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# Numerical approaches for some Nonlinear Eigenvalue Problems

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## Abstract

In this article we are interested for the numerical study of nonlinear eigenvalue problems. We begin with a review of theoretical results obtained by functional analysis methods, especially for the Schrödinger pencils. Some recall are given for the pseudospectra. Then we present the numerical methods and results obtained for eigenvalues computation with spectral methods and finite difference discretization, in infinite or bounded domains. Comparison with theoretical results is done. The main difficulty here is that we have to compute eigenvalues of strongly non-self-adjoint operators which are very unstable.

**Keywords :** nonlinear eigenvalue problems, spectra, pseudospectra, finite difference methods, Galerkin spectral method, Hermite functions.

## 1 Introduction

We are interested here in equations like  $L(\lambda)u = 0$  where  $L(\lambda)$  is a linear operator on some linear space  $\mathcal{E}$ , depending on a complex parameter  $\lambda$ . When  $L(\lambda) = L_0 - \lambda\mathbb{I}$ , this is the usual eigenvalue problem : find  $\lambda \in \mathbb{C}$  and  $u \in \mathcal{E}$ ,  $u \neq 0$  such that  $L(\lambda)u = 0$ .

In many applications, in particular for dissipative problems in mechanics, it is necessary to consider more general dependance in the complex parameter  $\lambda$ . A particular interesting case is a quadratic dependence :  $L(\lambda) = \lambda^2 L_2 + \lambda L_1 + L_0$ . We shall say that  $L(\lambda)$  is a quadratic pencil.

Let us consider the second order differential equation

$$\frac{d^2 u}{dt^2} L_2 + \frac{du}{dt} L_1 + u L_0 = 0 \quad (1.1)$$

Equation (1.1) is a model in mechanics for small oscillations of a continuum system in the presence of an impedance force [15].

Now looking for stationary solutions of (1.1),  $u(t) = u_0 e^{\lambda t}$ , we have the following equation

$$(\lambda^2 L_2 + \lambda L_1 + L_0) u_0 = 0 \quad (1.2)$$

So equation (1.2) is a non linear eigenvalue problem in the spectral parameter  $\lambda \in \mathbb{C}$ .

The operator  $L_1$  represent a damping term as we see in the following simple example.

Let us consider the perturbed wave equation

$$\frac{\partial^2}{\partial t^2} u - \frac{\partial^2}{\partial x^2} u - 2a \frac{\partial}{\partial t} u = 0 \quad (1.3)$$

where  $t \in \mathbb{R}$  and  $x \in \mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ . The damping term  $a < 0$  is here constant. So we have to solve (1.3) with periodical boundary conditions.

The stationary problem is reduced to the equation

$$\lambda^2 + k^2 - 2a\lambda = 0, \quad k \in \mathbb{Z}$$

Then we have for  $k^2 \geq a^2$  the damped solutions of (1.3) :

$$u_k(t, x) = \exp\left((a + i\sqrt{k^2 - a^2})t + ikx\right)$$

When  $a$  is a function of  $x$  we have no explicit formula so we need numerical approximations to compute the damping modes. It is the main goal of this work, in particular concerning the Schrödinger pencil  $L_{V,a}(\lambda)$ .

We say that  $\lambda$  is a non linear eigenvalue if there exists  $u_0 \neq 0$  satisfying (1.2).

Such generalized eigenvalue problems have appeared in a completely different way. The question was to decide if a class of P.D.E with analytic coefficients preserves or not the analyticity property. To be more explicit, let us consider a P.D.E :  $Pu = f$ . Assume that  $f$  is analytic in some open set  $\Omega$ , is-it true that  $u$  is analytic in  $\Omega$  ? This is true for elliptic operators.

For some example, this question can be reduce to the following (see [12] for more details):

Does there exist  $\lambda \in \mathbb{C}, 0 \neq u \in \mathcal{S}(\mathbb{R})$  such that

$$\left(-\frac{d^2}{dx^2} + (x^2 - \lambda)^2\right)u = 0 \quad ? \quad (1.4)$$

Existence of non null solutions for (1.2) and (1.4) is a non trivial problem. For (1.4) it was solved in [19] where it is proved that the generalized eigenfunctions span the Hilbert space  $L^2(\mathbb{R})$ . On the other side we can prove that the equation

$$\left(-\frac{d^2}{dx^2} + (x - \lambda)^2\right)u = 0$$

has only the trivial solution  $u \equiv 0$  in  $L^2(\mathbb{R}), \forall \lambda \in \mathbb{C}$ .

Our aim in this work is to present several numerical approaches concerning this kind of non linear eigenvalue problems.

For simplicity we only consider quadratic pencil such that  $L_0 = \mathbb{I}$ . We can reduce to this case if  $L_0$  or  $L_2$  are invertible in the linear space  $\mathcal{E}$ .

To every quadratic pencil  $L(\lambda)$  we can associate a linear operator  $\mathcal{A}_L$  in  $\mathcal{E} \times \mathcal{E}$  such that  $\lambda$  is a non linear eigenvalue for  $L$  if and only if  $\lambda$  is a usual eigenvalue for  $\mathcal{A}_L$ .

$\mathcal{A}_L$  is called a linearization of  $L(\lambda)$ . It is easy to see that we can choose

$$\mathcal{A}_L = \begin{pmatrix} 0 & \mathbb{I} \\ -L_0 & -L_1 \end{pmatrix}$$

So non-linear eigenvalue problems (for polynomial operator pencils) can be reduced to usual eigenvalue problems but it is useful to take care of their particular structure. There exist infinitely many linearizations.

We are mainly interested here in the multidimensional case called Schrödinger pencils:

$$L_{V,a}(\lambda) = -\Delta + V - 2a\lambda + \lambda^2$$

in the Hilbert space  $L^2(\mathbb{R}^d)$ .  $V$  and  $a$  are smooth real functions on  $\mathbb{R}^d$  such that  $\lim_{|x| \rightarrow +\infty} V(x) = +\infty$

and  $|a| \leq \sqrt{V}$ .

The main questions we want to discuss is the location in the complex plane  $\mathbb{C}$  of the eigenvalues

of  $L_{V,a}$ . In the first part of this work we shall recall some known theoretical results and in the second part we shall discuss several numerical approaches for the computation of the eigenvalues of  $L_{V,a}$ . We shall see that accurate theoretical results on the location of the eigenvalues have been obtained for 1D pencils  $L_{V,a}$  but in the multidimensional case very few results are known on the eigenvalues of  $L_{V,a}$  when  $a$  is of the same order of  $\sqrt{V}$ .

In Section 2, we present a review of theoretical results obtained by functional analysis methods. In Section 3, we give more results for Schrödinger pencils. In Section 4 we recall some results on pseudospectra. In Section 5 we present the numerical methods and results obtained for eigenvalues computation with spectral methods and finite difference discretization, in infinite and bounded domain. Comparison with theoretical results is done. Then in Section 6 we give conclusions and open problems.

## 2 A review of theoretical results obtained by functional analysis methods

Most of these results was obtained by the Russian school between 1917 and 1970. For more details we refer to the book [18].

Let us consider the quadratic family of operators  $L(\lambda) = L_0 + \lambda L_1 + \lambda^2$  where  $L_0, L_1$  are operators in an Hilbert space  $\mathcal{H}$ .

If  $\mathcal{H}$  is of dimension  $N < +\infty$  the eigenvalues are the solutions of the polynomial equation  $\det(L(\lambda)) = 0$ . When  $N$  is large this could be a difficult problem at least for numerical computations.

In applications involving PDE,  $\mathcal{H}$  is a  $L^2$  space or a Sobolev space, which is infinite dimensional and there is no explicit equation for the generalized eigenvalues. Moreover, as we shall see later, the non linear eigenvalue problem is equivalent to a linear eigenvalue problem which, in general, is non self-adjoint hence unstable.

$L_0$  is assumed to be self-adjoint, positive, with a domain  $D(L_0)$  and  $L_1$  is  $\sqrt{L_0}$ -bounded. Moreover  $L_0^{-1/2}$  is in a Schatten class  $\mathcal{C}^p(\mathcal{H})^*$ , for some real  $p > 0$ .

The following results are well known.

**Theorem 2.1**  $L(\lambda)$  is a family of closed operators in  $\mathcal{H}$ .

$\lambda \mapsto L^{-1}(\lambda)$  is meromorphic in the complex plane.

The poles  $\lambda_j$  of  $L^{-1}(\lambda)$ , with multiplicity  $m_j$ , coincide with the eigenvalues with the same multiplicities, of the matrix operator  $\mathcal{A}_L$  in the Hilbert space  $\mathcal{H} \times D(L_0^{1/2})$ , with domain  $D(\mathcal{A}_L) = D(L_0) \times D(L_0^{1/2})$  where

$$\mathcal{A}_L = \begin{pmatrix} 0 & \mathbb{I} \\ -L_0 & -L_1 \end{pmatrix}$$

Assuming that  $V(x) \geq C|x|^{2m}$  and  $|a(x)| \leq C\sqrt{V(x)}$ ,  $C > 0$ , then the Schrödinger pencil  $L_{V,a}(\lambda)$  satisfies the above theorem for  $p > \frac{d(m+1)}{2m}$ .

If  $L_0$  is positive and non degenerate we have the symmetric linearization

$$\mathcal{A}_{SL} = \begin{pmatrix} 0 & \sqrt{L_0} \\ -\sqrt{L_0} & -L_1 \end{pmatrix}$$

Let us denote  $\text{Sp}[L]$  the eigenvalues of  $\mathcal{A}_L$  (which coincide with the poles of  $L^{-1}(z)$ ).

---

\*Recall that a compact operator  $A$  in an Hilbert space is in the Schatten class  $\mathcal{C}^p$  if the series  $s_j(A)$  of the eigenvalues of  $\sqrt{A^*A}$  satisfies  $\sum s_j(A)^p < +\infty$

**Remark 2.2** *It may happens that  $\text{Sp}[L]$  is empty (example :  $L(\lambda) = -\frac{d^2}{dx^2} + (x - \lambda)^2$ ).*

Let us remark that if  $L_1 = 0$  then  $\lambda \in \text{Sp}[L]$  if and only if  $-\lambda^2$  is in the spectrum of  $L_0$ . So if  $L_0$  has a point spectrum then  $\text{Sp}[L]$  is a subset of the imaginary axis.

We shall see now that when  $L_1$  is strictly smaller than  $\sqrt{L_0}$  then the eigenvalues are asymptotically close to the imaginary axis and the generalized eigenvectors is a dense set in the Hilbert space. When  $L_1$  has the same power of  $\sqrt{L_0}$  it may happens that there is no eigenvector at all for  $L(\lambda)$ .

If  $\lambda_0 \in \text{Sp}[L]$  we denote by  $\mathcal{E}_L(\lambda_0)$  the linear space of the solutions  $\{u_0, u_1, \dots, u_k, \dots\}$  of the equations

$$L(\lambda_0)u_0 = 0, \quad L(\lambda)u_1 + L'(\lambda_0)u = 0, \quad L(\lambda_0)u_{k+2} + L'(\lambda_0)u_{k+1} + \frac{1}{2}L''(\lambda_0)u_k = 0, \quad k \geq 0$$

The dimension of  $\mathcal{E}_L(\lambda_0)$  is the multiplicity of  $\lambda_0$  (for details see [19]).

Assume that  $L_0, L_1$  are self-adjoint,  $L_0$  is positive non degenerate and that there exist  $\kappa \geq 0$  and  $\delta \geq 0$  such that  $L_1 L_0^{\delta-1/2}$  is a bounded operator on  $\mathcal{H}$  and

$$\|L_1 L_0^{\delta-1/2}\| \leq \kappa$$

Assume that  $L_0^{-1}$  is in the Schatten class  $C^p$ ,  $p \geq 1$ .

**Theorem 2.3** *If  $0 < \delta \leq 1/2$  then the spectra of  $L$  is the domain*

$$\Omega_\delta = D_R \cup \{\lambda \in \mathbb{C}, |\Re \lambda| \leq \kappa |\lambda|^{1-2\delta}\}$$

and  $\bigoplus_{\lambda \in \text{Sp}[L]} \mathcal{E}_L(\lambda)$  is dense in  $\mathcal{H}$ .

If  $\delta = 0$  and if

$$\left| \frac{\pi}{2} - \arccos \kappa \right| \leq \frac{\pi}{2p}$$

then  $\bigoplus_{\lambda \in \text{Sp}[L]} \mathcal{E}_L(\lambda)$  is also dense in  $\mathcal{H}$ .

For  $\delta > 0$  we get that the eigenvalues are localized in a vertical parabolic domain in the imaginary direction. For  $\delta = 0$  and  $\kappa$  small the eigenvalues are localized in a small sector around the imaginary axis. Notice that for  $\kappa$  of order 1 the above theorem does not give any information on the location of  $\text{Sp}[L]$ ; we only know that it is a discrete and infinite subset of  $\mathbb{C}$ .

### A sketch of proof of Theorem (2.3)

The idea is to consider  $L(\lambda)$  as a perturbation of  $L_0 + \lambda^2$ . We know that  $L_0 + \lambda^2$  has a spectrum in  $i\mathbb{R}$  because  $L_0$  is self-adjoint.

We have

$$L(\lambda) = (\mathbb{I} + \lambda L_1)(L_0 + \lambda^2)^{-1} (L_0 + \lambda^2)$$

So if  $\lambda \notin i\mathbb{R}$  then  $L(\lambda)$  is invertible if and only if  $(\mathbb{I} + \lambda L_1)(L_0 + \lambda^2)^{-1}$  is invertible. To check this property it is enough to choose  $\lambda$  such that  $\|\lambda L_1 (L_0 + \lambda^2)^{-1}\| < 1$ .  $\square$

Moreover If  $L_1$  has a sign we have easily

**Proposition 2.4** *If  $L_1 \geq 0$  then  $\text{Sp}[L] \subseteq \{\lambda \in \mathbb{C}, \Re \lambda \leq 0\}$ .*

*If  $L_1 \leq 0$  then  $\text{Sp}[L] \subseteq \{\lambda \in \mathbb{C}, \Re \lambda \geq 0\}$ .*

**Proof.** If  $L(\lambda)u = 0$  then  $\langle u, L(\lambda)u \rangle = 0$ . Taking the imaginary part of this equality we get the proposition.  $\square$

The above result applies for example to

$$L(\lambda) = -\frac{d^2}{dx^2} + x^6 + \alpha x^2 \lambda + \lambda^2$$

For this example we have  $\delta = \frac{5}{6}$  hence the spectra is localized inside the parabolic region  $\{\lambda \in \mathbb{C}, |\Im \lambda| \geq C |\Re \lambda|^{5/2}\}$ .

For Schrödinger pencils  $L_{V,a}$  we can say more.

### 3 More results for Schrödinger pencils

Let us recall our definition of Schrödinger pencils:  $L_{V,a}(\lambda) = -\Delta + V - 2a\lambda + \lambda^2$ .

In all this article we assume that the pair of functions  $(V, a)$  satisfies the following technical conditions. We do not try here to discuss the optimality of this conditions.

[cond( $V, a$ )].  $V, a$  are smooth  $C^\infty$  functions on  $\mathbb{R}^d$ . There exists  $k > 0$  such that

$$|\partial_x^\alpha V(x)| \leq C_\alpha \langle x \rangle^{k-|\alpha|}, \quad |\partial_x^\alpha a(x)| \leq C_\alpha \langle x \rangle^{k/2-|\alpha|}, \quad (3.5)$$

$$|a(x)| \leq \sqrt{V(x)}, \quad V(x) \geq 0, \quad V(x) \geq c \langle x \rangle^k, \quad \text{for } |x| \geq 1 \quad (3.6)$$

with  $C_\alpha > 0$  and  $c > 0$ . Under these conditions we know that  $L_0 = -\Delta + V$  is an unbounded self-adjoint operator in  $L^2(\mathbb{R}^d)$  and for every  $\lambda \in \mathbb{C}$   $L_{V,a}(\lambda)$  is a closed and Fredholm operator with domain the following weighted Sobolev space:  $\mathcal{H}_V = \{u \in L^2(\mathbb{R}^d), \Delta u \in L^2(\mathbb{R}^d), Vu \in L^2(\mathbb{R}^d)\}$ . Moreover the set  $\text{Sp}[L]$  of eigenvalues of  $L_{V,a}$  is a discrete set (empty or not), each eigenvalue having a finite multiplicity and the only possible accumulation point in the complex plane is  $\infty$ . Notice that  $\lambda$  is an eigenvalue then its complex conjugate  $\bar{\lambda}$  is also an eigenvalue.

**Proposition 3.1** *Assume that  $(V, a)$  satisfies [cond( $V, a$ )] and that  $a \leq 0$ ,  $a(x^0) < 0$  for some  $x^0 \in \mathbb{R}^d$ . Then  $\text{Sp}[L]$  is in the open sector  $\{\lambda \in \mathbb{C}; \Im(\lambda) > 0, \Re(\lambda) \neq 0\}$ .*

**Proof** Let  $u \in L^2(\mathbb{R}^d)$ ,  $u \neq 0$  such that  $L_{V,a}(\lambda)u = 0$ . Set  $\lambda = r + is$ . We know that  $r \geq 0$ . Assume that  $r = 0$ . Reasoning by contradiction we first prove that  $s = 0$ . If  $s \neq 0$  that we get that  $\int_{\mathbb{R}^d} a(x)|u|^2(x)dx = 0$  hence  $u$  vanishes in a non empty open set of  $\mathbb{R}^d$  and applying the uniqueness Calderon theorem for second order elliptic equation we get  $u = 0$  on  $\mathbb{R}^d$  and a contradiction.

