Harmonic oscillators with Neumann condition on the half-line

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Abstract

This paper is devoted to the computation of the minimum Θ_0 of the first eigenvalues for the Neumann realization of harmonic oscillators on the half-line. We propose an algorithm to determine this minimum and we estimate the accuracy of these computations. We also give numerical computations of constants appearing in superconductivity theory.

1 Introduction

Before motivating our analysis, we first define the parameters Θ_0 and $\Phi(0)$. We consider the operator $-d^2/dt^2 + (t-\zeta)^2$ on $(0,+\infty)$. Its Friedrichs extension from $C_0^\infty([0,+\infty))$ is denoted by $H(\zeta)$ and defined on

$$\mathcal{D} = \{u \in H^2(0,+\infty) |\ t^2 u \in L^2(\mathbb{R}^+) \text{ and } u'(0) = 0\}.$$

We denote by $\mu_k(\zeta)$ the k-th eigenvalue of this operator arranged in the ascending order with the multiplicity taken into account. The behavior of the first eigenvalue is well known (see, for example, [12]):

Proposition 1.1. *There exists $\zeta_0 > 0$ such that μ_1 is strictly decreasing from $(-\infty, \zeta_0)$ onto $(+\infty, \Theta_0)$ and strictly increasing from $[\zeta_0, +\infty)$ onto $[\Theta_0, 1)$. Furthermore, if Φ denotes a normalized positive eigenvector associated with $\mu_1(\zeta_0)$, then*

$$\int_0^\infty (|\Phi'(t)|^2 + (t-\zeta_0)^2 |\Phi(t)|^2)\, dt = \Theta_0, \qquad \int_0^\infty (t-\zeta_0)|\Phi(t)|^2\, dt = 0,$$

$$|\Phi(0)|^2 = \frac{\mu_1''(\zeta_0)}{2\zeta_0}, \qquad \Theta_0 = \zeta_0^2.$$

An estimate of Θ_0 by 0.59010 was already given in [13], using the Weber functions but there is no mention of the accuracy of this estimate. Using an integral representation [11], Chapman approximates Θ_0 by 0.59 without any estimate of the error. In the literature, we can find some estimates of Θ_0 but there is no mention of the accuracy of the computations. To our knowledge, we do not find any computation of $\Phi(0)$. The aim of this article is to give accurate estimates of Θ_0 and $\Phi(0)$ and of the error between exact values and numerical computations. The numerical method implemented here is very standard since we use finite difference and element methods.

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In Section 2, we remind of some results concerning the localization of the superconductivity and we notice that the parameters Θ_0 and $\Phi(0)$ appear frequently (see Propositions 2.1, 2.5). The analysis of the onset of superconductivity is based on those of the low-lying eigenmodes for the Schrödinger operator (see [7, 8, 17, 30] and Propositions 2.2, 2.3, 2.4, 2.6).
To estimate the error of the computations, we establish in Section 3 error estimates on eigenmodes: Theorem 3.2 quantifies the gap between the eigenvalue Θ_0 and the energy associated with a quasi-mode for the operator $H(\zeta)$. In Theorem 3.3, we prove H^1-estimate between the normalized eigenfunction Φ associated with Θ_0 for the operator $H(\zeta_0)$ and a normalized quasi-mode for $H(\zeta)$. We deduce in Theorem 3.5 an estimate of $\Phi(0)$. In Section 4, we construct an adequate quasi-mode combining the finite difference method and analysis of the ODE theory for the differential equations depending on parameters. We implement this method in Subsection 4.5 and obtain an accurate approximation of Θ_0 and $\Phi(0)$:

Theorem 1.2.

$$|\Theta_0 - 0.590106125| \leq \times 10^{-9} \qquad \textit{and} \qquad |\Phi(0) - 0.87304| \leq 5 \times 10^{-5}.$$

Section 5 presents computations with the finite element method. From a numerical point of view, we also mention papers [4, 3] which deal with the numerical computations for the bottom of the spectrum of $-d^2/dt^2 + (t-\zeta)^2$ on a symmetric interval using a finite difference method.

2 Motivation

To highlight how is important to compute accurately these parameters Θ_0 and $\Phi(0)$, we recall some results about superconductivity modelled by Ginzburg-Landau theory. It is well-known that superconductors of type II lose their superconducting property when submitted to a sufficiently strong external magnetic field. This transition takes place for a value H_{C_3}[1] of the field which appears as a function of a material-dependent parameter κ. We recall here results about the calculation of this critical field for large values of κ in two situations: smooth domains and domains with corners.
Let $\Omega \subset \mathbb{R}^2$ be a bounded simply-connected domain with Lipschitz boundary. The Ginzburg-Landau functional reads

$$\mathcal{E}_{\kappa,H}[\psi,\mathcal{A}] = \int_\Omega \Big\{ |(-i\nabla - \kappa H\mathcal{A})\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4 \Big\}\, dx + \kappa^2 H^2 \int_{\mathbb{R}^2} |\mathrm{curl}\,\mathcal{A} - 1|^2\, dx\ ,$$

with $(\psi,\mathcal{A}) \in W^{1,2}(\Omega;\mathbb{C}) \times \{\mathcal{A} = \mathcal{A}_0 + \tilde{\mathcal{A}} \text{ with } \tilde{\mathcal{A}} \in \dot{H}^1(\mathbb{R}^2,\mathbb{R}^2), \mathrm{div}\,\tilde{\mathcal{A}} = 0\}$, $\mathcal{A}_0(x) = 1/2(-x_2,x_1)$. We use the notation $\dot{H}^1(\mathbb{R}^2)$ for the homogeneous Sobolev spaces. We define the critical field H_{C_3} as the value of H where the transition between the normal and superconducting state takes place:

$$H_{C_3}(\kappa) = \inf\{H > 0\ :\ (0,\mathcal{A}_0) \text{ is a minimizer of } \mathcal{E}_{\kappa,H}\}\ .$$

The calculation of this critical field H_{C_3} for large values of κ has been the focus of much activity (see [22, 2, 27, 28, 29, 25, 14, 15, 16]). In the works [14, 15, 16, 17], the definition of H_{C_3} in the case of samples with smooth section has been clarified and the asymptotic is given by:

Proposition 2.1 (see [16])**.** *Suppose Ω is a bounded simply-connected domain in $\mathbb{R}^2$ with smooth boundary. Let κ_{max} be the maximal curvature of $\partial\Omega$. Then*

$$H_{C_3}(\kappa) = \frac{\kappa}{\Theta_0} + \frac{C_1}{\Theta_0^{3/2}}\kappa_{max} + \mathcal{O}(\kappa^{-1/2}) \qquad \textit{with} \qquad C_1 = \frac{\Phi^2(0)}{3}.$$

[1] The first rigorous definition of the critical field H_{C_3} appeared in [28].

