 1 + \eta \\ \psi'_\varepsilon(y_\eta) \end{bmatrix}. \quad (20)$$

We then use the following simplified version of more general comparison results on systems of differential inequalities [25, 26]. In the sequel, the inequality  $a \geq b$  for two vectors  $a, b \in \mathbb{R}^d$  means that  $a_i \geq b_i$  for all  $1 \leq i \leq d$ .

**Theorem 6.** (See e.g. [25, p. 112]). *Let  $d \geq 1$  and  $G : \mathbb{R}^d \rightarrow \mathbb{R}^d$  be locally Lipschitz and quasimonotone in the sense that for all  $X, Z \in \mathbb{R}^d$ ,*

$$(Z_i = X_i \text{ and } X_j \leq Y_j \text{ for } j \neq i) \Rightarrow (G(X) \leq G(Z)).$$

*Let  $0 \leq y_0 < y_M \leq \infty$  and  $\Phi \in C^1([y_0, y_M], \mathbb{R}^d)$  and  $\Psi \in C^1([y_0, y_M], \mathbb{R}^d)$  satisfying respectively the ODE*

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

*and the differential inequality*

$$\Psi'(y) \geq G(\Psi(y)), \quad \Psi(y_0) = \Phi(y_0).$$

*Then we have*

$$\Psi(y) \geq \Phi(y).$$

*on  $[y_0, y_M]$ .*

To apply this result to (20), we introduce the function  $G_\varepsilon : \mathbb{R}^2 \rightarrow \mathbb{R}^2$  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  $\Phi_\varepsilon$  to

$$\Phi'_\varepsilon(y) = G_\varepsilon(\Phi_\varepsilon(y)), \quad \Phi_\varepsilon(y_\eta) = \begin{bmatrix} 1 + \eta \\ \psi'_\varepsilon(y_\eta) \end{bmatrix}. \quad (21)$$

As  $\sinh(y) \geq 0$  for all  $y \geq 0$ , we have the following differential inequality:

$$\Psi'_\varepsilon(y) \geq G_\varepsilon(\Psi_\varepsilon(y)), \quad \Psi_\varepsilon(y_\eta) = \Phi_\varepsilon(y_\eta).$$

Note that, by convexity,  $\psi_\varepsilon(y) \geq \psi_\varepsilon(y_\eta) > 1$  for  $y \geq y_\eta$ :  $G_\varepsilon$  is indeed quasimonotone on the domain of interest. We are now ready to compute an upper bound of  $Y_\varepsilon$  with the use of Theorem 6, which yields

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

This leads us to the study of the ODE

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

We have

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

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

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

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,  $C(\eta) \geq \frac{1}{4}$  and we have

$$\frac{\varepsilon}{2}(\phi'_\varepsilon)^2 \geq \frac{1}{4}\phi_\varepsilon^4 - \frac{1}{2}\phi_\varepsilon^2 + \frac{1}{4} = \frac{1}{4}(\phi_\varepsilon^2 - 1)^2,$$

hence

$$\phi'_\varepsilon \geq \frac{1}{\sqrt{2\varepsilon}}(\phi_\varepsilon^2 - 1) \quad \text{on } [y_\eta, Y_\varepsilon].$$