If  $s = 0$  we get

$$(-\Delta + V - 2ra + r^2)u = 0$$

and  $\int_{\mathbb{R}^d} (V(x) - 2ra(x) + r^2)|u(x)|^2 dx = 0$ . Using that  $V \leq a^2$  we have  $\int_{\mathbb{R}^d} (r - a)^2 |u(x)|^2 dx = 0$ . So again we get that  $u$  vanishes on a non empty open set and a contradiction like above.  $\square$

Let us remark that the general results given in Theorem 2.3 apply if there exists  $\delta \geq 0$  such that  $|a|(x) \leq CV(x)^{1/2-\delta}$  or  $|a|(x) \leq \kappa V(x)^{1/2}$  with  $\kappa$  small enough.

For 1D Schrödinger pencils accurate results were obtained by M. Christ [6, 7] et by [5]. Let us recall here some of their results. They consider the pencils

$$L_k(\lambda) = -\frac{d^2}{dx^2} + (x^k - \lambda)^2$$

with  $k \in \mathbb{N}$ . Here we shall only consider  $k$  even. The above assumptions are satisfied.

**Proposition 3.2 (M. Christ [8])** *For every  $k \geq 2$ ,  $k$  even, the set  $\text{Sp}[L_k]$  is included in the two sectors  $\{\lambda \in \mathbb{C}, |\arg(\lambda)| \geq \frac{k\pi}{2(k+1)}\}$ .*

The second result say that the eigenvalues of large modulus are close to the lines  $\{\lambda \in \mathbb{C}, |\arg(\lambda)| \geq \frac{k\pi}{2(k+1)}\}$ .

**Theorem 3.3 (Y. Ching-Chau, [5], Theorem 1)** *Let  $\{\lambda_n\}_{n \in \mathbb{N}}$  be the set  $\text{Sp}[L_k]$  such that  $|\lambda_1| < |\lambda_2| < \dots < |\lambda_n| < |\lambda_{n+1}| < \dots$ .*

*Then we have for  $n \rightarrow +\infty$ ,*

$$\lambda_n = \left( \frac{\pm(n + \frac{1}{2})\pi i - \log(2)}{\frac{2k}{k+1}} \right)^{\frac{k}{k+1}} + O\left(\frac{1}{\sqrt{n}}\right) \quad (3.7)$$

This result was proved using ODE methods in the complex plane.

By an elementary computation of the argument for the complex number in the r.h.s of (3.7) we can see that  $|\arg(\lambda_n)|$  is close to  $\frac{k\pi}{2(k+1)}$  when  $n \rightarrow +\infty$ . We also have the following result

**Theorem 3.4** ([19, 1]) *The linear space span by the generalized eigenfunctions associated with the eigenvalues  $\{\lambda_n\}$  is dense in  $L^2(\mathbb{R})$ .*

In [19] the proof was given for  $L_2(\lambda)$  and for  $L_k(\lambda, k > 2$ , even in [1], [2].

In the following result we shall see that the spectral set  $\text{Sp}(L_k)$  is very unstable under perturbations. M. Christ [7] has consider the following model:

$$L_P^\#(\lambda) = (P - \lambda + \frac{d}{dx})(P - \lambda - \frac{d}{dx})$$

We also have  $L_P^\#(\lambda) = -\frac{d^2}{dx^2} + (P - \lambda)^2 + P'$ ; where  $P$  is a polynomial. Assume that the degree  $k$  of  $P$  is even,  $P(x) = x^k + a_{k-1}x^{k-1} + \dots + a_1x + a_0$ .

**Proposition 3.5** *We have  $\text{Sp}[L_P^\#] = \emptyset$ . In other words for every  $\lambda \in \mathbb{C}$ , the equation  $L_P^\#(\lambda)u = 0$  has only the trivial solution  $u \equiv 0$  <sup>†</sup> in the Schwartz space  $\mathcal{S}(\mathbb{R})$ .*

#### A sketch of proof of Proposition (3.5)

We have

$$L_P^\#(\lambda) = (P - \lambda + \frac{d}{dx})(P - \lambda - \frac{d}{dx})$$

So, we have to solve the two equations

$$(P - \lambda + \frac{d}{dx})v = 0 \tag{3.8}$$

$$(P - \lambda - \frac{d}{dx})u = v \tag{3.9}$$

Set  $Q(x) = \int_0^x (P(s) - \lambda)ds$  and using standard ODE methods we get that

$$u(x) = C_1 e^{Q(x)} + C_2 e^{Q(x)} \int_x^{+\infty} e^{-2Q(s)} ds \tag{3.10}$$

where  $C_1, C_2$  are constants. If  $u$  is in the Schwartz space then  $u$  is in particular bounded but (3.10) shows that this is possible only if  $C_1 = C_2 = 0$ .  $\square$

## 4 Pseudospectra for linear pencils

As we have seen above the eigenvalues of Schrödinger pencils are very unstable. As propose some times ago by Thefthen [22] it is useful to replace the spectra of non-self adjoint operators by something more stable which is called the pseudospectra.

### 4.1 A short review

Let  $A$  be closed operator in the Hilbert space  $\mathcal{H}$  with domain  $D(A)$  dense in  $\mathcal{H}$ . Recall that  $D(A)$  is an Hilbert space for the graph norm  $\|u\|_{D(A)} = \sqrt{\|u\|_{\mathcal{H}}^2 + \|Au\|_{\mathcal{H}}^2}$ .

**Definition 4.1** *The complex number  $z$  is in resolvent set  $\rho(A)$  of  $A$  if and only if  $A - z\mathbb{I}$  is invertible from  $D(A)$  into  $\mathcal{H}$  and  $(A - z\mathbb{I})^{-1} \in \mathcal{L}(\mathcal{H})$  where  $\mathcal{L}(\mathcal{H})$  is the Banach space of linear and continuous maps in  $\mathcal{H}$ .*

*The spectrum  $\sigma(A)$  is defined as  $\sigma(A) = \mathbb{C} \setminus \rho(A)$*

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<sup>†</sup>it is known that every solution in  $L^2(\mathbb{R})$  of  $L_P^\#(\lambda)u = 0$  is in the Schwartz space  $\mathcal{S}(\mathbb{R})$  (see [19])

**Definition 4.2** Fix  $\varepsilon > 0$ . The  $\varepsilon$ -spectrum  $\sigma_\varepsilon(A)$  of  $A$  is defined as follows. A complex number  $z \in \sigma_\varepsilon(A)$  if and only if  $z \in \sigma(A)$  or if  $\|(A - z\mathbb{I})^{-1}\|_{\mathcal{L}(\mathcal{H})} > \varepsilon^{-1}$ . It is convenient to write  $\|(A - z\mathbb{I})^{-1}\|_{\mathcal{L}(\mathcal{H})} = \infty$  if  $z \in \sigma(A)$  and denote  $A - z = A - z\mathbb{I}$ .

There are several equivalent definitions of  $\sigma_\varepsilon(A)$  for details see the introduction of the book [23]. The following characterization is useful for numerical computations.

Assume that  $\dim \mathcal{H} < +\infty$ . Recall that the singular values for  $A \in \mathcal{L}(\mathcal{H})$  are the eigenvalues of the non negative matrix  $\sqrt{A^*A} := |A|$ . Denote  $s(A) = \sigma(|A|)$ .

**Proposition 4.3** For any matrix  $A$  we have  $z \in \sigma_\varepsilon(A)$  if and only if  $s_{\min}(A - z) < \varepsilon$ , where we have denoted  $s_{\min}(A) := \min[s(A)]$ .

**Proof** It is known that  $\|A\| = s_{\max}(A)$  for every  $A \in \mathcal{L}(\mathcal{H})$ . But  $AA^*$  and  $A^*A$  have the same non zero eigenvalues, so if  $A$  is invertible we have we have  $\|A^{-1}\| = \frac{1}{s_{\min}(A)}$  and the proposition follows.  $\square$ .

## 4.2 Pseudospectra for quadratic pencils

Our numerical computations (see hereafter Section 5) show that the spectra of quadratic pencils is much more unstable than the spectra of linear pencils (rotated harmonic oscillator, see [9]).

Let us recall the basic definitions and properties concerning pseudospectra for quadratic pencils. A more general setting is explained in [13, 14] for pencils of matrices.

The following result gives an idea about the pseudospectra of the Schrödinger pencil  $L(\lambda) = -\frac{d^2}{dx^2} + (x^2 - \lambda)^2$ :

**Theorem 4.4** [8] Assume that  $\theta \in \mathbb{R}$ ,  $0 < |\theta| \leq \frac{\pi}{2}$  and denote  $\lambda_0 = \rho e^{i\theta}$ . Then there exists  $C < +\infty$ ,  $\delta > 0$  and for every  $\rho \geq 1$  a Schwartz function  $g$ ,  $\|g\| = 1$  such that :

$$\|L(\lambda_0)g\|_{\mathcal{L}^2(\mathbb{R})} \leq C e^{-\delta \rho^{\frac{3}{2}}} \quad (4.11)$$

i.e. for  $\rho$  large enough the complex number  $\lambda_0$  is, in some sense, an almost eigenvalue or a pseudospectral point of  $L(\lambda)$ . On the line of direction  $\theta \in ]0, \pi/2]$  we have for  $|\lambda|$  large enough,

$$\|L(\lambda)^{-1}\| \geq \frac{1}{C} e^{|\lambda|^{3/2}}$$

In order to capture more details for the localization in the complex plane of large modulus pseudospectral points of  $L(\lambda)$  we can consider the following tentative definition of pseudospectra.

Let us consider a quadratic pencil  $L(\lambda)$  satisfying the assumptions of Theorem 2.1.

**Definition 4.5** Let  $\varepsilon > 0$ ,  $\delta \geq 0$ ,  $\mu > 3/2$ . Define the pseudospectra of order  $(\varepsilon, \delta, \mu)$  as follows

$$\text{Sp}_{\varepsilon, \delta, \mu}[L] = \{\lambda \in \mathbb{C}, \|L(\lambda)^{-1}\| \geq \varepsilon^{-1} \exp(\delta|\lambda|^\mu)\} \quad (4.12)$$

For  $\delta = 0$  we recover the definition given by Threfeten.

It is clear that  $\lambda \in \text{Sp}_{\varepsilon, \delta, \mu}[L]$  if and only if there exists  $u \in D(L_0)$ ,  $u \neq 0$ , such that

$$\|L(\lambda)u\| \leq \varepsilon \exp(-\delta|\lambda|^\mu)\|u\|$$

**Remark 4.6** Later we shall compute pseudospectra with this definition and see how it behaves according the parameter  $0 \leq \mu < \infty$ .

## 5 Eigenvalues computation with spectral methods and finite difference discretization

The aim of this section is to present the numerical computation of the spectrum of linear operator with quadratic dependence (quadratic pencil), see (1.2) :

$$L(\lambda) = L_0 + \lambda L_1 + \lambda^2$$

where  $L_0$  and  $L_1$  are operators on some Hilbert space  $\mathcal{H}$ . So we are interested to solve the following nonlinear eigenvalue problem :

$$L(\lambda)u = 0 \quad , \quad \lambda \in \mathbb{C}, \quad u \in \mathcal{H}.$$

In a first step, in order to validate the numerical approaches proposed, we consider the rotated harmonic oscillator in  $L^2(\mathbb{R})$ (see Davies [9]) :

$$-h \frac{d^2}{dx^2} + cx^2 \tag{5.13}$$

where  $h$  is a real positive parameter and  $c$  is a complex number with positive real and imaginary parts,  $c = \exp(i\alpha)$ , for  $0 \leq \alpha < \pi/2$ .

Here after, for each operator considered, we compute spectra and pseudospectra and we discuss the numerical results obtained.

### 5.1 The rotated harmonic oscillator

#### 5.1.1 Eigenvalue computations with Hermite spectral method (unbounded domain)

We look for an approximation of  $\lambda \in \mathbb{C}$  solution of the following linear eigenvalue problem ( $h = 1$ ) :

$$-\frac{d^2 u}{dx^2}(x) + cx^2 u(x) = \lambda u(x) \quad , \quad x \in \mathbb{R} \tag{5.14}$$

Here the computational domain is unbounded ( $\Omega = \mathbb{R}$ ). So we use a spectral Galerkin method using Hermite functions (see Appendix A) *i.e.* we look for an approximation :

$$u_N(x) = \sum_{k=0}^N \tilde{u}_k \varphi_k(x) \tag{5.15}$$

of  $u$  such that :

$$\left\langle -\frac{d^2 u_N}{dx^2} + cx^2 u_N - \lambda_N u_N, \varphi_l \right\rangle = 0 \quad , \quad l = 0, \dots, N$$

where  $\langle \cdot, \cdot \rangle$  is the scalar product in  $L^2(\mathbb{R})$  (method of weighted residuals, MWR, see for example, [11], [4]). Using the orthogonality properties (A.53) of the Hermite functions in  $L^2(\mathbb{R})$  and the relations (A.57) we obtain the following eigenvalue problem :

$$\mathcal{A}_N U_N = \lambda_N U_N \tag{5.16}$$

with  $\mathcal{A}_N$  the square tridiagonal symmetric matrix of order  $N + 1$  such that  $\mathcal{A}_N(k, k - 2) = (c - 1)\sqrt{k(k - 1)}$ ,  $\mathcal{A}_N(k, k) = (c + 1)(2k + 1)$  and  $U_N$  is the vector containing the coefficients  $\tilde{u}_k$ ,  $k = 0, \dots, N$  of  $u_N$ .

For the numerical computation of the spectrum of  $\mathcal{A}_N$  we use the function ZGEEV of the library LAPack.

We recall that for the continuous operator (5.14) the eigenvalues are (see [24]) :

$$\exp(i\alpha/2)(2n+1) \quad , \quad n = 0, 1, \dots \quad (5.17)$$

inducing that the eigenvalues, in the complex plane, are aligned on a straight with a slope  $\frac{\lambda_i}{\lambda_r} = \tan(\alpha/2)$ , where  $\lambda_r$  (resp.  $\lambda_i$ ) is the real (resp. imaginary) part of the eigenvalues  $\lambda$ . Here we have chosen  $\alpha = \pi/4$  so  $\frac{\lambda_i}{\lambda_r} = \tan(\pi/8) = 0.4$ .

Now we present the numerical results obtained with the Hermite spectral method. On Figure 1 we can see the spectrum of the matrix  $\mathcal{A}_N$  associated with the eigenvalue problem (5.16) for  $N = 50$ ,  $c = \exp(i\alpha)$  with  $\alpha = \pi/4$ . We can see that the slope  $\lambda_{N,i}/\lambda_{N,r} = \tan(\alpha/2)$  is obtained for  $|\lambda_{N,r}| \leq 100$ . Then a bifurcation appears in the spectrum, which is in agreement with [9], [24]. If we choose a larger value of  $N$ , for example  $N = 100$ , the slope of  $\tan(\alpha/2)$  appears for larger value of  $|\lambda_{N,r}| \leq 200$  (see Figure 1) which is in agreement with the fact that  $u_N$  converges to  $u$  when  $N$  increases (see (A.58), (A.59)).

### 5.1.2 Eigenvalue computations with finite difference method (bounded domain)

The rotated harmonic oscillator is defined for functions  $u \in H^2(\mathbb{R})$  such that  $x^2u(x) \in L_2(\mathbb{R})$ . So  $u(x)$  decreases when  $x^2$  increases and we want to consider the problem (5.14) on a bounded domain, with homogeneous Dirichlet boundary conditions :

$$\begin{cases} -\frac{d^2u(x)}{dx^2} + cx^2u(x) = \lambda u(x) \quad , \quad x \in \Omega \\ u(\pm L) = 0 \end{cases} \quad (5.18)$$

where  $\Omega = (-L, +L)$ ,  $L$  being chosen sufficiently large. More precisely, if we retain  $N$  modes in the Hermite development (5.15), the Hermite function of highest degree is  $\varphi_N$  and the zeroes  $h_n$  of  $\varphi_N$  verify (see [3]) :

$$h_n \leq \sqrt{2N-2} \quad , \quad n = 1, \dots, N$$

So the size of the containment area is  $2L = 2\sqrt{2N-2}$  and we retain as value for the bounded domain  $\Omega$  :

$$L = \sqrt{2N-2} \quad (5.19)$$

To obtain a numerical approximation  $\lambda_N$  of the eigenvalues of problem (5.18) we discretize the second order spatial derivative using a standard second order centered finite difference scheme :

$$\frac{d^2u(x_j)}{dx^2} = \frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1}))}{\Delta x^2} + o(\Delta x^2)$$

where  $\Delta x = 2L/N$  is the spatial step of the meshgrid  $x_j = -L + j\Delta x$ ,  $j = 0, \dots, N$ , on the domain  $\Omega$ . So we obtain the following linear eigenvalue problem to solve :

$$\mathcal{A}_N U_N = \lambda_N U_N \quad (5.20)$$

where  $\mathcal{A}_N$  is a tridiagonal symmetric matrix of order  $N-1$  such that  $\mathcal{A}_N(k, k-1) = \mathcal{A}_N(k, k+1) = -\frac{1}{\Delta x^2}$ ,  $\mathcal{A}_N(k, k) = \frac{2}{\Delta x^2} + cx_k^2$  and  $U_N$  is the vector containing the approximations  $u_N(x_j)$  of  $u(x_j)$ ,  $j = 1, \dots, N-1$  ( $u_N(x_0) = u_N(x_N) = 0$ ).