It was realized that the asymptotics of the critical field is completely determined by the linear eigenvalue problem. Indeed, if we denote by $\mu^{(n)}(h)$ the n-th eigenvalue of the magnetic Neumann operator $P_h = (-ih\nabla - \mathcal{A}_0)^2$ defined on $\mathcal{D}(P_h) = \{u \in H^2(\Omega) | \nu \cdot (-ih\nabla - \mathcal{A}_0)u_{|\partial\Omega} = 0\}$, then the asymptotics of $\mu^{(n)}(h)$ was established by Fournais-Helffer in [15]:

Proposition 2.2 (see [15]). *Suppose that Ω is a smooth bounded and simply connected domain of $\mathbb{R}^2$, that the curvature $\partial\Omega \ni s \mapsto \kappa(s)$ at the boundary has a unique maximum κ_{max} reached at $s = s_0$ and that the maximum is non-degenerate, i. e. $k_2 := -\kappa''(s_0) \neq 0$. Then for all $n \in \mathbb{N}$, there exists a sequence $\{\xi_j^{(n)}\}_{j=1}^{\infty} \subset \mathbb{R}$ such that $\mu^{(n)}(h)$ admits the following asymptotic expansion (for $h \to 0$):*

$$\mu^{(n)}(h) \sim \Theta_0 h - \kappa_{max} C_1 h^{3/2} + C_1 \Theta_0^{1/4} \sqrt{\frac{3k_2}{2}} (2n-1) h^{7/4} + h^{15/8} \sum_{j=0}^{\infty} h^{j/8} \xi_j^{(n)}.$$

To carry through an analysis of the critical field H_{C_3} in the case of domains with corners, a linear spectral problem, studied in depth in [5, 6, 7, 8], is usefull. Let us first give estimates for the Schrödinger operator in a model geometry: the infinite sector.

Proposition 2.3 (see [6]). *Let G^α be the sector in $\mathbb{R}^2$ with opening α and Q^α be the Neumann realization of the Schrödinger operator $-(\nabla - i\mathcal{A}_0)^2$ on G^α. We denote by $\mu_k(\alpha)$ the k-th smallest element of the spectrum given by the max-min principle. Then:*

1. *The infimum of the essential spectrum of Q^α is equal to Θ_0.*
2. *For all $\alpha \in (0, \pi/2]$, $\mu_1(\alpha) < \Theta_0$ and $\mu_1(\pi) = \Theta_0$.*
3. *Let $\alpha \in (0, 2\pi)$, $k \geq 1$ be such that $\mu_k(\alpha) < \Theta_0$ and Ψ_k^α an associated normalized eigenfunction. Then Ψ_k^α satisfies the following exponential decay estimate:*

$$\forall \varepsilon > 0, \exists C_{\varepsilon,\alpha} > 0, \ \| e^{(\sqrt{\Theta_0 - \mu_k(\alpha)} - \varepsilon)|x|} \Psi_k^\alpha \|_{L^2(G^\alpha)} \leq C_{\varepsilon,\alpha}.$$

Thanks to the model situation given by the analysis of the angular sector, we are able to determine the asymptotic expansion of the low-lying eigenmodes of the Schrödinger operator on curvilinear polygons:

Proposition 2.4 (see [7]). *Let Ω be a bounded curvilinear polygon, Σ be the set of its vertices, α_{s} be the angle at the vortex s. We denote by Λ_n the n-th eigenvalue of the model operator $\oplus_{\mathsf{s}\in\Sigma} Q^{\alpha_{\mathsf{s}}}$, and $\mu^{(n)}(h)$ the n-th smallest eigenvalue of P_h. Let n be such that $\Lambda_n < \Theta_0$. There exist $h_0 > 0$ and $(m_j)_{j\geq 1}$ such that for any $N > 0$ and $h \leq h_0$,*

$$\mu^{(n)}(h) = h\Lambda_n + h \sum_{j=1}^{N} m_j h^{j/2} + \mathcal{O}(h^{\frac{N+1}{2}}).$$

If Ω is a bounded convex polygon, there exists $r_n > 0$ and for any $\varepsilon > 0$, $C_\varepsilon > 0$ such that

$$\left| \mu^{(n)}(h) - h\Lambda_n \right| \leq C_\varepsilon \exp\left(-\frac{1}{\sqrt{h}} (r_n \sqrt{\Theta_0 - \Lambda_n - \varepsilon}) \right).$$

For non constant magnetic field, the low-lying eigenvalues admit an asymptotic expansion in power of $\sqrt{h}$. These results highlight the importance of comparing $\mu_k(\alpha)$ with Θ_0 and then of computing precisely Θ_0. It is also natural to wonder for which angle α we have $\mu_k(\alpha) < \Theta_0$. It was conjectured in [1, 8] that

μ_1 is strictly increasing from $(0,\pi)$ onto $(0,\Theta_0)$ and is equal to Θ_0 on $[\pi,2\pi)$. This conjecture is based on numerical computations and could be strengthened with an accurate estimate of Θ_0.
As in the case of smooth domains, spectral informations produce results about the minimizers of the Ginzburg-Landau functional for domains with corners. We obtain in particular a complete asymptotics of H_{C_3} for large values of κ in terms of linear spectral data and precise estimates on the location of nucleation of superconductivity for magnetic field strengths just below the critical field:

Proposition 2.5 (see [10]). *Let Ω be a curvilinear polygon and $\Lambda_1 = \min_{\mathsf{s}\in\Sigma}\mu_1(\alpha_{\mathsf{s}})$. There exists a real-valued sequence $\{\eta_j\}_{j=1}^{\infty}$ such that*

$$H_{C_3}(\kappa) = \frac{\kappa}{\Lambda_1}\left(1+\sum_{j=1}^{\infty}\eta_j\kappa^{-j}\right), \quad \text{for } \kappa\to+\infty.$$

Let $\mu\in(\Lambda_1,\Theta_0)$ and define $\Sigma'=\{\mathsf{s}\in\Sigma|\mu_1(\alpha)\leq\mu\}$. There exist constants κ_0, M, C, $\varepsilon>0$ such that if $\kappa\geq\kappa_0$, $H/\kappa\geq\mu^{-1}$, and $(\psi,\mathcal{A})$ is a minimizer of $\mathcal{E}_{\kappa,H}$, then

$$\int_\Omega e^{\epsilon\sqrt{\kappa H}\mathrm{dist}(x,\Sigma')}\left(|\psi(x)|^2+\frac{1}{\kappa H}|(\nabla-i\kappa H\mathcal{A})\psi(x)|^2\right)dx\leq C\int_{\{x:\sqrt{\kappa H}\mathrm{dist}(x,\Sigma')\leq M\}}|\psi(x)|^2\,dx.$$

This Agmon type estimate describes how superconductivity can nucleate successively in the corners, ordered according to their spectral parameter $\mu_1(\alpha_{\mathsf{s}})$ seeing that $\mu_1(\alpha_{\mathsf{s}})<\Theta_0$. This reinforces the interest to compare precisely $\mu_1(\alpha)$ and Θ_0.