Finally, we consider the ODE

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

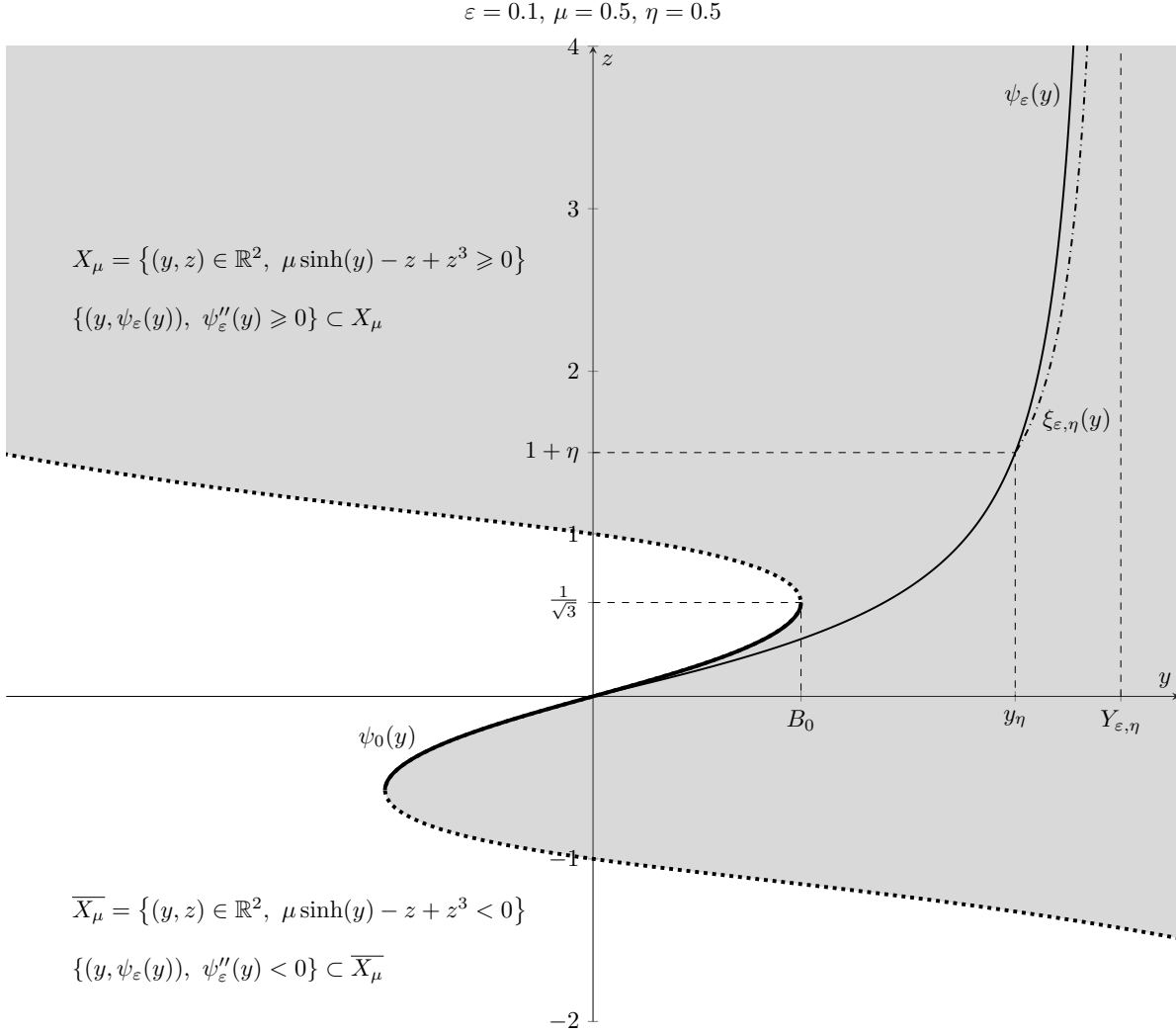
whose solution is

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

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 6](#), we have that  $\phi_\varepsilon(y) \geq \xi_{\varepsilon,\eta}(y)$  for any  $y \geq y_\eta$  such that both functions are still finite. Putting everything together, we obtain that  $\psi_\varepsilon$  is only defined up to some  $Y_\varepsilon$  with  $B_0 < Y_\varepsilon \leq Y_{\varepsilon,\eta} < \infty$  and that

$$\forall y \in [y_\eta, Y_\varepsilon), \quad \psi_\varepsilon(y) \geq \xi_{\varepsilon,\eta}(y). \quad (22)$$

These results are illustrated on [Figure 5](#), where we plotted the lower bound  $\xi_{\varepsilon,\eta}$  for  $\varepsilon = 0.1$  and  $\eta = 0.5$  as well as a numerical approximation of  $\psi_\varepsilon$ .



**FIGURE 5** – Description of  $X_\mu$  for  $\mu = 0.5$ , along with the plot of  $\psi_\varepsilon$  and the lower bound  $\xi_{\varepsilon,\eta}$  for  $\varepsilon = 0.1$ ,  $\eta = 0.5$ . While  $y < B_0$ ,  $\psi_\varepsilon$  can possibly oscillate around  $\psi_0$ , but as soon as  $y \geq B_0$ ,  $\psi_\varepsilon$  is strictly convex and has no other choice than to explode in finite time  $Y_\varepsilon \leq Y_{\varepsilon,\eta}$ , where  $Y_{\varepsilon,\eta}$  is the explosion time of the lower bound  $\xi_{\varepsilon,\eta}$ .



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