As previously for the Hermite spectral method, we use the function ZGEEV of the library LAPack for the numerical computation of the spectrum.

Now we present the numerical results obtained with the method based on finite difference discretization. As for the Hermite spectral method, we have chosen  $N = 50$  and  $N = 100$ . On Figure

2 we present the spectrum of the matrix  $\mathcal{A}_N$  of the eigenvalue problem (5.20) obtained for  $N = 50$ ,  $L = 10$  in accordance with (5.19) and  $c = \exp(i\alpha)$  with  $\alpha = \pi/4$ . We can see that the slope  $\lambda_{N,i}/\lambda_{N,r} = \tan(\alpha/2)$  is obtained for  $|\lambda_{N,r}| \leq 25$ . Then, as for the Hermite spectral method, a bifurcation appears in the spectrum. If we choose a larger value of  $N$ , for example  $N = 100$  and  $L = 15$  following (5.19), the slope of  $1/2$  appears in the spectrum for larger value of  $|\lambda_{N,r}| \leq 75$  (see Figure 2) which is in agreement with the fact that accuracy of the difference scheme increases with  $N$ .

Now if we compare, for a same value of  $N$  ( $N = 50$ ) the numerical results obtained with Hermite spectral method and with finite difference scheme, we can see on Figure 3 that the slope  $\frac{\lambda_{N,i}}{\lambda_{N,r}} = \tan(\alpha/2)$ , which is in agreement with the continuous operator (see (5.17)), appears for larger values of  $\lambda_{N,r}$  with the spectral method than with the finite difference method. This is coherent with the fact that the Hermite spectral method is more accurate than the finite difference method for a same value of the parameter  $N$  (spectral accuracy due to the fast decrease, in modulus, of the coefficients  $\tilde{u}_k$  when  $k$  increases, see Proposition (A.1)).

Now we try to analyze the bifurcation phenomenon appearing on the spectrum for eigenvalues with large real part  $\lambda_{N,r}$ . When we discretize with a finite difference scheme, we consider that  $x$  is constant over one spatial step  $\Delta x = \frac{2L}{N}$ . So, in a first step, we consider an operator deduced from the rotated harmonic oscillator in which  $x^2$  is chosen constant equal to  $b^2$  over all the domain  $\Omega$ . So we obtain the following problem deduced from (5.18) :

$$-\frac{d^2u}{dx^2} + cb^2u = \lambda u \quad , \quad x \in \Omega \quad (5.21)$$

If we consider periodic boundary conditions  $u(-L) = u(+L)$ , we look for eigenfunctions of (5.21) such as :

$$u(x) = \hat{u}_k \exp(ik'x) \quad (5.22)$$

with the wavenumber  $k' = \frac{k\pi}{L}$ ,  $k = 0, \dots, N-1$ . Substituting (5.22) in (5.21) we obtain :

$$\lambda = k'^2 + cb^2$$

So, since  $c = \exp(i\alpha)$  we have :

$$\begin{cases} \lambda_r = k'^2 + \cos(\alpha)b^2 \\ \lambda_i = \sin(\alpha)b^2 \end{cases}$$

We can see that  $\lambda_i$  is constant and that  $\lambda_r$  depends of the wavenumber  $k'$ .

Now we consider that  $x$  is constant over  $N_b$  spatial steps  $\Delta x$ , so in the rotated harmonic oscillator we replace  $x^2$  with  $b(x)^2$  where  $b(x) = b_j = -L + jN_b\Delta x$  for  $x \in [-L + jN_b\Delta x, -L + (j+1)N_b\Delta x]$ ,  $j = 0, \dots, N/N_b - 1$ . We obtain :

$$\begin{cases} \lambda_r = k'^2 + \cos(\alpha)b_j^2 \\ \lambda_i = \sin(\alpha)b_j^2 \end{cases} \quad (5.23)$$

with the wavenumber  $k' = \frac{k\pi}{L}$ ,  $k = 0, \dots, N_b - 1$ . So the spectrum is constituted of different steps, each step corresponding to  $N_b$  eigenvalues  $\lambda$ , with  $\lambda_i$  constant while  $\lambda_r$  is wavenumber dependent. We can observe on (5.23) that for  $k' = 0$  the corresponding eigenvalues  $\lambda$ ,  $j = 0, \dots, N/N_b - 1$  are aligned on a straight with a slope  $\lambda_i/\lambda_r = \tan(\alpha)$ . This can be seen on Figure 4, corresponding to  $N = 100$ ,  $L = 20$ ,  $\alpha = \pi/4$  and  $N_b = 5$ . On Figure 5, corresponding to  $N = 100$ ,  $L = 15$ ,  $\alpha = \pi/4$  and  $N_b = 5$  ( $\Delta x$  is decreased in comparison with Figure 4), we can see that some numerical artefacts appear on the computation of the eigenvalues  $\lambda$  having small modulus. In order to avoid

this, we try to impose in the spectrum that two consecutive steps, corresponding to two different values of  $b_j$ , are not recovered for the real part  $\lambda_r$ . So we must have :

$$\left(\frac{N}{2L}\right)^2 \leq \cos(\alpha)N_b^2(\Delta x)^2$$

So, since  $\Delta x = \frac{2L}{N}$  we deduce the following inequality :

$$\left(\frac{N}{L}\right)^2 \leq 4N_b\sqrt{\cos(\alpha)} \quad (5.24)$$

which is a constraint on  $\Delta x^{-1}$ .

As it has been said previously for the finite difference scheme we have  $N_b = 1$ . So, in agreement with (5.23) we expect that the eigenvalues computed with the finite difference scheme (5.20) are aligned on a straight with a slope  $\lambda_i/\lambda_r = \tan(\alpha) = 1$  for  $\alpha = \pi/4$ . This is what we obtain if we choose  $N = 50$  and  $L = 50$  (see Figure 6). We can note that with this choice of the parameters, the inequality (5.24) is satisfied. Now, in order to test the convergence of the finite difference scheme we reduce the spatial step  $\Delta x$ . So we choose  $N = 500$  and  $L = 50$  (see Figure 7). With this choice of the parameters, the inequality (5.24) is not satisfied. We can see that some numerical artefacts appear near the origin, where we can observe a slope  $\frac{\lambda_{N,i}}{\lambda_{N,r}} = \tan(\alpha/2)$ , which is in agreement with (5.17). This can be interpreted as an intermediate slope between the slope  $\frac{\lambda_{N,i}}{\lambda_{N,r}} = \tan(\alpha)$  and the slope  $\frac{\lambda_{N,i}}{\lambda_{N,r}} = \tan(0) = 0$  of each step.

**Remark 5.1** Let  $H(b_j)$  the operator deduced from the rotated harmonic oscillator,  $H(b_j) = -\frac{d^2}{dx^2} + cb_j^2$  and  $\lambda_{j,i}$ ,  $u_{j,i}$  the eigenvalues and eigenvectors associated :  $H(b_j)u_{j,i} = \lambda_{j,i}u_{j,i}$ . We denote  $u = \sum_{j=0}^{N/N_b-1} u_j \mathbb{1}_{[x_j, x_{j+1}]}$  and  $b = \sum_{j=0}^{N/N_b-1} b_j \mathbb{1}_{[x_j, x_{j+1}]}$ , with  $x_j = -L + jN_b\Delta x$  and  $\mathbb{1}_{[x_j, x_{j+1}]}$  the characteristic function associated with the interval  $[x_j, x_{j+1}]$ . We consider the operator  $H(b) = \oplus H(b_j)$ . If  $\lambda$  is an eigenvalue of  $H(b)$ , so there exists  $(j, i)$  such that  $\lambda = \lambda_{j,i}$ .

Now, in order to study the numerical instability of the finite difference scheme in function of the meshgrid  $x_j$ ,  $j = 0, \dots, N$ , we consider a small perturbation on each point of the grid,  $x_j + \varepsilon$ ,  $j = 0, \dots, N$ , where  $\varepsilon$  is a small parameter. The matrix  $\mathcal{A}_N$  (see (5.20)) is replaced with the matrix :

$$\mathcal{A}_{N,\varepsilon} = \mathcal{A}_N + \varepsilon \mathcal{E}_N$$

where  $\mathcal{E}_N$  is the diagonal matrix of order  $N-1$  such that  $\mathcal{E}_N(k, k) = 2 \exp(i\alpha)x_k$  (we have neglected the terms in  $\varepsilon^2$ ). If we compare the eigenvalues  $\lambda_N$  of the matrix  $\mathcal{A}_N$  with the eigenvalues  $\lambda_{N,\varepsilon}$  of  $\mathcal{A}_{N,\varepsilon}$  we have :

$$\mathcal{A}_{N,\varepsilon} U_{N,\varepsilon} = (\mathcal{A}_N + \varepsilon \mathcal{E}_N) U_{N,\varepsilon} = \lambda_{N,\varepsilon} U_{N,\varepsilon}$$

where  $U_{N,\varepsilon}$  is a right eigenvector of  $\mathcal{A}_{N,\varepsilon}$ . So we deduce (see [21]) :

$$\mathcal{A}_N \frac{dU_{N,\varepsilon}}{d\varepsilon}(\varepsilon) + \mathcal{E}_N U_{N,\varepsilon}(\varepsilon) + \varepsilon \mathcal{E}_N \frac{dU_{N,\varepsilon}}{d\varepsilon}(\varepsilon) = \frac{d\lambda_{N,\varepsilon}}{d\varepsilon}(\varepsilon) U_{N,\varepsilon}(\varepsilon) + \lambda_{N,\varepsilon}(\varepsilon) \frac{dU_{N,\varepsilon}}{d\varepsilon}(\varepsilon)$$

For  $\varepsilon = 0$  we obtain :

$$\mathcal{A}_N \frac{dU_{N,\varepsilon}}{d\varepsilon}(0) + \mathcal{E}_N U_{N,\varepsilon}(0) = \frac{d\lambda_{N,\varepsilon}}{d\varepsilon}(0) U_{N,\varepsilon}(0) + \lambda_{N,\varepsilon}(0) \frac{dU_{N,\varepsilon}}{d\varepsilon}(0)$$

If we multiply on the left the previous equality with  $V_N$  a left eigenvector of  $\mathcal{A}_N$  we obtain :

$$\frac{d\lambda_{N,\varepsilon}}{d\varepsilon}(0) = \frac{V_N^* \mathcal{E}_N U_N}{V_N^* U_N} \quad (5.25)$$

where  $V_N^* = \overline{V_N}^t$  and  $U_N$  is a right eigenvector of  $\mathcal{A}_N$ . The equality (5.25) measures the sensivity of the eigenvalue  $\lambda_N$  of the matrix  $\mathcal{A}_N$  in function of a perturbation  $\varepsilon$  on the meshgrid (condition number of the eigenvalue  $\lambda_N$ ). On Figure 8 we have represented the condition number of the eigenvalues  $\lambda_N$  in function of the modulus of the eigenvalues, for  $N = 100$  and  $L = 15$ . We can see that the condition number is small for eigenvalues with small modulus and then it increases with the modulus. However, the values are small in comparison with the results obtain for a nonlinear eigenvalue problem (see Section 5.2.2, Figure 15), which implies that the numerical computation is stable if we consider a perturbation on the meshgrid points.

### 5.1.3 Pseudospectra

In this subsection we present numerical pseudospectra computations for the rotated harmonic oscillator. Notice that a theoretical analysis of this problem has been performed in [20]. In a first step we consider the matrix from the Hermite spectral method (5.16) and in a second step the matrix from the finite difference scheme (5.20). It is known that the numerical computation of the pseudospectra is more stable than for the spectra (see Section 4).

To obtain the pseudospectra, following Definition 4.2 we look for  $z \in \mathbb{C}$  such that  $\|(\mathcal{A}_N - z\mathbb{I}_N)^{-1}\| = s_{\min}^{-1}(\mathcal{A}_N - z\mathbb{I}_N)$  is large, *i.e.* the distance of  $z$  to the spectrum of  $\mathcal{A}_N$  is small :

$$s_{\min}(\mathcal{A}_N - z\mathbb{I}_N) \leq \varepsilon \quad (5.26)$$

where  $\|-\|$  is the matricial norm associated with the Euclidean norm,  $\varepsilon$  is a small parameter,  $\mathbb{I}_N$  is the identity matrix and  $s_{\min}(\mathcal{A}_N - z\mathbb{I}_N)$  is the smallest singular value of the matrix  $\mathcal{A}_N - z\mathbb{I}_N$ . So we consider a mesh on the complex plane. For each point  $z$  of the mesh we compute the singular value of  $\mathcal{A}_N - z\mathbb{I}_N$ , using the function ZGESVD of the LAPack Library.

For the computation of the pseudospectra (5.26), we have retained complex values  $z$  lying on the meshgrid in the area of the complex plane corresponding to  $[0, 140] \times [0, 80]$ . The step retained is  $dx = 1$  and  $dy = 1$  in the real and imaginary directions. On Figure 9 (resp. Figure 10) we can see the computation corresponding to the matrix  $\mathcal{A}_N - z\mathbb{I}_N$ , with  $\mathcal{A}_N$  corresponding to the Hermite spectral method (resp. finite difference scheme). The choice of the parameters are  $\alpha = \pi/4$ ,  $N = 100$  for unbounded and bounded domains,  $L = 15$  for the bounded domain. We can see on these two figures that the spectrum of the continuous operator (slope equal to  $\lambda_i/\lambda_r = \tan(\alpha/2) = 0.4$  (see (5.17)) is contained in the area of the pseudospectra corresponding to the smallest values of the parameter  $\varepsilon$ , *i.e.* in the area where the distance of  $z$  to the eigenvalues of matrix  $\mathcal{A}_N$  is the smallest. This is especially true for the Hermite spectral method.

Now we consider here the computation of the pseudospectra based on Definition 4.5 (see (4.12)) instead of Definition 4.2 as previously. So we look for  $z \in \mathbb{C}$  such that :

$$\|(\mathcal{A}_N - z\mathbb{I}_N)^{-1}\| = s_{\min}^{-1}(\mathcal{A}_N - z\mathbb{I}_N) \geq \varepsilon^{-1} \exp(\delta|z|^\mu) \quad (5.27)$$

where  $\varepsilon$ ,  $\delta$  and  $\mu$  are real parameters. For  $\delta = 0$  we retrieve (5.26). The majoration in (5.27) depends on  $|z|$ , in opposition with (5.26) : the constraint appearing in (5.27) is stronger when  $|z|$  is increased. On Figure 11 we present the pseudospectra corresponding to the matrix  $\mathcal{A}_N - z\mathbb{I}_N$ , where  $\mathcal{A}_N$  is the matrix obtained with the finite difference scheme, for  $\delta = 0.5$ ,  $\mu = 0.5$  and for different values of the parameter  $\varepsilon$ . As before we have retained complex values  $z$  lying on the meshgrid in the area of the complex plane corresponding to  $[0, 140] \times [0, 80]$ . The step retained is  $dx = 1$  and  $dy = 1$  in the real and imaginary directions. The numerical results obtained are in agreement with the results presented on Figure 10.

## 5.2 Nonlinear eigenvalue problems

In this section we consider the following operator :

$$L_a(\lambda) = -\frac{d^2}{dx^2} + x^4 - 2a\lambda x^2 + \lambda^2 \quad (5.28)$$

where  $a$  is a real parameter. We want to solve the following problem :

$$L_a(\lambda)u = 0 \quad , \quad x \in \mathbb{R} \quad (5.29)$$

For  $a = 1$  we recover the problem (1.4).

The problem (5.29) can be reformulated as an eigenvalue problem. Indeed, if we set  $v = \lambda u$  we can rewrite (5.29) as :

$$\mathcal{A}_a \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix} \quad (5.30)$$

where :

$$\mathcal{A}_a = \begin{pmatrix} 0 & \mathbb{I} \\ -L_0 & -L_{1_a} \end{pmatrix}$$

with the operators  $L_0 = -\frac{d^2}{dx^2} + x^4$  and  $L_{1_a} = -2ax^2$ .

### 5.2.1 Eigenvalue computations with Hermite spectral method (unbounded domain)

We look for an approximation  $u_N$  of  $u$  such that  $L_a(\lambda)u_N = 0$ , with  $u_N = \sum_{k=0}^N \tilde{u}_k \varphi_k$ , with  $\varphi_k$  Hermite functions (spectral Galerkin approximation, see Appendix A). Then, in order to obtain  $u_N$ , we use a method of weighted residuals (MWR, see for example, [11], [4]) :

$$(L_a(\lambda)u_N, \varphi_l) = 0 \quad , \quad l = 0, \dots, N$$

where  $(.,.)$  is the scalar product in  $L^2(\mathbb{R})$ . Setting  $v_N = \lambda u_N$ , using the orthogonality properties of the Hermite function in  $L^2(\mathbb{R})$  and the relations (A.57), we obtain the following eigenvalue problem :

$$\mathcal{A}_{a,N} \begin{pmatrix} U_N \\ V_N \end{pmatrix} = \lambda_N \begin{pmatrix} U_N \\ V_N \end{pmatrix}$$

which is an approximation of the eigenvalue problem (5.30).  $U_N$  (resp.  $V_N$ ) is the vector containing the coefficients  $\tilde{u}_k$  (resp.  $\tilde{v}_k$ ) of  $u$  (resp.  $v$ ),  $k = 0, \dots, N$ . The matrix  $\mathcal{A}_{a,N}$  is the square matrix of order  $(2N + 2)$  :

$$\mathcal{A}_{a,N} = \begin{pmatrix} 0 & \mathbb{I}_N \\ -L_{0_N} & -L_{1_{a,N}} \end{pmatrix} \quad (5.31)$$

where  $L_{0_N}u_N = (L_0u_N, \varphi_l)$  and  $L_{1_{a,N}}v_N = (L_{1_a}v_N, \varphi_l)$ ,  $l = 0, \dots, N$ , with  $L_0u_N = -\frac{d^2u_N}{dx^2} + x^4u_N$  and  $L_{1_a}v_N = -2ax^2v_N$ .