When we consider the Schrödinger operator in dimension 3, see [23, 24, 30], we have to analyze some new operators: the Neumann realization of $h^2D_s^2+h^2D_t^2+(hD_r+t\cos\theta-s\sin\theta)^2$ on $\mathbb{R}^3_+=\{(r,s,t)\in\mathbb{R}^3:t>0\}$ where $\theta\in[0,\frac{\pi}{2}]$ is the angle that makes the magnetic field with the boundary at each point (approximated by the tangent plane). We first make a Fourier transform in r. When $\theta=0$, we are led to the so-called de Gennes operator $H(\zeta)$ on the half-line (see [12] and this present paper). If $\theta\neq0$, we perform a translation in s and a rescaling. Thus we are reduced to a Schrödinger operator with an electric potential on the half-plane $\mathbb{R}^2_+=\{(s,t)\in\mathbb{R}^2:t>0\}$:

$$\mathcal{L}_\theta = D_s^2+D_t^2+(t\cos\theta-s\sin\theta)^2.$$

This operator is deeply studied in [9], both theoretically and numerically. The authors prove an isotropic estimate and anisotropic estimate for the eigenvectors. They also analyze the asymptotics when $\theta\to0$. In particular, they prove the following result:

Proposition 2.6. *We have the following upper-bound for the n-th eigenvalue $\sigma_n(\theta)$ of $\mathcal{L}_\theta$:*

$$\sigma_n(\theta)\leq\Theta_0\cos\theta+(2n-1)\sin\theta,\qquad\forall n\geq1. \tag{2.1}$$

For all $M_0\geq1$, there exist $h_0>0$ and $C(M_0)>0$ such that for all $0<\theta\leq h_0$ and $1\leq n\leq M_0$:

$$|\sigma_n(\theta)-\Theta_0-\theta\,a_1\,(2n-1)|\leq C(M_0)\,\theta^{3/2},\qquad\text{with}\quad a_1=\sqrt{\frac{\mu_1''(\zeta_0)}{2}}=\Phi(0)\Theta_0^{1/4}. \tag{2.2}$$

If we denote by $n(\theta)$ the number of eigenvalues of $\mathcal{L}_\theta$ below the essential spectrum, we have with (2.1):

$$n(\theta)\geq\frac{1-\Theta_0\cos\theta}{2\sin\theta}+\frac{1}{2}. \tag{2.3}$$

If we bound from below Θ_0 by 1, 0.6, 0.591, we lower-bound shows that $n(\pi/2000)$ is greater than 0, 127 and 130 respectively. A greater approximation of Θ_0 we have, a greater lower-bound of $n(\theta)$ we deduce.

3 Error estimates on eigenmodes

This section concerns the analysis of the operator $H(\zeta)$ and error estimates between Θ_0 and the energy associated with a quasi-mode for $H(\zeta)$.

Notation 3.1. *For any $\zeta \in \mathbb{R}$, we define q_1^ζ and q_2^ζ on $\mathcal{D}$ by*

$$q_1^\zeta(u) = \int_{\mathbb{R}^+} (t-\zeta)|u(t)|^2\, dt, \qquad q_2^\zeta(u) = \int_{\mathbb{R}^+} (t-\zeta)^2|u(t)|^2\, dt. \tag{3.1}$$

Let $\zeta \in \mathbb{R}$ and φ_ζ be a normalized positive function of $\mathcal{D}$. We define $\breve{\mu}(\zeta)$ and r_ζ by

$$\breve{\mu}(\zeta) = \langle H(\zeta)\varphi_\zeta, \varphi_\zeta\rangle, \qquad r_\zeta = H(\zeta)\varphi_\zeta - \breve{\mu}(\zeta)\varphi_\zeta.$$

We denote also

$$\eta_\zeta = \breve{\mu}(\zeta) + 2(\zeta-\zeta_0)q_1^\zeta(\varphi_\zeta) + (\zeta-\zeta_0)^2, \tag{3.2}$$

$$a_\zeta = \left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2|\zeta-\zeta_0|\sqrt{q_2^\zeta(\varphi_\zeta)}\right)^2. \tag{3.3}$$

With these Notation 3.1, we have

$$H(\zeta)\varphi_\zeta = \breve{\mu}(\zeta)\varphi_\zeta + r_\zeta \qquad \text{with} \qquad \langle r_\zeta, \varphi_\zeta\rangle = 0.$$

Theorem 3.2. *Let $\zeta \in \mathbb{R}$ and φ_ζ be a normalized positive function of $\mathcal{D}$. With Notation 3.1, we assume*

$$\eta_\zeta \le \mu_2(\zeta_0).$$

Then we can compare Θ_0 and $\breve{\mu}(\zeta)$:

$$\eta_\zeta - \frac{a_\zeta - 4(\zeta-\zeta_0)^2 q_1^\zeta(\varphi_\zeta)^2}{\mu_2(\zeta_0)-\eta_\zeta} \le \Theta_0 \le \breve{\mu}(\zeta).$$

Proof. The upper-bound is trivial: by definition of the minimum Θ_0, $\Theta_0 = \mu_1(\zeta_0) \le \mu_1(\zeta)$ and by the min-max principle $\mu_1(\zeta) \le \breve{\mu}(\zeta) = \langle H(\zeta)\varphi_\zeta, \varphi_\zeta\rangle$. Thus:

$$\Theta_0 = \mu_1(\zeta_0) \le \mu_1(\zeta) \le \breve{\mu}(\zeta).$$

To prove the lower-bound, we bring to mind the Temple inequality (see [26], [19, Theorem 1.15]): Let A be self-adjoint and $\Psi \in \mathcal{D}(A)$, $\|\Psi\| = 1$. Suppose that λ is the unique eigenvalue of A in an interval (α,β). Let $\eta = \langle \Psi, A\Psi\rangle$ and $\varepsilon^2 = \|(A-\eta)\Psi\|^2$. If $\varepsilon^2 < (\beta-\eta)(\eta-\alpha)$, then

$$\eta - \frac{\varepsilon^2}{\beta-\eta} \le \lambda \le \eta + \frac{\varepsilon^2}{\eta-\alpha}. \tag{3.4}$$

We apply this inequality with $A = H(\zeta_0)$, $\Psi = \varphi_\zeta$. Since Θ_0 is the first eigenvalue for $H(\zeta_0)$, we can choose $\alpha = -\infty$, $\beta = \mu_2(\zeta_0)$. We rewrite $H(\zeta_0)$ with $H(\zeta)$:

$$H(\zeta_0) = H(\zeta) + 2(\zeta-\zeta_0)(t-\zeta) + (\zeta-\zeta_0)^2.$$

Since φ_ζ is normalized and $\langle r_\zeta, \varphi_\zeta\rangle = 0$, we obtain $\eta = \langle \varphi_\zeta, H(\zeta_0)\varphi_\zeta\rangle = \eta_\zeta$ with definition (3.2). The assumption $\varepsilon^2 < (\beta-\eta)(\eta-\alpha)$ is then obviously fulfilled. Consider now ε^2.

$$\begin{aligned}\varepsilon^2 &= \int_{\mathbb{R}^+} \left| r_\zeta(t) + 2(\zeta-\zeta_0)(t-\zeta)\varphi_\zeta(t) - 2(\zeta-\zeta_0)q_1^\zeta(\varphi_\zeta)\varphi_\zeta(t)\right|^2 dt \\ &\leq \left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2|\zeta-\zeta_0|\sqrt{q_2^\zeta(\varphi_\zeta)}\right)^2 - 4(\zeta-\zeta_0)^2 q_1^\zeta(\varphi_\zeta)^2. \end{aligned} \tag{3.5}$$

Temple inequality (3.4) gives

$$\eta_\zeta - \frac{\varepsilon^2}{\mu_2(\zeta_0)-\eta_\zeta} \leq \mu_1(\zeta_0) \leq \eta_\zeta\ .$$

□

Let us now prove an estimate on the eigenfunction.

Theorem 3.3. *Let $\zeta \in \mathbb{R}$ and φ_ζ be a normalized and positive function of $\mathcal{D}$. With Notation 3.1, we assume $\eta_\zeta \leq \mu_2(\zeta_0)$. Then*

$$\begin{aligned}\|\varphi_\zeta - \Phi\|_{L^2(\mathbb{R}^+)} &\leq 2\sqrt{2}\frac{\left(a_\zeta + (\zeta-\zeta_0)^3\left(\zeta-\zeta_0+4q_1^\zeta(\varphi_\zeta)\right)\right)^{1/2}}{\mu_2(\zeta_0)-\breve{\mu}(\zeta)}, \\ \|\varphi_\zeta' - \Phi'\|_{L^2(\mathbb{R}^+)} &\leq \left(\frac{a_\zeta - 4q_1^\zeta(\varphi_\zeta)^2(\zeta-\zeta_0)^2}{\mu_2(\zeta_0)-\eta_\zeta} + \breve{\mu}(\zeta)\|\Phi-\varphi_\zeta\|^2_{L^2(\mathbb{R}^+)}\right)^{1/2}.\end{aligned}$$

To prove this result, we use an estimate of quasi-modes established in [21, Proposition 4.1.1, p. 30] :

Proposition 3.4. *Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Let $I \subset \mathbb{R}$ be a compact interval, $\Psi_1, \ldots, \Psi_N \in \mathcal{H}$ linearly independent in $\mathcal{D}(A)$ and $\mu_1, \ldots, \mu_N \in I$ such that $A\Psi_j = \mu_j\Psi_j + r_j$ with $\|r_j\|_{\mathcal{H}} \leq \varepsilon$. Let $a > 0$ and assume that $\mathrm{Sp}(A) \cap (I + \mathcal{B}(0,2a) \setminus I) = \emptyset$. Then if E is the space spanned by $\Psi_1, \ldots, \Psi_N$ and if F is the space associated to $\sigma(A) \cap I$, we have*

$$d(E,F) \leq \frac{\varepsilon\sqrt{N}}{a\sqrt{\lambda_S^{\min}}},$$

where $\lambda_S^{\min}$ is the smallest eigenvalues of $S = (\langle \Psi_j, \Psi_k\rangle_{\mathcal{H}})$ and d the non-symmetric distance defined by $d(E,F) = \|\Pi_E - \Pi_F\Pi_E\|_{\mathcal{H}}$, with Π_E, Π_F the orthogonal projections on E and F.

Proof of Theorem 3.3. We apply Proposition 3.4 with $N = 1$, $A = H(\zeta_0)$, $\Psi_1 = \varphi_\zeta$, E the space spanned by φ_ζ and F the space spanned by Φ.
We first connect the distance d with the norm $\|\varphi_\zeta - \Phi\|_{L^2(\mathbb{R}^+)}$ by noticing that

$$d(E,F) = ||\varphi_\zeta - \langle\varphi_\zeta, \Phi\rangle\Phi||_{L^2(\mathbb{R}^+)} = \sqrt{1-|\langle\varphi_\zeta,\Phi\rangle|^2} \geq \frac{1}{\sqrt{2}}\|\varphi_\zeta - \Phi\|_{L^2(\mathbb{R}^+)}. \tag{3.6}$$

Writing

$$H(\zeta_0)\varphi_\zeta = \breve{\mu}(\zeta)\varphi_\zeta + \tilde{r}_\zeta \quad \text{with} \quad \tilde{r}_\zeta = (H(\zeta_0) - H(\zeta))\varphi_\zeta + r_\zeta,$$

we estimate $\|\tilde{r}_\zeta\|_{L^2(\mathbb{R}^+)}$ using the orthogonality relation $\langle r_\zeta, \varphi_\zeta\rangle = 0$:

$$\begin{aligned} ||\tilde{r}_\zeta||^2_{L^2(\mathbb{R}^+)} &= \int_{\mathbb{R}^+} \left|2(\zeta-\zeta_0)(t-\zeta)\varphi_\zeta(t) + (\zeta-\zeta_0)^2\varphi_\zeta(t) + r_\zeta(t)\right|^2 \, dt \\ &\leq a_\zeta + (\zeta-\zeta_0)^3\left(\zeta-\zeta_0+4q_1^\zeta(\varphi_\zeta)\right). \end{aligned} \tag{3.7}$$

Relations (3.6), (3.7) and Proposition 3.4 with $a = (\mu_2(\zeta_0) - \breve{\mu}(\zeta))/2$ give the L^2-estimate of $(\varphi_\zeta - \Phi)$. Let us now estimate the L^2-norm of $(\varphi'_\zeta - \Phi')$. An integration by parts gives:

$$\langle H(\zeta_0)(\Phi-\varphi_\zeta), \Phi-\varphi_\zeta\rangle_{L^2(\mathbb{R}^+)} \geq \|\Phi'-\varphi'_\zeta\|^2_{L^2(\mathbb{R}^+)} \, . \tag{3.8}$$