$L_{0_N}$  is a pentadiagonal symmetric matrix such that  $L_{0_N}(j, j) = (\frac{2j+1}{2}) + \frac{1}{4}c_j$ ,  $L_{0_N}(j, j-2) = -\frac{1}{2}\sqrt{j(j-1)} + \frac{1}{4}b_{j-2}$  and  $L_{0_N}(j, j-4) = \frac{1}{4}a_{j-4}$  for  $j = 0, \dots, N$ , where  $a_j = \sqrt{j(j-1)(j-2)(j-3)}$ ,  $b_j = (4j-2)\sqrt{j(j-1)}$  and  $c_j = (6j^2 + 2j + 3)$ .

$L_{1_{a,N}}$  is a tridiagonal symmetric matrix such that  $L_{1_{a,N}}(j, j) = -(2j+1)$  and  $L_{1_{a,N}}(j, j-2) = -\sqrt{j(j-1)}$ .

For the numerical computation of the spectrum of  $\mathcal{A}_{a,N}$  we use the function DGEEV of the LAPack library.

For  $a = 1$ , in order to analyze the spectrum of the continuous operator (1.4), we consider a simplified operator, deduced from the operator (5.28) for  $a = 1$ , where  $x$  is replaced with a real constant  $b$ . We obtain the following problem :

$$\lambda^2 u - \frac{d^2 u}{dx^2} - 2b^2 \lambda u + b^4 u = 0 \quad (5.32)$$

We look for a solution  $u(x)$  of the problem (5.32) of the form  $u = \tilde{u}_k \varphi_k$ . Substituting in (5.32) and using the relations (A.57), we obtain :

$$\lambda_N^2 \varphi_k - \frac{1}{2} \sqrt{k(k-1)} \varphi_{k-2} + \left(\frac{2k+1}{2k+2}\right) \varphi_k - \frac{1}{2} \sqrt{(k+1)(k+2)} \varphi_{k+2} - 2b^2 \lambda_N \varphi_k + b^4 \varphi_k = 0 \quad (5.33)$$

Using the scalar product in  $L^2(\mathbb{R})$  of (5.33) with  $\varphi_k$  we obtain :

$$\lambda_N^2 + \frac{2k+1}{2} - 2b^2 \lambda_N + b^4 = 0 \quad (5.34)$$

We deduce from (5.34) that  $\lambda_N = b^2 \pm i \sqrt{k+1/2}$ , so :

$$\begin{cases} \lambda_{N,r} = b^2 \\ \lambda_{N,i} = \pm \sqrt{k+1/2} \end{cases} \quad (5.35)$$

The imaginary part  $\lambda_{N,i}$  of  $\lambda_N$  is wavenumber independent. From (5.35) it comes that the spectrum is contained in the part of the complex plane defined by  $\lambda_{N,r} = b^2$  and  $-\sqrt{N} \leq \lambda_{N,i} \leq \sqrt{N}$  since  $k = 0, \dots, N$ .

Now, on Figure 12 we present the spectrum of the matrix (5.31) for  $N = 50$  and  $a = 1$ . Firstly we can note that, as for the rotated harmonic oscillator (see Figure 1), a bifurcation appears in the spectrum when the modulus of the eigenvalues is increased (see also Figure 16). Then theoretical results give that the eigenvalues of the continuous operator (5.28), for  $a = 1$ , are included in the two sectors  $\{\lambda \in \mathbb{C}, |\arg(\lambda)| \geq \frac{\pi}{3}\}$  (see Section 3). We can see on Figure 12 that computed eigenvalues are not all included in these two sectors. This reflects numerical instabilities leading to spurious eigenvalues (spectral pollution, see [10]). We can note that we have  $-\sqrt{N} \leq \lambda_{N,i} \leq \sqrt{N}$ , in agreement with the previous analyze when  $x = b$  is constant (see (5.35)). Moreover, in the previous analyze we have  $\lambda_{N,r} = b^2$ . Here, for  $N = 50$  following (5.19) we deduce that the size of the containment domain is  $2L$  with  $L \simeq 10$  and, on Figure 12, we can see that  $0 \leq \lambda_{N,r} \leq L^2$ .

### 5.2.2 Eigenvalue computations with finite difference method (bounded domain)

The operator  $L_a(\lambda)$  (see (5.28)) is defined on the domain  $D(\mathcal{A}) = \{u \in H^2(\mathbb{R}), x^4 u \in L^2(\mathbb{R})\}$ . So  $u$  is decreasing when  $x^4$  is increasing and the decrease is faster than for the rotated harmonic oscillator (5.13). So we want to consider the following nonlinear eigenvalue problem in bounded domain with Dirichlet homogeneous boundary conditions : find  $\lambda \in \mathbb{C}$  such that :

$$\begin{cases} L_a(\lambda)u = 0, & x \in \Omega \\ u(\pm L) = 0 \end{cases} \quad (5.36)$$

where  $\Omega = (-L, +L)$  with  $L$  sufficiently large. More precisely we retain  $L = \sqrt{2N-2}$  (see (5.19)).

As before, the problem (5.36) can be reformulated as an eigenvalue problem :

$$\mathcal{A}_a \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix} \quad (5.37)$$

where :

$$\mathcal{A}_a = \begin{pmatrix} 0 & \mathbb{I} \\ -L_0 & -L_{1_a} \end{pmatrix}$$

with  $v = \lambda u$  and the operators  $L_0 = -\frac{d^2}{dx^2} + x^4$ ,  $L_{1_a} = -2ax^2$ .

We consider on the domain  $\Omega$  a meshgrid with a mesh  $\Delta x = 2L/N$  on  $\Omega$  and we note  $x_j = -L + j\Delta x$ ,  $j = 0, \dots, N$  the points of the grid. We have retained homogeneous Dirichlet boundary conditions for  $x = \pm L$ , so  $u(x_0) = u(x_N) = 0$ . We look for an approximation  $u_N$ ,  $v_N$  of  $u$  and  $v = \lambda u$  such that :

$$\mathcal{A}_{a,N} \begin{pmatrix} U_N \\ V_N \end{pmatrix} = \lambda_N \begin{pmatrix} U_N \\ V_N \end{pmatrix}$$

with  $U_N$  and  $V_N$  two vectors containing respectively the approximations  $u_N(x_j)$ ,  $v_N(x_j)$  of  $u(x_j)$ ,  $v(x_j)$  and  $\mathcal{A}_{a,N}$  is the square matrix of order  $2N - 2$  :

$$\mathcal{A}_{a,N} = \begin{pmatrix} 0 & \mathbb{I}_N \\ -L_{0,N} & -L_{1_{a,N}} \end{pmatrix} \quad (5.38)$$

where  $L_{0,N}u_N(x_j) = -\left(\frac{u_N(x_{j+1}) - 2u_N(x_j) + u_N(x_{j-1}))}{\Delta x^2} + x_j^4 u_N(x_j)\right)$  is the discretization of the operator  $L_0$  with a centered finite difference scheme and  $L_{1_{a,N}}v_N(x_j) = -2ax_j^2 v_N(x_j)$ .

$L_{0,N}$  is a tridiagonal symmetric matrix such that  $L_{0,N}(j, j) = \frac{2}{\Delta x^2} + x_j^4$  and  $L_{0,N}(j, j-1) = -\frac{1}{\Delta x^2}$ .

$L_{1_{a,N}}$  is a diagonal matrix such that  $L_{1_{a,N}}(j, j) = -2ax_j^2$ .

For the numerical computation of the spectrum of the matrix  $\mathcal{A}_{a,N}$  we use the function DGEEV of the LAPack library.

Now, we are interested to analyze the dependence of the spectrum of the operator (5.28) in function of the real parameter  $a$ . For this, we consider an approximation of the infinite dimensional domain as a bounded domain with periodic boundary conditions. We look for eigenfunction  $u_k(x) = \hat{u}_k \exp(ik'x)$ , with  $k' = \frac{k\pi}{L}$ , of the continuous operator (5.28). Computing  $L_a(\lambda)u_k(x)$  we obtain the following equation :

$$\lambda^2 - 2a\lambda x^2 + x^4 + k'^2 = 0$$

The discriminant  $\Delta = 4(a^2 - 1)x^4 - 4k'^2$  is negative for  $0 \leq a \leq 1$  and the solutions are :

$$\lambda^\pm = \frac{2ax^2 \pm i\sqrt{-\Delta}}{2}$$

When  $a$  is increased from 0 to 1 the ratio of the imaginary part over the real part of  $\lambda$ ,  $\frac{|\lambda_i|}{|\lambda_r|} = \frac{\sqrt{k'^2 - (a^2 - 1)x^4}}{ax^2}$  is decreased and it is infinite for  $a = 0$ . We can observed this on the numerical simulations corresponding to  $a = 0$ ,  $a = 0.5$ ,  $a = 0.9$  and  $a = 1.0$  obtained with the finite difference scheme for  $N = 50$  and  $L = 10$  (see Figure 13 ).

We are now interested with the operator  $L_a(\lambda)$  for  $a = 1$ . We look for the spectrum of the discretized operator, using finite difference method, where  $x$  is replaced with a real constant  $b$  (see (5.32)). We have :

$$\lambda_N^2 u(x_j) - \frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1}))}{\Delta x^2} - 2b^2 \lambda_N u(x_j) + b^4 u(x_j) = 0 \quad (5.39)$$

If we consider periodic boundary conditions, we look for a solution of (5.39) of the form  $u(x) = \hat{u}_k \exp(ik'x)$ , with  $k' = \frac{k\pi}{L}$ . Substituting in (5.39) and supposing that  $\hat{u}_k \neq 0$  we obtain :

$$\lambda_N^2 \Delta x^2 - 2b^2 \lambda_N \Delta x^2 + b^4 \Delta x^2 - 2 \cos(k' \Delta x) + 2 = 0$$

Finally we have  $\lambda_N = \lambda_{N,r} + i\lambda_{N,i}$  with  $\lambda_{N,r} = b^2$  is wavenumber independent and  $\lambda_{N,i} = \pm \frac{\sqrt{2 - 2 \cos(k' \Delta x)}}{\Delta x}$  is wavenumber dependent. So the spectrum of the discretized operator is located in the part of the plan complex such that  $\lambda_{N,r} = b^2$  and  $-|k'_{\max}| \leq \lambda_{N,i} \leq |k'_{\max}|$  since  $\cos(k' \Delta x) \simeq 1 - \frac{k'^2 \Delta x^2}{2}$  for  $\Delta x$  sufficiently small.

Here since  $\Omega = (-L, +L)$  and  $N$  is the number of grid points retained, the highest wavenumber  $k'_{\max}$  we can take into account with this meshgrid is  $k'_{\max} = \frac{N}{2L} = \Delta x^{-1}$ . Since  $L \simeq \sqrt{2N-2}$  (see (5.19)) we have  $k'_{\max} = O(\sqrt{N})$ , which is in agreement with the Hermite spectral method for unbounded domain (see (5.35)).

On Figure 14 we present the spectrum of the matrix (5.38) for  $N = 50$ ,  $L = 10$  and  $a = 1$ . Comparison with Figure 12 shows that the results obtained for Hermite spectral method (unbounded domain) and for finite difference method (bounded domain) are quite similar. We have chosen  $L = 10$  for the size of the bounded domain, in agreement with (5.19). As it has been said previously, theoretical results give that the eigenvalues of the continuous operator (5.28), for  $a = 1$ , are included in the two sectors  $\{\lambda \in \mathbb{C}, |\arg(\lambda)| \geq \frac{\pi}{3}\}$  (see Section 3). But we can see on Figure 14 (as on Figure 12) that computed eigenvalues are not all included in these two sectors, which can be imputed to numerical instabilities leading to spurious eigenvalues (spectral pollution, see [10]).

In order to analyze these numerical instabilities, we study the stability of the eigenvalues in function of a perturbation on the points of the mesh grid retained for the discretization. The equality (5.25) measures the sensivity of the eigenvalue  $\lambda_N$  of the matrix  $\mathcal{A}_N$  in function of a perturbation  $\varepsilon$  on the meshgrid (condition number of the eigenvalue  $\lambda_N$ ). Here the matrix  $\mathcal{E}_N$  is the matrix of order  $2N - 2$  :

$$\mathcal{E}_N = \varepsilon \begin{pmatrix} 0 & 0 \\ \mathcal{E}_{0,N} & \mathcal{E}_{1,N} \end{pmatrix}.$$

where  $\mathcal{E}_{0,N}$  (resp.  $\mathcal{E}_{1,N}$ ) is the diagonal matrix with the elements  $-4x_j^3$  (resp.  $4ax_j$ ) on the diagonal,  $j = 1, \dots, N - 1$  (we have neglected in  $\mathcal{E}_N$  the terms in  $\varepsilon^n$ , with  $n > 1$ ).

On Figure 15 we have represented the condition number of the eigenvalues  $\lambda_N$  in function of the modulus  $|\lambda_N|$  for  $N = 50$ ,  $L = 10$  and  $a = 1$ . We can see that eigenvalues are ill conditioned, excepted for the eigenvalues with small modulus. This can explain the convergence problem when  $N$  is increased. In comparison with the rotated harmonic oscillator (see Figure 8) we can see that the condition numbers of the eigenvalues are much greater for the operator (5.28) than for the rotated harmonic oscillator (5.13). A small perturbation on the grid points induces large perturbations on the eigenvalue computations. However the eigenvalues are independent of  $x$ . So, in order to decrease this dependence of the eigenvalues in function of a perturbation on the points of the mesh grid, we have considered several grids for the finite difference discretization, with a shift on the mesh points, but with the same step  $\Delta x$  for the mesh grid :  $y_j = x_j + \varepsilon$ . Then we compute an average on the eigenvalues obtained with these staggered grids. The results obtained are presented on Figure 16, which corresponds to  $a = 1$ ,  $N = 1000$  and  $L = 10$ . The number of staggered grids retained is 11. We can see that spurious eigenvalues have disappeared. The computed eigenvalues after averaging are now essentially contained in the area  $\{\lambda \in \mathbb{C}, |\arg(\lambda)| \geq \frac{\pi}{3}\}$  in agreement with theoretical results (see Section 3). We can note on Figure 16 that on the imaginary axis we have

limited the imaginary part of  $\lambda_N$  to  $|\lambda_{N,i}| \leq \frac{N}{2L} = 50$ . Indeed, as it has been said previously,  $\lambda_{N,i}$  is function of the wavenumber and the highest wavenumber we can take into account on the grids is  $\frac{N}{2L}$ .

For the use of staggered meshes to avoid spectral pollution, we may mention the following reference [17].

Now we consider the pseudospectra (5.26) since it is known that the numerical computation of the pseudospectra is more stable than for the spectra (see Section 4). For the computation of the pseudospectra, we have retained complex values  $z$  in (5.26) lying on the meshgrid in the part of the complex plane corresponding to  $[0, 100] \times [0, 100]$ . The step retained is  $dx = dy = 1$  in the real and imaginary directions. On Figure 17 we can see the computation for the matrix  $\mathcal{A}_{a,N} - z\mathbb{I}_N$  with  $\mathcal{A}_{a,N}$  corresponding to the matrix (5.38), for  $N = 1000$ ,  $L = 10$  and  $a = 1$ . We can note that, in agreement with the theoretical results (see Section 3), the two sectors  $\{\lambda \in \mathbb{C}, |\arg(\lambda)| \geq \frac{\pi}{3}\}$  of the spectrum of the continuous operator (5.28) are essentially contained in the area of the pseudospectra corresponding to the smallest values of the parameter  $\varepsilon$ , *i.e.* in the area where the distance of  $z$  to the eigenvalues of the matrix (5.38) is the smallest.

The pseudospectra computation is very expensive. So we use parallel computation in order to accelerate the computation. The numerical solution is done thanks to the linear algebra library LAPack which contains specialized algorithms for singular values problems, especially the one called ZGESVD for complex matrices in double precision. As the matrix (5.38) is quite huge, and computing time a bit long, a parallelization by MPI (Message Passing Interface) is implemented with the client/server model. One process (the server) distributes values of the complex parameter  $z$  (see (5.26)) to the other processes (the clients) which sample the domain. The server renews their data as the work progresses. Each client builds the matrix to be study and sends to the server, at the end of the computation, the smallest value. This system has the advantage of being dynamically balanced. As there is no communication (in MPI sense) between the clients, the efficiency of the parallelization is complete. As an example, the simulation corresponding to the parameters  $N = 5000$ ,  $L = 1000$ ,  $a = 1$  and to an area of the complex plane  $[0, 150] \times [0, 150]$  with a mesh step  $dx = 1$  and  $dy = 1$  in the real and imaginary directions has needed 40 cores (Intel Xeon E5-2670 at 2.5GHz) during quite 40 days.