On the other hand,

$$\begin{aligned} \langle H(\zeta_0)(\varphi_\zeta-\Phi), \varphi_\zeta-\Phi\rangle_{L^2(\mathbb{R}^+)} &= \langle H(\zeta_0)\varphi_\zeta, \varphi_\zeta\rangle_{L^2(\mathbb{R}^+)} - 2\Theta_0\langle\Phi, \varphi_\zeta\rangle_{L^2(\mathbb{R}^+)} + \Theta_0 \\ &= \eta_\zeta - \Theta_0 + \Theta_0\|\Phi-\varphi_\zeta\|^2_{L^2(\mathbb{R}^+)}. \end{aligned} \tag{3.9}$$

We deduce from (3.8), (3.9) and Theorem 3.2 a upper-bound for the L^2-norm of $\Phi' - \varphi'_\zeta$:

$$\|\Phi'-\varphi'_\zeta\|^2_{L^2(\mathbb{R}^+)} \leq \frac{a_\zeta - 4q_1^\zeta(\varphi_\zeta)^2(\zeta-\zeta_0)^2}{\mu_2(\zeta_0)-\eta_\zeta} + \breve{\mu}(\zeta)\|\Phi-\varphi_\zeta\|^2_{L^2(\mathbb{R}^+)}.$$

□

We deduce now an estimate for $\varphi_\zeta - \Phi$ at point $t = 0$.

Theorem 3.5. *Using the same notation and assumptions as Theorem 3.3, we have*

$$|\Phi(0)-\varphi_\zeta(0)|^2 \leq 2\|\Phi-\varphi_\zeta\|_{L^2(\mathbb{R}^+)} \, \|\Phi'-\varphi'_\zeta\|_{L^2(\mathbb{R}^+)}. \tag{3.10}$$

Proof. As $\Phi - \varphi \in H^1(\mathbb{R}^+)$, it suffices to write

$$|\Phi(0)-\varphi_\zeta(0)|^2 = 2\int_0^\infty |\Phi(t)-\varphi_\zeta(t)||\Phi'(t)-\varphi'_\zeta(t)| \, dt.$$

We conclude with the Cauchy-Schwarz inequality. □

4 Construction of a quasi-mode by a finite difference method

Theorem 3.2 gives bounds for Θ_0 as soon as we get quasi-modes for the operator $H(\zeta)$. Of course, the closer ζ is from ζ_0, the better the bounds. A heuristic approach based on finite difference method and the ODE theory gives a sequence of approximated values for φ_ζ. Then we use this sequence to construct a test-function with energy as small as possible and thus try and give a good approximation of Θ_0. We organize this approximation in several steps:

1. Reduce the problem to a finite interval,
2. Write a finite difference scheme,
3. Study the dependence of the discrete solution on the parameter ζ,
4. Construct a regular function on $\mathbb{R}^+$ from the discrete solution,
5. Deduce an algorithm to approximate Θ_0,
6. Estimate the accuracy of the computations.

4.1 Reduction to a finite interval

In a first step, we reduce the domain $\mathbb{R}^+$ to an interval $[0, L]$: We know that the eigenvector is exponentially decreasing so, if L is large enough, the error due to cut-off is exponentially small. Let φ_ζ be a normalized eigenvector associated with $\mu_1(\zeta)$ for the operator $H(\zeta)$. This function φ_ζ is decreasing like $t \mapsto \exp\left(-\frac{t^2}{2}\right)$ as $t \to +\infty$. Therefore there exists a positive constant C such that, for $L > 0$,

$$\int_a^\infty |\varphi_\zeta(t)|^2 dt \leq 2\frac{C}{L}\int_L^\infty te^{-t^2}\, dt = \frac{Ce^{-L^2}}{L}. \tag{4.1}$$

Consequently, to approximate $\|\varphi_\zeta\|_{L^2(\mathbb{R}^+)}$ by $\displaystyle\int_0^L |\varphi_\zeta(t)|^2\, dt$ with a better accuracy than 10^{-N}, it is enough that L satisfies

$$\frac{e^{-L^2}}{L} \leq \frac{10^{-N}}{C}.$$

It is equivalent to find L such that $L^2 + \ln L \geq N \ln 10 + \ln C$. So it is reasonnable to restrict the study to the interval $(0, 10)$ for numerical computations. The numerical quasi-mode will be extend by 0 on $(L, +\infty)$ to define a function on $\mathbb{R}^+$. We will control the error due to the cut-off.
We conclude this section with a comparaison between the fundamental energy on a finite interval and Θ_0.

Lemma 4.1. *Let $L > 0$. We denote by $\mu^{N,N}(\zeta, L)$ and $\mu^{N,D}(\zeta, L)$ the smallest eigenvalue of $-d^2/dt^2 + (t-\zeta)^2$ with Neumann condition at $t = 0$ and respectively Neumann and Dirichlet condition at $t = L$. Then $\mu^{N,D}(\zeta, L)$ is decreasing with respect to L and for any $L > 0$,*

$$\mu^{N,D}(\zeta, L) \geq \mu_1(\zeta) \geq \Theta_0. \tag{4.2}$$

For L large enough, the function $\mu^{N,N}(\zeta, \cdot)$ is increasing on $(L, +\infty)$ and

$$\mu^{N,N}(\zeta, L) \leq \mu_1(\zeta). \tag{4.3}$$

Proof. The monotonicity of $L \mapsto \mu^{N,D}(\zeta, L)$ is obvious: For $L' \geq L$, we extend the functions of $\{u \in H^1(0, L) | u(L) = 0\}$ by 0 on (L, L') and use the min-max principle.
To deal with $\mu^{N,N}(\zeta, L)$, we compute the derivative of $\mu^{N,N}(\zeta, L)$ with respect to L:

$$\partial_L \mu^{N,N}(\zeta, L) = ((L-\zeta)^2 - \mu^{N,N}(\zeta, L))|u_{\zeta,L}(L)|^2, \tag{4.4}$$

with $u_{\zeta,L}$ a normalized eigenvector associated with $\mu^{N,N}(\zeta, L)$. The positivity of the first derivative is directly deduced for L large enough. □

4.2 Finite difference scheme

Instead of looking for a normalized eigenfunction, we impose the value of Φ at $t = 0$. Therefore, we try to determine $(\zeta_0, \Phi) \in \mathbb{R}^+ \times \mathcal{D}$ such that:

$$\left\{\begin{array}{rcl} H(\zeta_0)\Phi(t) &=& \zeta_0^2\Phi(t), \quad \forall t > 0, \\ \Phi(0) &=& 1, \\ \Phi'(0) &=& 0. \end{array}\right. \tag{4.5}$$