Now, as for the rotated harmonic oscillator, we consider here the computation of the pseudospectra based on Definition 4.5 (see (4.12)) instead of Definition 4.2 as previously. So we look for  $z \in \mathbb{C}$  such that :

$$\|A_{a,N}^{-1}(z)\| = s_{\min}^{-1}(A_{a,N}(z)) \geq \varepsilon^{-1} \exp(\delta|z|^\mu) \quad (5.40)$$

where  $A_{a,N}(z)$  is the matrix obtained with the finite difference discretization of the operator  $L_a(z)$  (see (5.28));  $\varepsilon$ ,  $\delta$  and  $\mu$  are real parameters. The majoration in (5.40) depends on  $|z|$ , in opposition with (5.26), *i.e.* the constraint appearing in (5.40) is stronger when  $|z|$  is increased. As before we have retained  $N = 1000$ ,  $L = 10$ ,  $a = 1$  and complex values  $z$  lying on the meshgrid in the area of the complex plane corresponding to  $[0, 100] \times [0, 100]$ . The step retained is  $dx = 1$  and  $dy = 1$  in the real and imaginary directions. In order to look for the influence of the parameters  $\delta$  and  $\mu$  on the pseudospectra (5.40), we have presented on Figure 18 the pseudospectra computed with different values of the parameters  $\delta$  and  $\mu$ . We can see that when the parameter  $\mu$  is increased, eigenvalues with large modulus are eliminated in the pseudospectra computed with (5.40). Moreover, the CPU time required to compute pseudospectra with Definition 4.5 (see (5.40)) is much lower than if we use Definition 4.2 (see (5.26)). Indeed, the matrix  $A_{a,N}(z)$  is of order  $N + 1$  instead of  $2N + 2$  for the matrix  $\mathcal{A}_{a,N}$ .

### 5.2.3 Eigenvalue computations with Legendre spectral Galerkin method (bounded domain)

In order to obtain a higher accurate numerical scheme in bounded domain, we propose a spectral numerical scheme using Legendre Galerkin basis.

We consider the problem (5.36). This problem is reformulated as an eigenvalue problem (5.37). But instead of using a finite difference scheme to obtain an approximation  $u_N$ ,  $v_N$  of  $u$  and  $v = \lambda u$ , we use a spectral method with Legendre Galerkin basis  $\Phi_l$ . Such basis is obtained as a linear combination of Legendre polynomials :

$$\Phi_l(x) = c_l(L_l(x) - L_{l+2}(x))$$

with  $L_l$  the Legendre polynomial of degree  $l$  and  $c_l = \frac{1}{\sqrt{4l+6}}$  (see [16]). Such a basis verify homogeneous Dirichlet boundary conditions  $\Phi_l(\pm 1) = 0$ . In particular, with the scalar product in  $L_2(\Omega)$  we have :

$$(\Phi_k, \Phi_j) = \begin{cases} c_k c_j \left( \frac{2}{2j+1} + \frac{2}{2j+5} \right) , & k = j \\ -c_k c_j \frac{2}{2k+1} , & k = j + 2 \\ 0 , & \text{otherwise} \end{cases} \quad (5.41)$$

and

$$(\Phi'_k, \Phi'_j) = \begin{cases} 1 , & k = j \\ 0 , & k \neq j \end{cases} \quad (5.42)$$

Moreover, we need the expressions of  $x^2\Phi_l$  and  $x^4\Phi_l$  as linear combination of the Legendre polynomials. We have :

$$x^2 L_l(x) = \frac{1}{2l+1} \left( \frac{l+1}{2l+3} ((l+2)L_{l+2}(x) + (l+1)L_l(x)) + \frac{l}{2l-1} (lL_l(x) + (l-1)L_{l-2}(x)) \right) \quad (5.43)$$

and

$$x^4 L_l(x) = \alpha_l L_{l-4}(x) + \beta_l L_{l-2}(x) + \gamma_l L_l(x) + \delta_l L_{l+2}(x) + \eta_l L_{l+4}(x) \quad (5.44)$$

with

$$\begin{aligned} \alpha_l &= \frac{1}{2l+1} \left( \frac{l(l-1)(l-2)(l-3)}{(2l-1)(2l-3)(2l-5)} \right) \\ \beta_l &= \frac{1}{2l+1} \left( \left( \frac{(l+1)^2}{(2l+3)(2l+1)} + \frac{l^2}{(2l-1)(2l+1)} \right) \left( \frac{l(l-1)}{2l-1} \right) + \frac{l(l-1)^3}{(2l-1)^2(2l-3)} + \frac{l(l-1)(l-2)^2}{(2l-1)(2l-3)(2l-5)} \right) \\ \gamma_l &= \frac{1}{2l+1} \left( \left( \frac{(l+1)^2(l+2)^2}{(2l+3)^2(2l+5)} + \left( \frac{(l+1)^2}{(2l+1)(2l+3)} + \frac{l^2}{(2l-1)(2l+1)} \right) * \left( \frac{(l+1)^2}{(2l+3)} + \frac{l^2}{(2l-1)} \right) + \frac{l^2(l-1)^2}{(2l-1)^2(2l-3)} \right) \right) \\ \delta_l &= \frac{1}{2l+1} \left( \left( \frac{(l+1)^2}{(2l+3)(2l+1)} + \frac{l^2}{(2l-1)(2l+1)} \right) \left( \frac{(l+1)(l+2)}{2l+3} \right) + \frac{(l+1)(l+2)^3}{(2l+3)^2(2l+5)} + \frac{(l+1)(l+2)(l+3)^2}{(2l+3)(2l+5)(2l+7)} \right) \\ \eta_l &= \frac{1}{2l+1} \left( \frac{(l+1)(l+2)(l+3)(l+4)}{(2l+3)(2l+5)(2l+7)} \right) \end{aligned}$$

In order to adapt the previous basis  $\Phi_l$  to the Dirichlet boundary conditions  $\Phi_l(\pm L) = 0$ , we multiply the previous polynomials by a scale factor. As for the Hermite spectral method (see Section 5.2.1), we use a method of weighted residuals (MWR, see for example, [11], [4]) and relations (5.41), (5.42), (5.43), (5.44) to obtain the following generalized eigenvalue problem :

$$\mathcal{A}_{a,N} \begin{pmatrix} U_N \\ V_N \end{pmatrix} = \lambda_N \mathcal{B}_N \begin{pmatrix} U_N \\ V_N \end{pmatrix} \quad (5.45)$$

where  $U_N$  and  $V_N$  are the vectors containing respectively the coefficients  $\tilde{u}_l$  and  $\tilde{v}_l$ ,  $l = 0, \dots, N$ , of  $u_N = \sum_{l=0}^N \tilde{u}_l \Phi_l$  and  $v_N = \sum_{l=0}^N \tilde{v}_l \Phi_l$ .  $\mathcal{A}_{a,N}$  is the square matrix of order  $(2N + 2)$  :

$$\mathcal{A}_{a,N} = \begin{pmatrix} 0 & \mathbb{I}_N \\ -L'_{0_N} & -L'_{1_{a,N}} \end{pmatrix}$$

and  $\mathcal{B}_N$  is the square matrix of order  $(2N + 2)$  :

$$\mathcal{B}_N = \begin{pmatrix} B_{0_N} & 0 \\ 0 & B_{0_N} \end{pmatrix}$$

Here  $L'_{0_N} u_N = (L_0 u_N, \Phi_{l'})$  and  $L'_{1_{a,N}} v_N = (L_{1_a} v_N, \Phi_{l'})$ ,  $l' = 0, \dots, N$ , with  $L_0 u_N = -\frac{d^2 u_N}{dx^2} + x^4 u_N$  and  $L_{1_a} u_N = -2ax^2 u_N$ . As for  $B_{0_N} u_N = (u_N, \Phi_{l'})$ .

$L'_{0_N}$  is a symmetric matrix with seven diagonal and  $L'_{1_{a,N}}$  is a pentadiagonal symmetric matrix. As for  $B_{0_N} = (\Phi_l, \Phi_{l'})$  for  $l$  and  $l' = 0, \dots, N$  (see (5.41)).

To obtain the eigenvalues of the generalized eigenvalue problem (5.45) we use the function DGGEV of the LAPack library.

On Figure 19 we present the solutions  $\lambda_N$  of (5.45), computed with  $N = 50$ ,  $L = 10$  and  $a = 1$ . Comparison with the spectral Hermite method (Figure 12) and the finite difference method (Figure 14) is done. We can see that the numerical results are quite similar.

### 5.3 Another discretized nonlinear eigenvalue problem

In this section we consider the following operator :

$$\mathcal{L}u(x) = -\frac{d^2 u}{dx^2}(x) + (x^k - \lambda)^2 u(x) \quad (5.46)$$

For  $k = 2$  we retrieve the operator (1.4) studied in the previous section.

We discretize the problem  $\mathcal{L}u = 0$  using some techniques similar to finite difference methods, with a spatial step equal to one. For simplicity reasons we need to add either periodic boundary conditions or homogeneous boundary conditions. Also we replace  $\Delta u(n)$  by  $\delta\delta^*$  where:

$$\begin{aligned} \delta u(n) &= u(n+1) - u(n), \quad n \in \mathbb{N} \\ \delta^* u(n) &= u(n) - u(n-1), \quad n \in \mathbb{N} \end{aligned}$$

i.e.

$$(\delta\delta^*)u(n) = u(n-1) - 2u(n) + u(n+1)$$

So we have :

$$\mathcal{L}u(n) = -(\delta\delta^*)u(n) + (n^k - \lambda)^2 u(n), \quad n \in \mathbb{N} \quad (5.47)$$

#### 5.3.1 Finite difference method with periodic boundary conditions

In this section we are interested to study the problem (5.47) with periodic boundary conditions. So for some  $N \in \mathbb{N}$ , we study the following problem :

$$\begin{aligned} -(\delta\delta^*)u(n) + (n^k - \lambda)^2 u(n) &= 0, \quad n = 1, \dots, N \\ u(j) &= u(j+N), \quad j = 0, 1 \end{aligned}$$

For  $n = 1, \dots, N$  we have :

$$\begin{aligned}
n=1 & : & -u(0) + 2u(1) - u(2) + 1^{2k}u(1) - 2\lambda(1)^k u(1) + \lambda^2 u(1) & = 0 \\
n=2 & : & -u(1) + 2u(2) - u(3) + 2^{2k}u(2) - 2\lambda(2)^k u(2) + \lambda^2 u(2) & = 0 \\
n=j & : & -u(j-1) + 2u(j) - u(j+1) + j^{2k}u(j) - 2\lambda(j)^k u(j) + \lambda^2 u(j) & = 0 \\
n=N-1 & : & -u(N-2) + 2u(N-1) - u(N) + (N-1)^{2k}u(N-1) & \\
& & -2\lambda(N-1)^k u(N-1) + \lambda^2 u(N-1) & = 0 \\
n=N & : & -u(N-1) + 2u(N) - u(N+1) + (N)^{2k}u(N) - 2\lambda(N)^k u(N) + \lambda^2 u(N) & = 0
\end{aligned}$$

Using the periodic conditions  $u(0) = u(N)$  and  $u(N+1) = u(1)$ , we obtain the system :

$$\begin{aligned}
n=1 & : & -u(N) + 2u(1) - u(2) + 1^{2k}u(1) - 2\lambda(1)^k u(1) + \lambda^2 u(1) & = 0 \\
n=2 & : & -u(1) + 2u(2) - u(3) + 2^{2k}u(2) - 2\lambda(2)^k u(2) + \lambda^2 u(2) & = 0 \\
n=j & : & -u(j-1) + 2u(j) - u(j+1) + j^{2k}u(j) - 2\lambda(j)^k u(j) + \lambda^2 u(j) & = 0 \\
n=N-1 & : & -u(N-2) + 2u(N-1) - u(N) + (N-1)^{2k}u(N-1) & \\
& & -2\lambda(N-1)^k u(N-1) + \lambda^2 u(N-1) & = 0 \\
n=N & : & -u(N-1) + 2u(N) - u(1) + (N)^{2k}u(N) - 2\lambda(N)^k u(N) + \lambda^2 u(N) & = 0
\end{aligned}$$

This gives the following system :

$$A_0 + \lambda A_1 + \lambda^2 I = 0$$

where  $I$  is the  $N \times N$  identity matrix and  $A_1, A_0$  are given as follows :

$$A_1 = -2 \begin{pmatrix} 1 & 0 & \dots & & \dots & 0 \\ 0 & 2^k & 0 & \dots & \dots & 0 \\ \vdots & & \vdots & & \vdots & \vdots \\ 0 & \dots & & \dots & 0 & (N-1)^k & 0 \\ 0 & \dots & & \dots & \dots & 0 & N^k \end{pmatrix} \quad (5.48)$$

$$A_0 = A_{0,d} + A_{0,+1} + A_{0,-1} \quad (5.49)$$

with

$$A_{0,d} = \begin{pmatrix} 2+1 & 0 & 0 & \dots & & \dots & 0 & 0 \\ 0 & 2+2^{2k} & 0 & 0 & \dots & & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots & \vdots \\ 0 & \dots & \dots & 0 & 0 & 2+j^{2k} & 0 & 0 & \dots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots & \vdots \\ 0 & \dots & & \dots & 0 & 0 & 2+(N-1)^{2k} & 0 \\ 0 & 0 & \dots & & \dots & \dots & 0 & 0 & 2+N^{2k} \end{pmatrix}$$

$$A_{0,+1} = \begin{pmatrix} 0 & -1 & \dots & & \dots & -1 \\ 0 & 0 & -1 & \dots & \dots & 0 \\ \vdots & & \vdots & & \vdots & \vdots \\ 0 & \dots & & \dots & 0 & 0 & -1 \\ 0 & \dots & & \dots & 0 & 0 \end{pmatrix}, \quad A_{0,-1} = \begin{pmatrix} 0 & 0 & \dots & & \dots & 0 \\ -1 & 0 & 0 & \dots & \dots & 0 \\ 0 & -1 & 0 & \dots & \dots & 0 \\ \vdots & & \vdots & & \vdots & \vdots \\ 0 & \dots & & \dots & 0 & 0 & 0 \\ -1 & \dots & & \dots & -1 & 0 \end{pmatrix}$$

We start computing the eigenvalues for different values of  $N$  and for the operator  $\mathcal{L}$ . Then, we compute the eigenvalues for some perturbations of the operator  $\mathcal{L}$ , i.e. we study the discrete operator :

$$\mathcal{L}_c u(n) = A_0 u(n) + c\lambda A_1 u(n) + \lambda^2 I u(n), \quad n = 1, \dots, N$$

for  $0 \leq c \leq 1$  with the same previous periodic boundary conditions. For this we consider the linearization system problem in place of the non-linear problem, so we study the spectrum of the linear system  $\mathcal{A}_c U = \lambda U$  with :

$$\mathcal{A}_c = \begin{pmatrix} 0 & I \\ -A_0 & -cA_1 \end{pmatrix}, \quad 0 \leq c \leq 1$$

where  $U = (u_1, u_2, \dots, u_{N-1}, u_N, v_1, v_2, \dots, v_{N-1}, v_N)^t$ , with  $v_i = \lambda u_i$ ,  $i = 1, \dots, N$ .  $A_0$  and  $A_1$  are given in (5.49) and (5.48) respectively. For the computation of the eigenvalues, we use Matlab (or Scilab).

The results obtained for  $N = 100$ ,  $k = 2$  and  $c = 1$  are presented on Figure 20. The associated domain is  $[0, N]$ . This figure represents a zoom for the case  $c = 1$ . We note that the imaginary part of the eigenvalues  $\lambda_i$  lies between 1.38 and 1.42 in the positive part and between  $-1.42$  and  $-1.38$  in the negative part. Starting from a real part  $\lambda_r = 576$  all the eigenvalues are aligned on a straight parallel to the  $x$ -axis with  $\lambda_i = 1.4141$  and  $\lambda_i = -1.4141$ . The results obtained for  $N = 1000$ ,  $k = 2$  and  $c = 1$  are similar.

On Figure 21 we present the numerical results obtained for  $N = 1000$ ,  $k = 4$  and  $0 \leq c \leq 1$ . For the case  $c = 0$  we have pure imaginary eigenvalues (since in this case we have just a selfadjoint matrix). The positions of eigenvalues for the cases  $c = 0.2, 0.4$  confirm the theoretical results. For the cases  $c = 0.6, 0.8, 1$ , eigenvalues are localized in a sector delimited by an angle with the  $x$ -axis smaller than  $2\pi/6$ . This is not coherent with the theoretical results.