Varying parameter ζ_0 and working on a finite interval, it is natural to look for a function φ_ζ defined on $(0, L)$ and satisfying:

$$\left\{\begin{array}{rcl} H(\zeta)\varphi_\zeta(t) &=& \zeta^2\varphi_\zeta(t), \quad \forall t \in (0, L), \\ \varphi_\zeta(0) &=& 1, \\ \varphi'_\zeta(0) &=& 0. \end{array}\right. \tag{4.6}$$

The system (4.6) is numerically solved by a finite difference scheme. Let n be the number of discretization points in $(0, L)$ and $h = L/n$. We determine recursively an approximation $\tilde{\varphi}_j^\zeta$ of $\varphi_\zeta(jh)$ for any integer $j \in \{0, \dots, n\}$. For this, $\varphi''_\zeta(jh)$ and $\varphi'_\zeta(0)$ are classically approximated respectively by $(\tilde{\varphi}_{j+1}^\zeta - 2\tilde{\varphi}_j^\zeta + \tilde{\varphi}_{j-1}^\zeta)/h^2$ and $(\tilde{\varphi}_1^\zeta - \tilde{\varphi}_0^\zeta)/h$. The boundary condition at $t = 0$ determines completely the sequence $(\tilde{\varphi}_j^\zeta)_{j=0,\dots,n}$:

$$\left\{\begin{array}{rcl} \tilde{\varphi}_0^\zeta &=& 1, \\ \tilde{\varphi}_1^\zeta &=& 1, \\ \tilde{\varphi}_{j+1}^\zeta &=& (2 + jh^3(jh - 2\zeta))\tilde{\varphi}_j^\zeta - \tilde{\varphi}_{j-1}^\zeta, \ \forall j = 1, \dots, n-1. \end{array}\right. \tag{4.7}$$

4.3 Dependence on ζ of the sequence $(\tilde{\varphi}_j^\zeta)_{j=0,\dots,n}$

The change of variables $x = t - \zeta$ in the eigenmonde equation leads to the second order differential equation:

$$u''(x) - x^2 u(x) - \zeta^2 u(x) = 0. \tag{4.8}$$

The Sturm-Liouville equation (cf [18, 20, 31, 12]) admits a basis of fundamental solutions $u_\zeta^\pm$ with $u_\zeta^- = \mathcal{O}(\exp(-x^2/2))$ and $u_\zeta^+ = \mathcal{O}(x^{-(1+\zeta^2)/2}\exp(x^2/2))$ at infinity. By a change of variable, we deduce that the solution φ_ζ of problem (4.6) is a linear combination of an exponentially increasing function denoting by f_ζ^+ and an exponentially decreasing function f_ζ^-. Moreover $f_\zeta^+ \to +\infty$ and $f_\zeta^- \to 0$ as $t \to +\infty$. Thus, there exist constants a_ζ and b_ζ which depend continously on ζ such that:

$$\varphi_\zeta = a_\zeta f_\zeta^- + b_\zeta f_\zeta^+. \tag{4.9}$$

We now use this dependence on ζ to determine Θ_0. Indeed, for $\zeta = \zeta_0$, $\varphi_{\zeta_0} = \Phi$ is integrable and then $b_{\zeta_0} = 0$. To determine Θ_0, it is then enough to find the smallest ζ such that the solution φ_ζ is bounded. Furthermore, we know that the eigenvector Φ associated with the first eigenvalue Θ_0 and normalized with $\Phi(0) = 1$, holds strictly positive. The positivity of Φ gives a criterion to select functions which constitute a good quasi-modes. Indeed, if for some ζ, the sequence $(\tilde{\varphi}_j^\zeta)$ has positive and strictly negative coefficients, then the coefficient b_ζ in the decomposition (4.9) of the associated interpolated function $\tilde{\varphi}_\zeta$ is negative and consequently $\zeta > \zeta_0$. At the opposite, the parameter b_ζ is positive for $\zeta < \zeta_0$.

4.4 Construction of quasi-modes

Discretization (4.7) gives two behaviors for $(\tilde{\varphi}_j^\zeta)_j$ (see Figures 1 and 2) and we modify coefficients of $(\tilde{\varphi}_j^\zeta)_j$ consequently:

- The sequence $(\tilde{\varphi}_j^\zeta)_j$ remains positive (see Figure 1). We determine j_0 the smallest integer where the sequence $(\tilde{\varphi}_j^\zeta)_j$ reaches its minimum and we denote $L' = j_0 h$. The restriction of $\tilde{\varphi}_\zeta$ on $(0, L')$ makes a better quasi-mode than the function defined enterely on $(0, L)$ and we have $\mu^{N,N}(\zeta, L') \leq \tilde{\mu}(\zeta, L')$ with $\tilde{\mu}(\zeta, L')$ the energy of $(\tilde{\varphi}_j^\zeta)_j$ computed on $[0, L']$. Nevertheless, as we can not compare

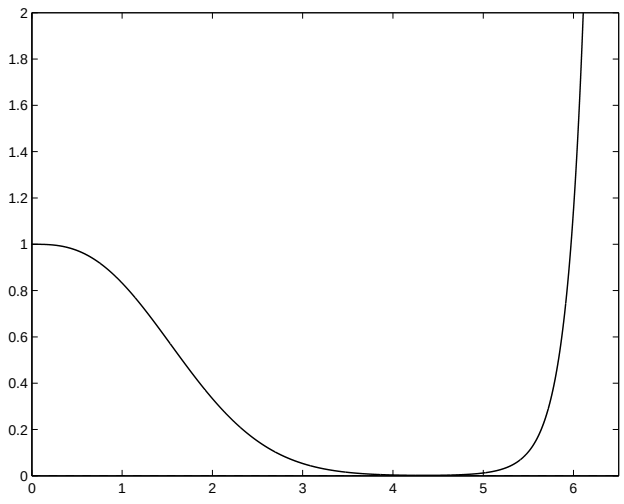

Figure 1: $(\tilde{\varphi}_j^\zeta)_j$ for $\zeta = 0.76818$.

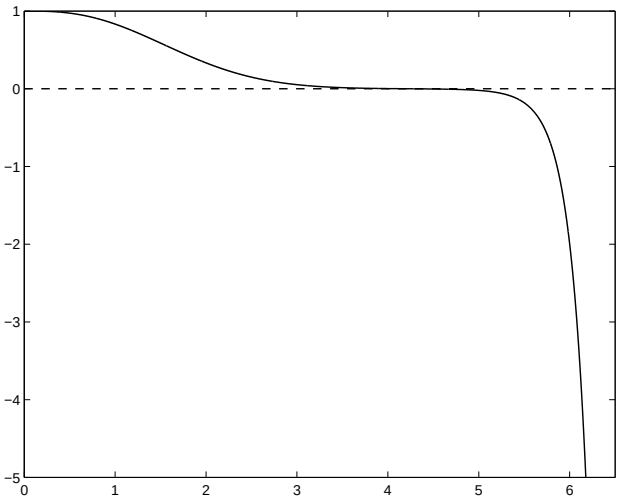

Figure 2: $(\tilde{\varphi}_j^\zeta)_j$ for $\zeta = 0.76819$.

$\mu^{N,N}(\zeta, L')$ and Θ_0 for any L', we modify the sequence by translation so that the minimum equals to 0 and dilation to keep the normalization $\tilde{\varphi}_1^\zeta = 1$. We then define the new sequence:

$$\varphi_j^\zeta = \begin{cases} \dfrac{\tilde{\varphi}_j^\zeta - \tilde{\varphi}_{j_0}^\zeta}{\tilde{\varphi}_1^\zeta - \tilde{\varphi}_{j_0}^\zeta} & \text{for } j = 1, \dots, j_0 - 1, \\ 0 & \text{for } j = j_0, \dots, n. \end{cases} \tag{4.10}$$

The energy associated with a regular interpolation of $(\varphi_j^\zeta)_j$ gives a upper-bound of Θ_0 according to Lemma 4.1. The initial sequence (see Figure 1) corresponds to $b_\zeta > 0$ in the decomposition (4.9).

- The sequence $(\tilde{\varphi}_j^\zeta)_j$ has positive and negative terms (see Figure 2). Let j_0 be the smallest integer such that $\tilde{\varphi}_{j_0}^\zeta < 0$. We set

$$\varphi_j^\zeta = \begin{cases} \tilde{\varphi}_j^\zeta & \text{for } j = 1, \dots, j_0 - 1, \\ 0 & \text{for } j = j_0, \dots, n. \end{cases} \tag{4.11}$$

Lemma 4.1 bounds from above Θ_0 by the energy of the function constructed from $(\varphi_j^\zeta)_j$. For the initial sequence, $b_\zeta < 0$ in the decomposition (4.9).

Let us now be more explicit about the interpolation of the sequence $(\varphi_j^\zeta)_j$ to construct the quasi-mode φ_ζ. If we make an interpolation of $(\varphi_j^\zeta)_j$ by a piecewise linear function, this function does not belong to $H^2(\mathbb{R}^+)$ and is necessarily not in the operator domain $\mathcal{D}$. So we interpolate $(\varphi_j^\zeta)_j$ on $[0, L]$ by a piecewise polynomial function φ_ζ of degree 2 defined by:

$$\forall j = 0, \dots, n-1,\ \forall t \in [jh, (j+1)h], \quad \varphi_\zeta(t) = \alpha_j (t - jh)^2 + \tau_j (t - jh) + \varphi_j^\zeta, \tag{4.12}$$

with $\tau_0 = 0$ and

$$\begin{cases} \tau_{j+1} &= 2\dfrac{\varphi_{j+1}^\zeta - \varphi_j^\zeta}{h} - \tau_j, \\ \alpha_j &= \dfrac{\varphi_{j+1}^\zeta - \varphi_j^\zeta}{h^2} - \dfrac{\tau_j}{h}. \end{cases} \tag{4.13}$$

We notice that $\tau_j = \varphi'_\zeta(jh)$. We extend φ_ζ by 0 on $(L, +\infty)$. With such a construction, φ_ζ is continuous, its derivative is continuous, piecewise linear and the second derivative is constant on $[jh, (j+1)h]$ for $j = 0, \dots, n-1$. Furthermore, any computations (norm, energy, ...) are explicit. With the change of variables $x = t - jh$, we have:

$$\begin{aligned} ||\varphi_\zeta||^2_{L^2(\mathbb{R}^+)} &= \sum_{j=0}^{n-1} \int_0^h |\alpha_j x^2 + \tau_j x + \varphi_j^\zeta|^2 \, dx \\ &= h \sum_{j=0}^{n-1} \left(\frac{h^4}{5}\alpha_j^2 + \frac{h^3}{2}\alpha_j\tau_j + \frac{h^2}{3}(\tau_j^2 + 2\alpha_j\varphi_j^\zeta) + h\tau_j\varphi_j^\zeta + (\varphi_j^\zeta)^2 \right). \end{aligned} \tag{4.14}$$

Let us compute the energy of φ_ζ:

$$||\varphi'_\zeta||^2_{L^2(\mathbb{R}^+)} = \sum_{j=0}^{n-1} \int_0^h |2\alpha_j x + \tau_j|^2 \, dx = h \sum_{j=0}^{n-1} \left(\frac{4}{3}h^2\alpha_j^2 + 2h\alpha_j\tau_j + \tau_j^2 \right). \tag{4.15}$$

To compute $\displaystyle\int_{\mathbb{R}^+} (t-\zeta)^k |\varphi_\zeta(t)|^2 \, dt$, we define $\delta_j = jh - \zeta$. Put $x = t - jh$ gives:

$$\int_{\mathbb{R}^+} (t-\zeta)^k |\varphi_\zeta(t)|^2 dt = \sum_{j=0}^{n-1} \int_0^h (x+\delta_j)^k |(\alpha_j x^2 + \tau_j x + \varphi_j^\zeta|^2 \, dx.$$

Consequently

$$\begin{aligned} \int_{\mathbb{R}^+} (t-\zeta)|\varphi_\zeta(t)|^2 dt &= h \sum_{j=0}^{n-1} \left(\frac{h^5}{6}\alpha_j^2 + \frac{h^4}{5}\alpha_j(2\tau_j + \alpha_j\delta_j) + \frac{h^3}{4}(\tau_j^2 + 2\alpha_j\varphi_j^\zeta + 2\alpha_j\tau_j\delta_j) \right. \\ &\quad \left. + \frac{h^2}{3}(2\tau_j\varphi_j^\zeta + 2\alpha_j\varphi_j^\zeta\delta_j + \tau_j^2\delta_j) + \frac{h}{2}((\varphi_j^\zeta)^2 + 2\tau_j\delta_j\varphi_j^\zeta) + (\varphi_j^\zeta)^2\delta_j \right). \end{aligned} \tag{4.16}$$

$$\begin{aligned} ||(t-\zeta)\varphi_\zeta||^2_{L^2(\mathbb{R}^+)} &= h \sum_{j=0}^{n-1} \left(\frac{h^6}{7}\alpha_j^2 + \frac{h^5}{3}\alpha_j(\tau_j + \alpha_j\delta_j) + \frac{h^4}{5}((\tau_j + \alpha_j\delta_j)^2 + 2\alpha_j(\varphi_j^\zeta + \tau_j\delta_j)) \right. \\ &\quad + \frac{h^3}{2}(\alpha_j\varphi_j^\zeta\delta_j + (\tau_j + \alpha_j\delta_j)(\varphi_j^\zeta + \tau_j\delta_j)) \\ &\quad \left. + \frac{h^2}{3}((\varphi_j^\zeta + \tau_j\delta_j)^2 + 2\varphi_j^\zeta\delta_j(\tau_j + \alpha_j\delta_j)) + h\varphi_j^\zeta\delta_j(\varphi_j^\zeta + \tau_j\delta_j) + (\varphi_j^\zeta)^2\delta_j^2 \right) \end{aligned} \tag{4.17}$$