### 5.3.2 Finite difference method with homogeneous boundary conditions

In the following we consider the problem (5.47) with homogeneous boundary conditions. So we study the following problem :

$$\begin{aligned} -(\delta\delta^*)u(n) + (n^k - \lambda)^2 u(n) &= 0, \quad n = 1, \dots, N \\ u(0) = u(N+1) &= 0 \end{aligned} \quad (5.50)$$

So we obtain the following system :

$$A_0 + \lambda A_1 + \lambda^2 I = 0$$

where  $I$  is the  $N \times N$  identity matrix and  $A_1, A_0$  are given as follows :

$$A_1 = -2 \begin{pmatrix} 1 & 0 & \dots & & \dots & 0 \\ 0 & 2^k & 0 & \dots & \dots & 0 \\ \vdots & & \vdots & & \vdots & \vdots \\ 0 & \dots & & \dots & 0 & (N-1)^k & 0 \\ 0 & \dots & & \dots & \dots & 0 & N^k \end{pmatrix} \quad (5.51)$$

$$A_0 = A_{0,d} + A_{0,+1} + A_{0,-1} \quad (5.52)$$

where

$$A_{0,d} = \begin{pmatrix} 2+1 & 0 & 0 & \dots & & \dots & 0 & 0 \\ 0 & 2+2^{2k} & 0 & 0 & \dots & & \dots & 0 \\ & & \vdots & & & & & \vdots \\ 0 & \dots & \dots & 0 & 0 & 2+j^{2k} & 0 & 0 & \dots & 0 \\ \vdots & & \vdots & & & \vdots & & & & \vdots \\ 0 & \dots & & \dots & \dots & 0 & 0 & 2+(N-1)^{2k} & 0 \\ 0 & 0 & \dots & & \dots & \dots & 0 & 0 & 2+N^{2k} \end{pmatrix}$$

$$A_{0,+1} = \begin{pmatrix} 0 & -1 & \cdots & & \cdots & 0 \\ 0 & 0 & -1 & \cdots & & 0 \\ \vdots & & \vdots & & \vdots & \vdots \\ 0 & \cdots & & \cdots & 0 & 0 & -1 \\ 0 & \cdots & & & \cdots & 0 & 0 \end{pmatrix}, \quad A_{0,-1} = \begin{pmatrix} 0 & 0 & \cdots & & \cdots & 0 \\ -1 & 0 & 0 & \cdots & & 0 \\ 0 & -1 & 0 & \cdots & & 0 \\ \vdots & & \vdots & & \vdots & \vdots \\ 0 & \cdots & & \cdots & 0 & 0 & 0 \\ 0 & \cdots & & & \cdots & -1 & 0 \end{pmatrix}$$

We start by computing the eigenvalues for different values of  $N$  and for the operator  $\mathcal{L}$ . Then we compute the eigenvalues for some perturbations of the operator  $\mathcal{L}$ , i.e. we consider the discrete operator :

$$\mathcal{L}_c u(n) = A_0 u(n) + c\lambda A_1 u(n) + \lambda^2 I u(n), \quad n = 1, \dots, N$$

with  $0 \leq c \leq 1$  and the same previous homogeneous boundary conditions. We do this considering the linearization system problem in place of the non-linear problem. So we study the spectrum of the linear system  $\mathcal{A}_c U = \lambda U$  with :

$$\mathcal{A}_c = \begin{pmatrix} 0 & I \\ -A_0 & -cA_1 \end{pmatrix}, \quad 0 \leq c \leq 1$$

where  $U = (u_1, u_2, \dots, u_{N-1}, u_N, v_1, v_2, \dots, v_{N-1}, v_N)^t$ , with  $v_i = \lambda u_i$ ,  $i = 1, \dots, N$ .  $A_0$  and  $A_1$  are given in (5.52) and (5.51) respectively. We compute the eigenvalues using Matlab.

For the numerical simulations we have considered a domain  $[-L, +L]$  and a spatial step  $\Delta x = \frac{2L}{N}$ . For the case  $k = 4$ , the results obtained for  $L = 10$ ,  $N = 2000$  (resp.  $L = 20$ ,  $N = 10000$ ) and  $c = 1$  are presented on Figures 22 and 23 respectively. For the case  $k = 6$ , the numerical results obtained for the example (5.50) with  $N = 10000$ ,  $c = 1$  and  $L = 20$  (resp.  $L = 10$ ) are presented on Figure 24 and 25 respectively.

**Remark 5.2** *We can note that when the parameter  $k$  is increased, the numerical results obtained are in better agreement with the theoretical results given in Section 3, i.e the eigenvalues of the continuous operator (5.46) are included in the two sectors  $\{\lambda \in \mathbb{C}, |\arg(\lambda)| \geq \frac{k\pi}{2(k+1)}\}$ . This can be explained by the fact that the eigenvalues are better conditioned when  $k$  is increased.*

## 6 Conclusions and open problems

In this work we have presented a review of some theoretical results obtained for quadratic family of operators :

$$L(\lambda) = L_0 + \lambda L_1 + \lambda^2$$

where  $L_0$  and  $L_1$  are operators in an Hilbert space.

Then we have presented numerical methods to compute the spectrum of such operators. We reduce it to a non self-adjoint linear eigenvalue problem. The numerical methods proposed are spectral methods and finite difference methods, for bounded and unbounded domains. For bounded domain we consider homogeneous Dirichlet boundary conditions and periodic boundary conditions. Comparison with the results obtained in unbounded and bounded domains are done. They are based on the size of the containment domain, deduces from the zeroes of the Hermite functions.

The numerical results obtained are presented. In particular the numerical instabilities are highlighted. Comparisons of the numerical results obtained, with the theoretical results presented in the first part of this work, are done. These comparisons show the difficulties for the numerical computation of such problem. Elimination of the spectral pollution, using staggered grids, and the computation of pseudospectra allow to obtain numerical results in agreement with theoretical

results.

A future step in this work is the extension to the two dimensional case. This work is in progress and will be presented elsewhere.

### Acknowledgments

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## Appendix A Hermite spectral method

### A.1 The 1-D case

The basis  $\{\varphi_k\}_{k \in \mathbb{N}}$  of Hermite functions is obtained as an orthonormal basis of  $L^2(\mathbb{R})$  of the eigenfunctions of the harmonic oscillator :

$$H_{osc} = -\frac{d^2}{dx^2} + x^2$$

We recall briefly its construction (see the basic books of quantum mechanics).

Define the creation operator  $a^*$  and the annihilation operator  $a$

$$a^* = x - \frac{d}{dx}, \quad a = x + \frac{d}{dx}$$

We satisfy

$$[a, a^*] = 2\mathbb{I}, \quad H_{osc} = a^*a + \mathbb{I} = \frac{1}{2}(aa^* + a^*a)$$

where  $[a, a^*] = aa^* - a^*a$ .

Starting by the normalized Gaussian :

$$\varphi_0(x) = \pi^{-1/4} e^{-x^2/2}$$

verified  $a\varphi_0 = 0$  and then  $H_{osc}\varphi_0 = \varphi_0$  one define by induction for integer  $k$  the sequence  $\{\varphi_k\}_{k \in \mathbb{N}}$ :

$$\varphi_{k+1} = (2(k+1))^{-1/2} a^* \varphi_k$$

$$\varphi_k = 2^{-k/2} (k!)^{-1/2} (a^*)^k \varphi_0$$

We verify the following relation by using an algebraic calculation

$$a\varphi_{k+1} = (2k+1)^{1/2} \varphi_k \tag{A.53}$$

$$a^* \varphi_k = (2k+1)^{1/2} \varphi_{k+1} \tag{A.54}$$

$$H_{osc} \varphi_k = (2k+1) \varphi_k \tag{A.55}$$

$$\langle \varphi_k, \varphi_\ell \rangle = \delta_{k,\ell} \tag{A.56}$$

where  $\langle \cdot, \cdot \rangle$  denoted the scalar product in the (complex) Hilbert space  $L^2(\mathbb{R})$ .

We then show that  $\{\varphi_k\}_{k \in \mathbb{N}}$  is a Hilbertian basis of  $L^2(\mathbb{R})$ .

To do the projection of the differential operators in this basis we need to calculate the multiplication by  $x$  and the derivation  $\frac{d}{dx}$  of  $\varphi_k$ .

We use the relations  $x = \frac{a+a^*}{2}$  and  $\frac{d}{dx} = \frac{a-a^*}{2}$ . By the relations (A.53) we obtain :

$$\begin{aligned}
x\varphi_k &= 2^{-1/2}\sqrt{k}\varphi_{k-1} + \sqrt{k+1}\varphi_{k+1} \\
\frac{d}{dx}\varphi_k &= 2^{-1/2}\sqrt{k}\varphi_{k-1} - \sqrt{k+1}\varphi_{k+1} \\
x^2\varphi_k &= \frac{1}{2}\left(\sqrt{k(k-1)}\varphi_{k-2} + (2k+1)\varphi_k + \sqrt{(k+1)(k+2)}\varphi_{k+2}\right) \\
x^4\varphi_k &= \frac{1}{4}\left(\sqrt{k(k-1)(k-2)(k-3)}\varphi_{k-4} + (4k-2)\sqrt{k(k-1)}\varphi_{k-2} \right. \\
&\quad \left. + (6k^2 + 2k + 3)\varphi_k + (4k+6)\sqrt{(k+1)(k+2)}\varphi_{k+2} \right. \\
&\quad \left. + \sqrt{(k+1)(k+2)(k+3)(k+4)}\varphi_{k+4}\right) \\
\frac{d^2}{dx^2}\varphi_k &= \frac{1}{2}\left(\sqrt{k(k-1)}\varphi_{k-2} - (2k+1)\varphi_k + \sqrt{(k+1)(k+2)}\varphi_{k+2}\right)
\end{aligned} \tag{A.57}$$

We have used the following convention : when any integer become  $< 0$  we replace it by 0.

### Estimation of error

The suitable spaces are Sobolev spaces with weight are naturally associated to the harmonic oscillator  $H_{osc}$  because the usual spaces of Sobolev are associated with the Laplacian. For each integer  $m \geq 0$  we define the space  $\mathcal{B}_m$  of function  $u \in L^2(\mathbb{R})$  such that for any pair of integers  $k, l$  such that  $k + l \leq m$  we have  $x^k \frac{d^l}{dx^l} u \in L^2(\mathbb{R})$ .

$\mathcal{B}_m$  is a Hilbert space with the scalar product

$$\langle u, v \rangle_m = \sum_{k+l \leq m} \int_{\mathbb{R}} \left( \overline{x^k \frac{d^l}{dx^l} u} \right) \left( x^k \frac{d^l}{dx^l} v \right) dx$$

$\mathcal{B}_m$  is equal to the domain of  $H_{osc}^{m/2}$  and the scalar product is equivalent to

$$\langle u, v \rangle_m^* = \langle H_{osc}^{m/2} u, H_{osc}^{m/2} v \rangle = \langle H_{osc}^m u, v \rangle$$

We deduce a characterization of  $\mathcal{B}_m$  with the Hermite coefficient of  $u$ ,  $\alpha_k(u) := \langle \varphi_k, u \rangle$ .

**Proposition A.1**  $u \in \mathcal{B}_m$  if and only if  $\sum_{k \in \mathbb{N}} (2k+1)^m |\alpha_k|^2 < +\infty$ .

In addition, the scalar product is expressed as the following :

$$\langle u, v \rangle_m^* = \sum_{k \in \mathbb{N}} (2k+1)^m \overline{\alpha_k(u)} \alpha_k(v)$$

The proposition can be summarized by saying that  $\mathcal{B}_m$  is identical to the domain of the operator  $H_{osc}^{m/2}$ . By complex interpolation we deduce the intermediate spaces  $\mathcal{B}_s$  for all  $s$  positive reals hence by the duality for  $s$  negative reals. The arguments are identical to the case of usual Sobolev spaces. For  $s < 0$  the  $\mathcal{B}_s$  are the spaces of temperate distribution.

Then we set  $u_N = \sum_{0 \leq k \leq N} \alpha_k(u) \varphi_k$ , let  $u_N = \Pi_N u$ ,  $\Pi_N$  be the projections on the vector space  $V_N$  generated by  $\{\varphi_0, \varphi_1, \dots, \varphi_N\}$ . So we clearly have :

$$\|u - u_N\|^2 = \sum_{k > N} |\alpha_k|^2 \leq \frac{1}{(2N+1)^m} \sum_{k \in \mathbb{N}} (2k+1)^m |\alpha_k|^2$$

Hence if  $u \in \mathcal{B}_m$  we have

$$\|u - u_N\|^2 \leq (2N+1)^{-m} \|u\|_m^{*,2} \tag{A.58}$$

More generally we can estimate the error in the spaces  $\mathcal{B}_s$

$$\|u - u_N\|_s^{*,2} \leq (2N + 1)^{s-m} \|u\|_m^{*,2} \quad (\text{A.59})$$

It may be useful to have such Sobolev inequalities explaining the regularity and decay at infinity of  $u \in \mathcal{B}_s$  as soon as  $s$  is large enough. We do not search to obtain an optimal estimation.

**Proposition A.2** *Let  $m \in \mathbb{N}$ . There exists constants  $C_m > 0$ ,  $C_{s,m}$  ( $m < 2s - 2$ ) such that*

$$|x^\ell \frac{d^k}{dx^k} \varphi_j(x)| \leq C_m (2j + 1)^{(m+1)/2}, \quad \forall x \in \mathbb{R}, \quad k + \ell \leq m \quad (\text{A.60})$$

$$|x^\ell \frac{d^k}{dx^k} u(x)| \leq C_{s,m} \|u\|_s, \quad \forall x \in \mathbb{R}, \quad k + \ell \leq m, u \in \mathcal{S}(\mathbb{R}) \quad (\text{A.61})$$

*In particular if  $m$  is known and if  $s > m + 2$  then all  $u$  in  $\mathcal{B}_s$  are of class  $C^m$  on  $\mathbb{R}$  and verify the inequality (A.61).*

*Proof.* It is sufficient to consider the case  $k = 0$ .

For (A.60) starting from the usual Sobolev inequality (in one dimension the critical index  $1/2$ ).

Then

$$|x^m \varphi_j(x)| \leq C \|x^\ell \varphi_j\|_{H^1} \leq C \|\varphi_j\|_{m+1}$$

Since  $\|\varphi_j\|_m$  is of order  $(2j + 1)^{m/2}$ , hence (A.60).

For (A.61) by expanding  $u$  on the basis and by applying the Cauchy-Schwarz inequality

$$|x^m u(x)| \leq \left( \sum_j |\alpha_j|^2 (2j + 1)^s \right)^{1/2} \left( \sum_j (2j + 1)^{-s} |x^m \varphi_j(x)|^2 \right)^{1/2}$$

then one use (A.60) by choosing  $s > m + 2$

$$|x^m u(x)| \leq C_{s,m} \|u\|_s$$

The last assertion follows from the density of  $\mathcal{S}(\mathbb{R})$  in  $\mathcal{B}_s$  for all  $s \in \mathbb{R}$ .

The definition of derivatives does not cause a problem.

Thus we see that the functions  $u \in \mathcal{B}_m$  are both regular and decreasing to 0 at the infinity more rapidly when  $m$  is big (positive). □

## A.2 The multidimensional case

The results are similar up to complication of notations.

Let  $d \geq 2$ , we denote  $x = (x_1, x_2, \dots, x_d) \in \mathbb{R}^d$ ,  $k = (k_1, k_2, \dots, k_d) \in \mathbb{N}^d$  and

$$\varphi_k(x) = \varphi_{k_1}(x_1) \varphi_{k_2}(x_2) \cdots \varphi_{k_d}(x_d)$$

Then  $\{\varphi_k\}_{k \in \mathbb{N}^d}$  is an orthonormal basis of the Hilbert space  $L^2(\mathbb{R}^d)$ .

Then we have  $d$  annihilation operators  $a = (a_1, a_2, \dots, a_d)$  and  $d$  creation operators  $a^* = (a_1^*, a_2^*, \dots, a_d^*)$  with

$$a_k^* = x_k - \frac{\partial}{\partial x_k}, \quad a_k = x_k + \frac{\partial}{\partial x_k}$$

To define the spaces  $\mathcal{B}_m$  one replace  $k, \ell$  by multi-indices. The harmonic oscillator can be written as

$$H_{osc} = -\Delta + |x|^2 = a^* \cdot a + d = \frac{1}{2}(a^* \cdot a + a \cdot a^*)$$

where  $a^* \cdot a = \sum_{1 \leq k \leq d} a_k^* a_k$  and  $|x|^2 = x_1^2 + \dots + x_d^2$ .

Then we have

$$H_{osc} \varphi_k = 2(k_1 + \dots + k_d) + 1, \quad k = (k_1, \dots, k_d)$$

The space  $V_N$  is generated by  $\{\varphi_k, k_1 + \dots + k_d \leq N\}$ . We denote for all multiindex  $k$ ,  $|k| = k_1 + \dots + k_d$ .

The Hermite coefficients  $\alpha_k(u)$  are indexed on  $\mathbb{N}^d$ . The estimation of error is then formally unchanged.

Sobolev inequalities with weight depend naturally on the dimension  $d$ . For all  $m, s$  such that  $s > 1/2 + m + d$  there exists  $C_{s,m} > 0$  such that

$$|x^j u(x)| \leq C_{s,m} \|u\|_s$$

For  $|j| \leq m$  and  $u \in \mathcal{B}_s$ . Here  $x^j = x_1^{j_1} \dots x_d^{j_d}$  when  $j = (j_1, \dots, j_d)$ .

As for the case  $d = 1$  we have a similar inequality for the partial derivatives.

## Appendix B Figures

In this section we give the figures referenced in this article.

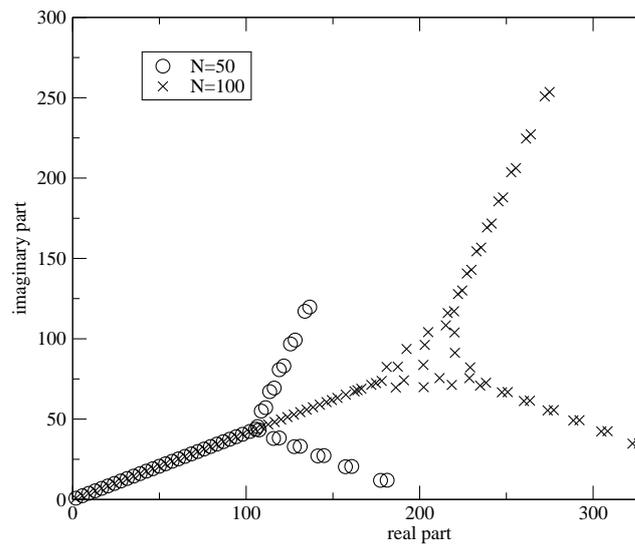


Figure 1: Spectrum of the matrix  $\mathcal{A}_N$  associated with the eigenvalue problem (5.16) (Hermite spectral method) for  $N = 50$  and  $N = 100$ ,  $c = \exp(i\alpha)$  with  $\alpha = \pi/4$ .

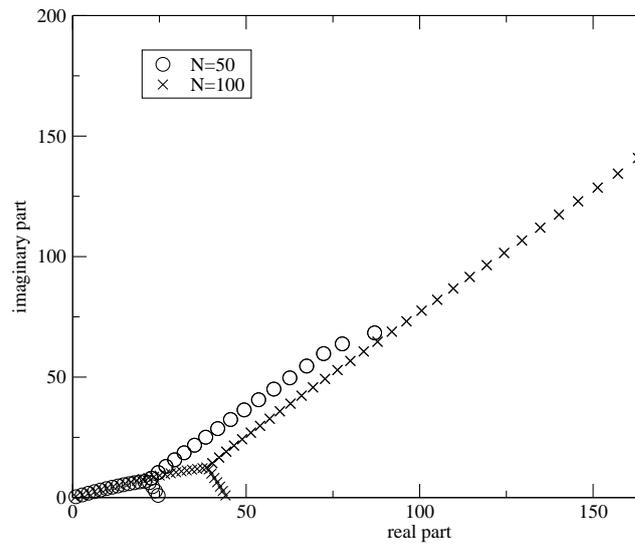


Figure 2: Spectrum of the matrix  $\mathcal{A}_N$  of the eigenvalue problem (5.20) (finite difference scheme) obtained for  $N = 50$  ( $L = 10$ ),  $N = 100$  ( $L = 15$ ) and  $c = \exp(i\alpha)$  with  $\alpha = \pi/4$ .

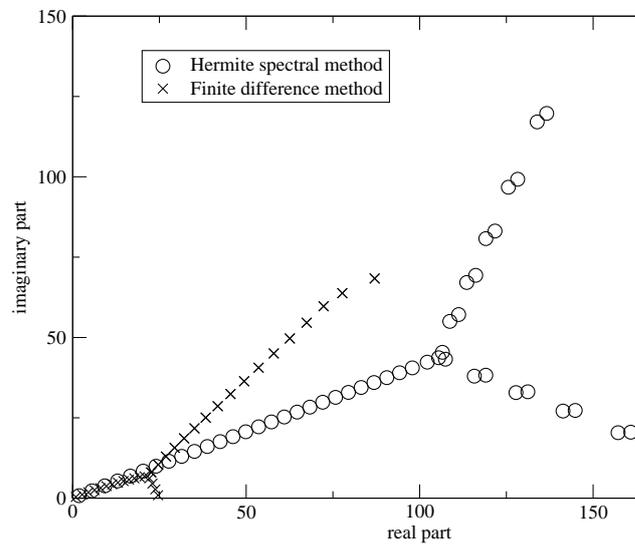


Figure 3: For  $N = 50$ , comparison of the numerical results obtained with the Hermite spectral method and with the finite difference scheme.

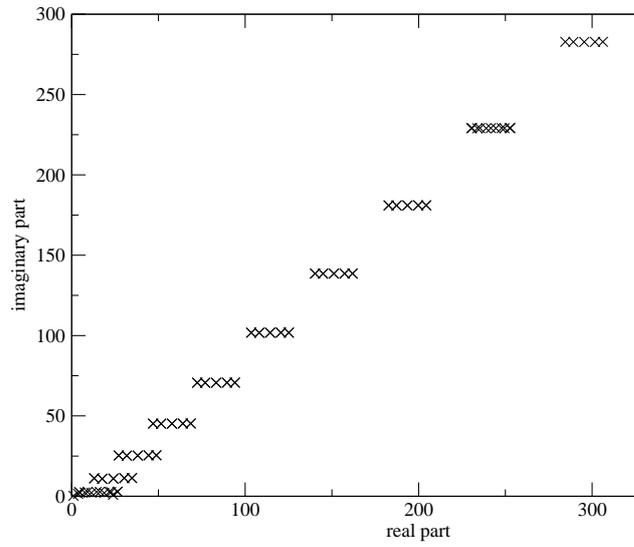


Figure 4: Eigenvalues computed with the finite difference scheme, corresponding to  $N = 100$ ,  $L = 20$ ,  $\alpha = \pi/4$  and  $N_b = 5$ .

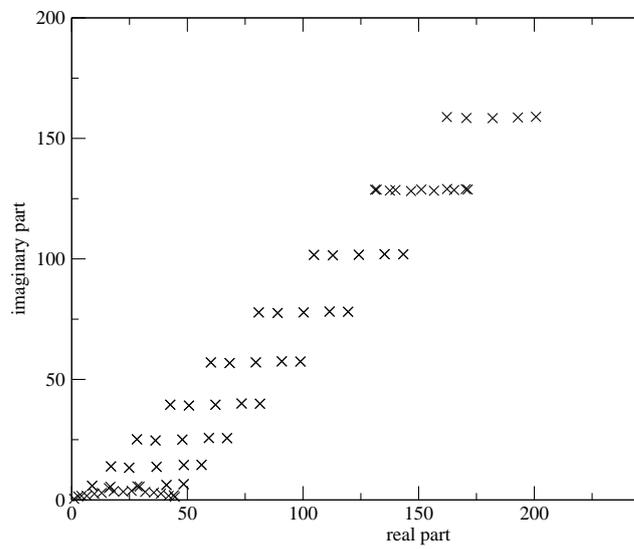


Figure 5: Eigenvalues computed with the finite difference scheme, corresponding to  $N = 100$ ,  $L = 15$ ,  $\alpha = \pi/4$  and  $N_b = 5$ .

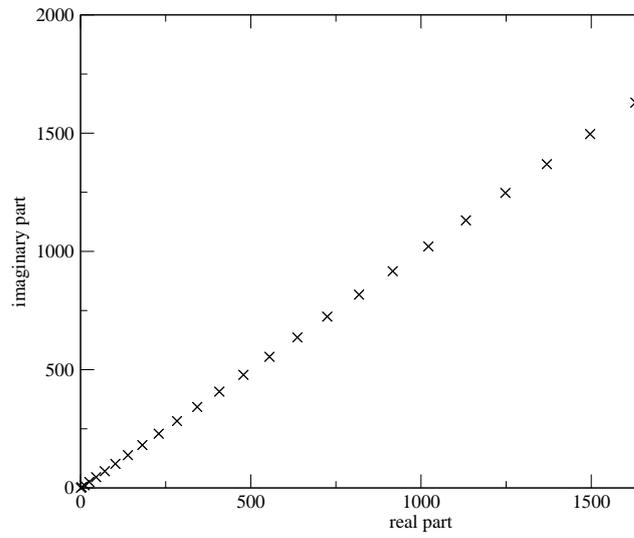


Figure 6: Eigenvalues computed with the finite difference scheme (5.20) for  $\alpha = \pi/4$ ,  $N = 50$  and  $L = 50$ .

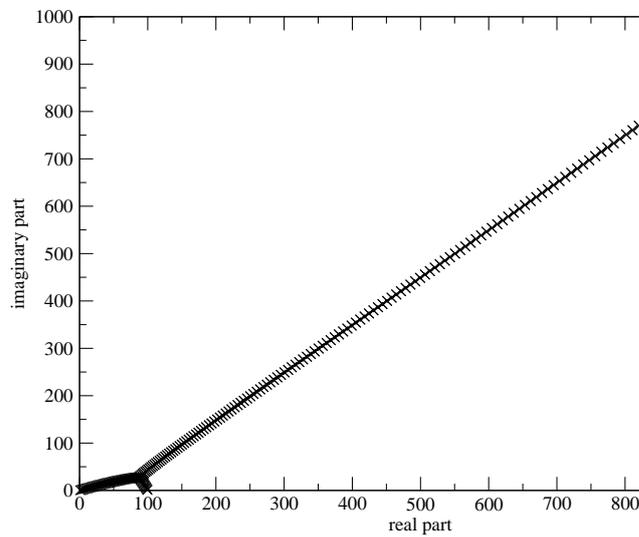


Figure 7: Eigenvalues computed with the finite difference scheme (5.20) for  $\alpha = \pi/4$ ,  $N = 500$  and  $L = 50$ .

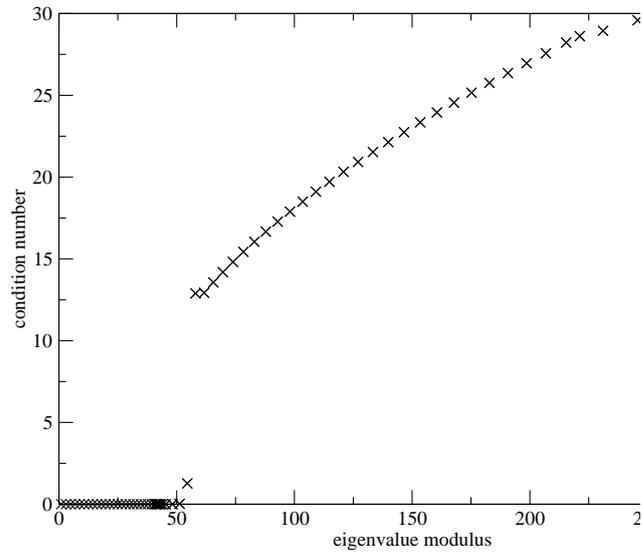


Figure 8: Condition number of the eigenvalues  $\lambda_N$  in function of the modulus of the eigenvalues, for  $N = 100$  and  $L = 15$ .

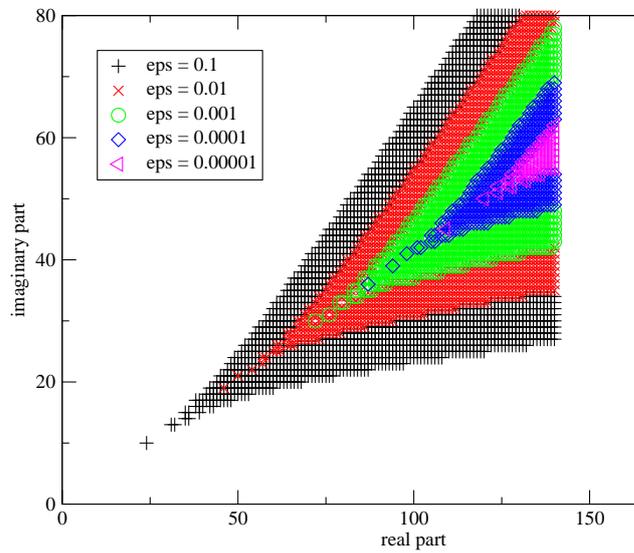


Figure 9: Computation of the pseudospectra (5.26) of the matrix  $\mathcal{A}_N$  corresponding to the Hermite spectral method for  $\alpha = \pi/4$ ,  $N = 100$ .

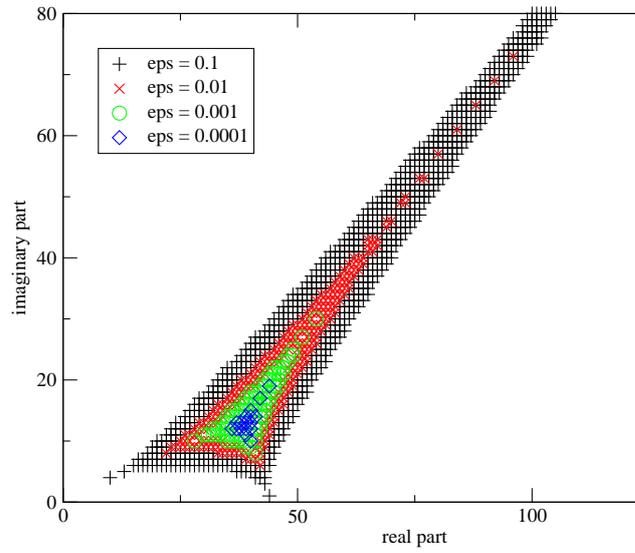


Figure 10: Computation of the pseudospectra (5.26) of the matrix  $\mathcal{A}_N$  corresponding to the finite difference scheme for  $\alpha = \pi/4$ ,  $N = 100$  and  $L = 15$ .

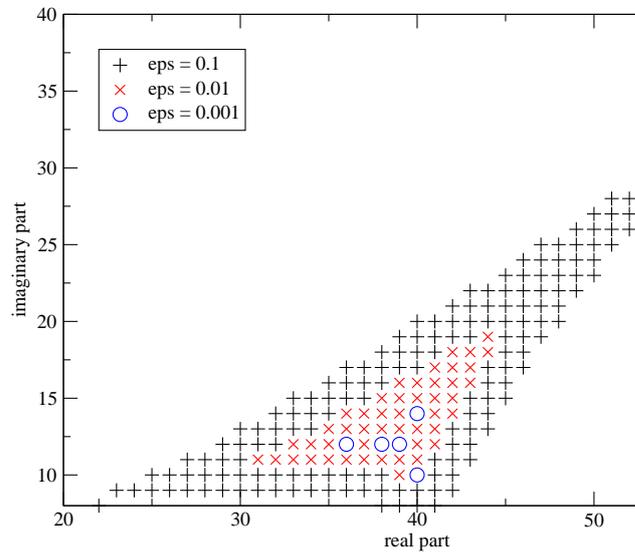


Figure 11: Computation of the pseudospectra (5.27) of the matrix  $\mathcal{A}_N$  corresponding to the finite difference scheme for  $\alpha = \pi/4$ ,  $N = 100$  and  $L = 15$ .

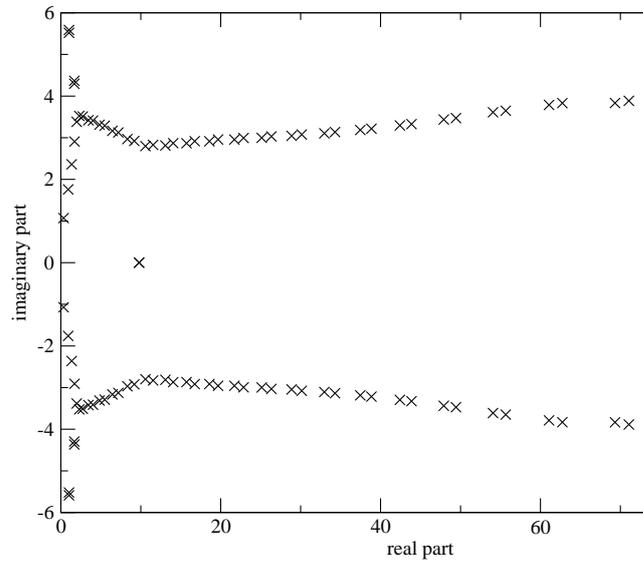


Figure 12: Spectrum of the matrix  $\mathcal{A}_{a,N}$  (5.31) (Hermite spectral method) for  $N = 50$  and  $a = 1$ .

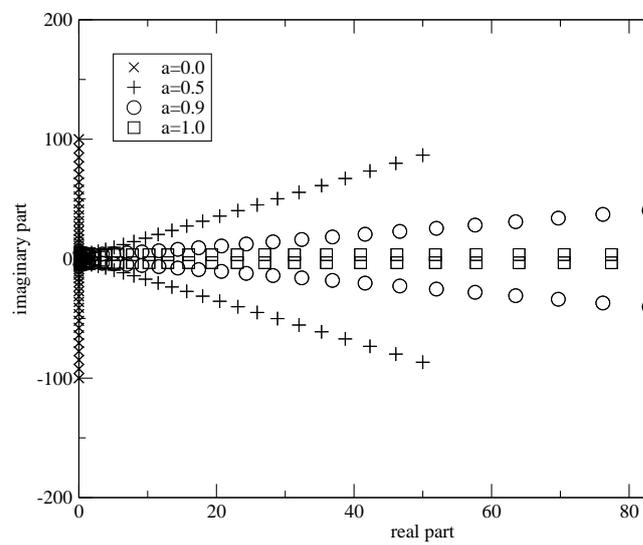


Figure 13: Spectrum obtained with the finite difference scheme for  $a = 0$ ,  $a = 0.5$ ,  $a = 0.9$ ,  $a = 1.0$ ,  $N = 50$  and  $L = 10$ .

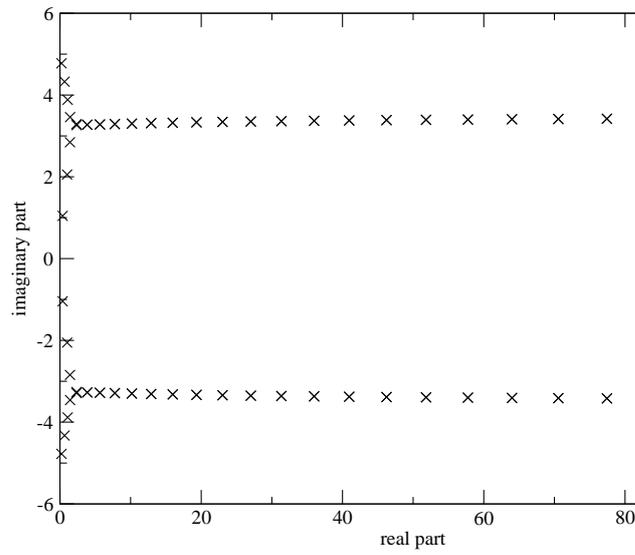


Figure 14: Spectrum of the matrix  $\mathcal{A}_{a,N}$  (5.38) (finite difference scheme) for  $N = 50$ ,  $L = 10$  and  $a = 1$ .

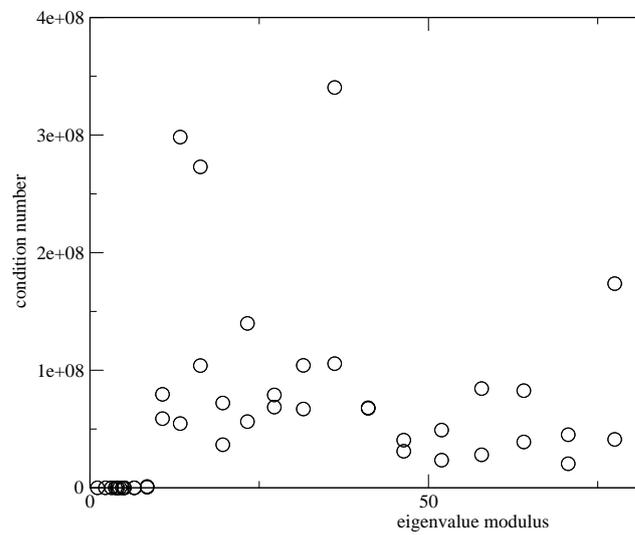


Figure 15: Condition number of the eigenvalues  $\lambda_N$  in function of the modulus  $|\lambda_N|$  for  $N = 50$ ,  $L = 10$  and  $a = 1$ .

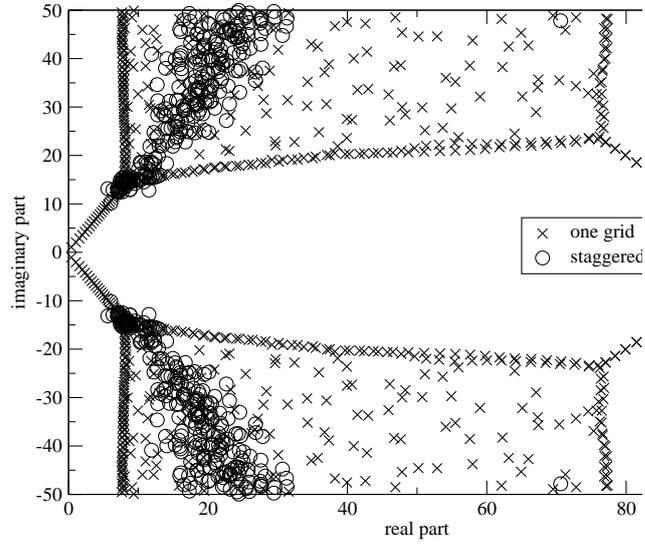


Figure 16: Average on the eigenvalues computed with the finite difference scheme using 11 staggered grids for  $a = 1$ ,  $N = 1000$  and  $L = 10$ .

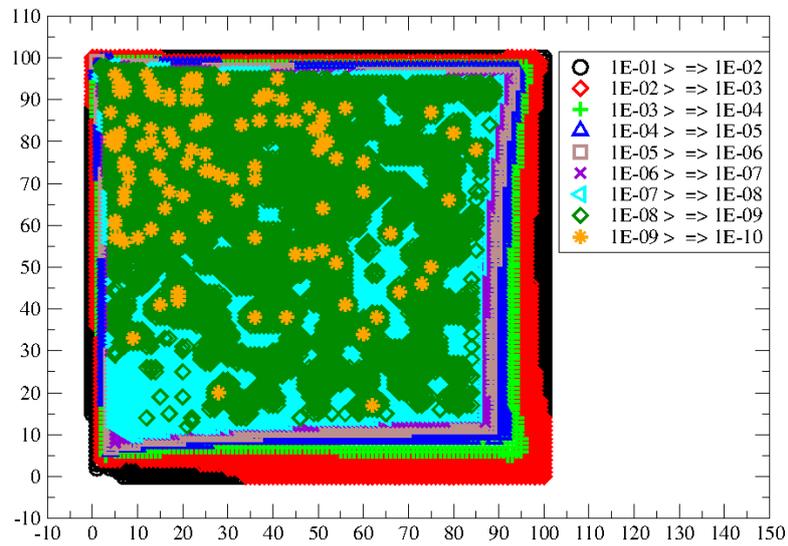


Figure 17: Computation of the pseudospectra (5.26) of the matrix  $\mathcal{A}_{a,N}$  (5.38) (finite difference scheme), for  $N = 1000$ ,  $L = 10$  and  $a = 1$ .

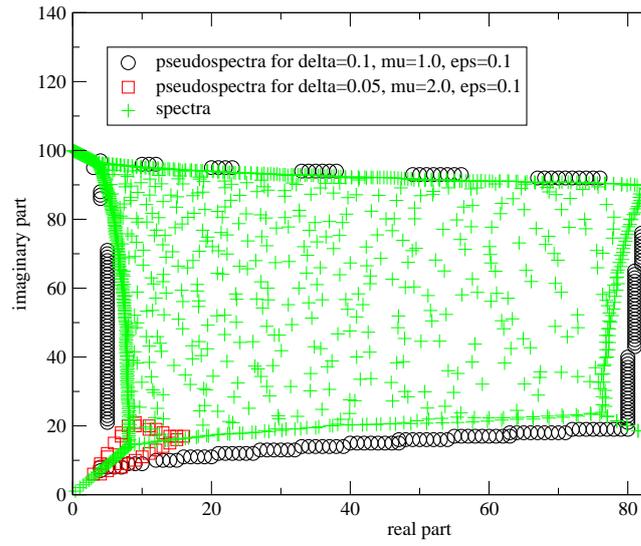


Figure 18: Computation of the pseudospectra (5.40) (finite difference scheme), for  $N = 1000$ ,  $L = 10$  and  $a = 1$ .

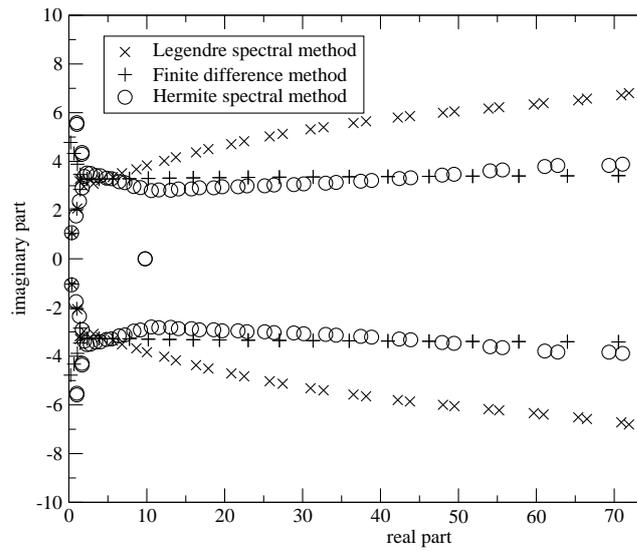


Figure 19: Computation of the eigenvalues for  $N = 50$ ,  $L = 10$  and  $a = 1$  with the Legendre spectral method. Comparison with the spectral Hermite method and the finite difference method is done.

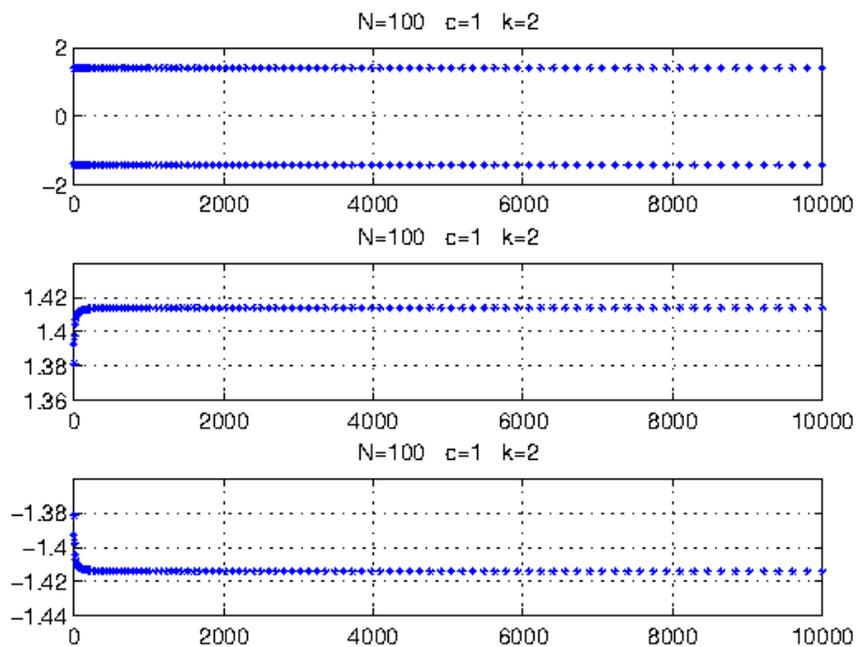


Figure 20: Eigenvalues of the matrix  $\mathcal{A}_c$  for  $N = 100$ ,  $c = 1$  and  $k = 2$ . This figure represents a zoom for the case  $c = 1$ .

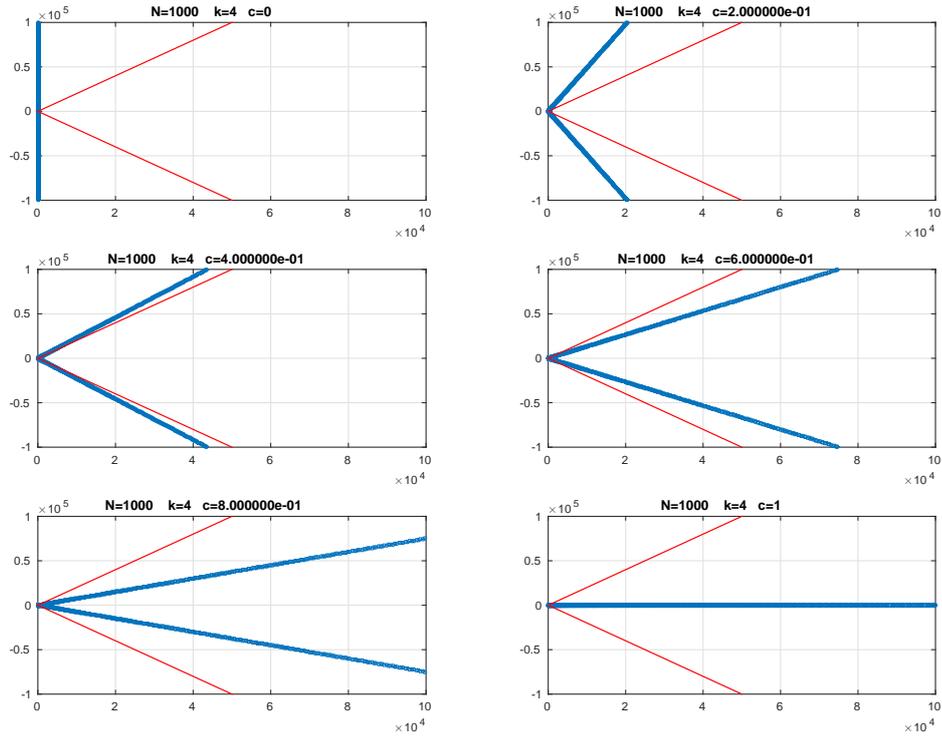


Figure 21: Eigenvalues of the matrix  $\mathcal{A}_c$  for  $N = 1000$ ,  $k = 4$  and  $c = 0, 0.2, 0.4, 0.6, 0.8, 1$ . In the first three figures we can see the cases  $c = 0, 0.2, 0.4$ . In the last three figures we can see the cases  $c = 0.6, 0.8, 1$ .

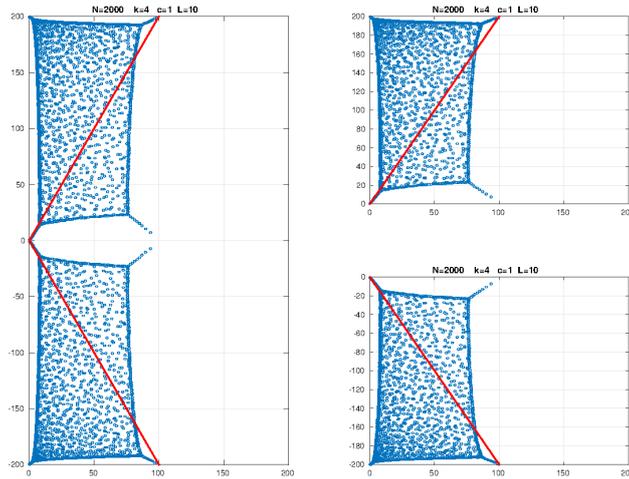


Figure 22: Eigenvalues of the matrix  $\mathcal{A}_c$  for  $N = 2000$ ,  $k = 4$ ,  $L = 10$ ,  $c = 1$ .

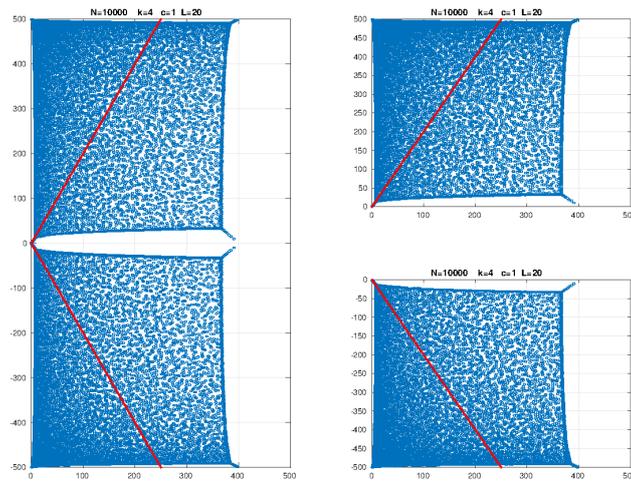


Figure 23: Eigenvalues of the matrix  $\mathcal{A}_c$  for  $N = 10000$ ,  $k = 4$ ,  $L = 20$ ,  $c = 1$ .

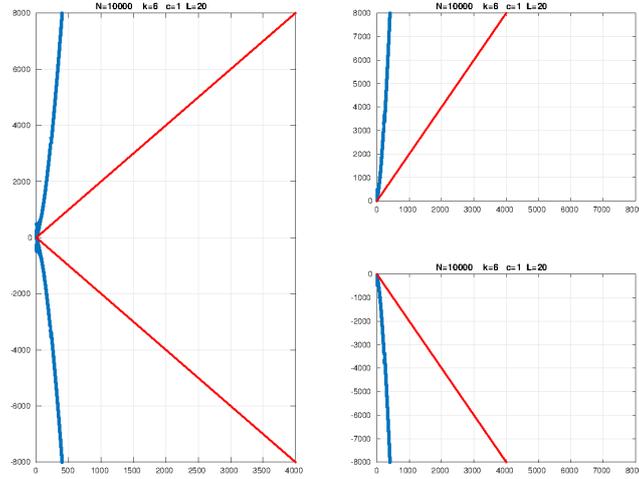


Figure 24: Eigenvalues of the matrix  $\mathcal{A}_c$  for  $N = 10000$ ,  $k = 6$ ,  $L = 20$ ,  $c = 1$ . The figure on the left corresponds to  $0 \leq \Re\lambda \leq 10000$  and  $-10000 \leq \Im\lambda \leq 10000$ . The two figures on the right correspond, up to  $0 \leq \Re\lambda \leq 10000$  and  $0 \leq \Im\lambda \leq 10000$ , down to  $0 \leq \Re\lambda \leq 10000$  and  $-10000 \leq \Im\lambda \leq 0$ .

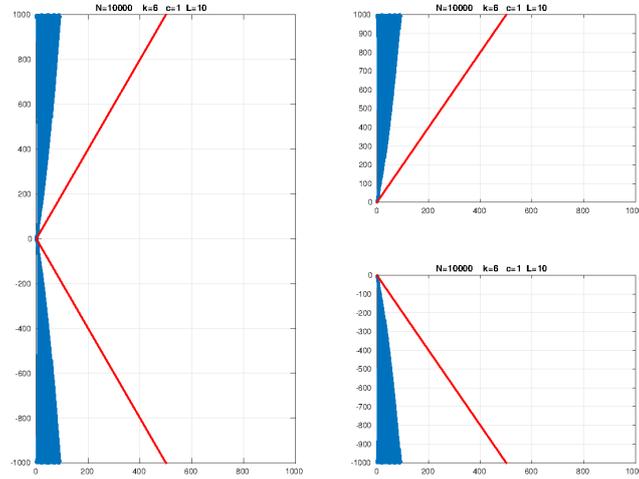


Figure 25: Eigenvalues of the matrix  $\mathcal{A}_c$  for  $N = 10000$ ,  $k = 6$ ,  $L = 10$ ,  $c = 1$ . The figure on the left corresponds to  $0 \leq \Re\lambda \leq 1500$  and  $-1500 \leq \Im\lambda \leq 1500$ . The two figures on the right correspond, up to  $0 \leq \Re\lambda \leq 1500$  and  $0 \leq \Im\lambda \leq 1500$ , down to  $0 \leq \Re\lambda \leq 1500$  and  $-1500 \leq \Im\lambda \leq 0$ .

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