Expressions (4.14), (4.15) and (4.17) present the main advantage to be exact. Let $\breve{\mu}(\zeta)$ be the Rayleigh quotient of φ_ζ:

$$\breve{\mu}(\zeta) = \frac{||\varphi'_\zeta||^2_{L^2(\mathbb{R}^+)} + ||(t-\zeta)\varphi_\zeta||^2_{L^2(\mathbb{R}^+)}}{||\varphi_\zeta||^2_{L^2(\mathbb{R}^+)}}. \tag{4.18}$$

To apply Theorem 3.2, we have to estimate the residus $\|r_\zeta\|^2_{L^2(\mathbb{R}^+)}$ with $r_\zeta := (H(\zeta) - \breve{\mu}(\zeta))\varphi_\zeta$. As we extend φ_ζ by 0 on $(L, +\infty)$, we have just to compute the norms on $(0, L)$. We notice that for any $j = 0, \dots, n-1$ and $t \in [jh, (j+1)h]$, we get:

$$r_\zeta(t) = -2\alpha_j + ((t-\zeta)^2 - \breve{\mu}(\zeta))(\alpha_j(t-jh)^2 + \tau_j(t-jh) + \varphi_j^\zeta).$$

As in (4.14), (4.15) and (4.17), the computation of $\|r_\zeta\|_{L^2(\mathbb{R}^+)}$ is explicit. For $j = 0, \dots, n-1$, we define:

$$\begin{array}{rclrcl} r_{0,j} &=& \varphi_j^\zeta(\delta_j^2 - \breve{\mu}(\zeta)) - 2\alpha_j, & r_{1,j} &=& 2\varphi_j^\zeta\delta_j + \tau_j\,(\delta_j^2 - \breve{\mu}(\zeta)), \\ r_{2,j} &=& \varphi_j^\zeta + 2\tau_j\delta_j + \alpha_j(\delta_j^2 - \breve{\mu}(\zeta)), & r_{3,j} &=& \tau_j + 2\alpha_j\delta_j. \end{array}$$

A change of variables gives:

$$||r_\zeta||^2_{L^2(\mathbb{R}^+)} = h\sum_{j=0}^{n-1}\left(\frac{h^8}{9}\alpha_j^2 + \frac{h^7}{4}\alpha_j r_{3,j} + \frac{h^6}{7}(2\alpha_j r_{2,j} + r_{3,j}^2) + \frac{h^5}{3}(\alpha_j r_{1,j} + r_{3,j}r_{2,j})\right.$$
$$\left. + \frac{h^4}{5}(2\alpha_j r_{0,j} + 2r_{3,j}r_{1,j} + r_{2,j}^2) + \frac{h^3}{2}(r_{3,j}r_{0,j} + r_{2,j}r_{1,j}) + \frac{h^2}{3}(2r_{2,j}r_{0,j} + r_{1,j}^2) + hr_{1,j}r_{0,j} + r_{0,j}^2\right). \tag{4.19}$$

4.5 Algorithm and results

We described how interpolate the sequence (φ_j^ζ) to construct an appropriate quasi-mode and proposed criteria to estimate Θ_0. Let us now explain the algorithm to determine Θ_0 accurately.

Algorithme 4.2.

1. *We choose a length L for the finite interval and a step h for the discretization for finite difference method.*
2. *We initialize a value for ζ with n decimals.*
3. *We construct the sequence (φ_j^ζ) by* (4.7)*.*
4. *If $(\varphi_j^\zeta)_j$ has negative coefficients, we return to the first step with a smaller value for ζ. Otherwise, we modify $(\varphi_j^\zeta)_j$ according to* (4.10)*.*
5. *While $(\varphi_j^\zeta)_j$ has only positive coefficients,*
   (a) *we define the function φ_ζ by relations* (4.12) *and* (4.13)*,*
   (b) *we compute the L^2-norm of φ_ζ thanks to* (4.14) *and deduce the value of $\varphi_\zeta(0)$ after normalization,*
   (c) *we compute the energy $\breve{\mu}(\zeta)$ associated with φ_ζ thanks to relations* (4.14)*,* (4.15)*,* (4.17) *and* (4.18)*,*
   (d) *we estimate the residus $\|r_\zeta\|_{L^2(\mathbb{R}^+)} = ||(H(\zeta) - \breve{\mu}(\zeta))\varphi_\zeta||_{L^2(\mathbb{R}^+)}$ with relation* (4.19)*,*
   (e) *we raise ζ of $10^{-(n+1)}$.*
6. *We go back to the first step with the last value of ζ with the $n+1$ decimals for which the sequence (φ_j^ζ) has only positive terms.*

Table 1 sums up the results obtained with this algorithm: we choose $h = 1/26000$ and $L = 7$. In each part, results given at the last line correspond to a function φ_ζ which takes negative values. The last colum gives $\breve{a}_1 = \varphi_j^\zeta(0)\sqrt{\zeta}$ which aims to approximate the constant a_1 in the asymptotics expansion (2.2).
Of course, a dichotomy method should be faster but we aim at determining decimals step by step.

ζ	$\breve{\mu}(\zeta)$	$\|r_\zeta\|_{L^2(\mathbb{R}^+)}$	$\min_j \tilde{\varphi}_j^\zeta$	$\varphi_j^\zeta(0)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\alpha}_1$
0.761	0.611266093453	4.009e-01	1.194e-01	0.900663817274	-3.215e-02	0.796379904345
0.762	0.608936310293	1.020e+00	1.098e-01	0.898608814736	-2.829e-02	0.793804656654
0.763	0.606516822831	1.017e+00	9.947e-02	0.896392499552	-2.435e-02	0.791059092651
0.764	0.603984720795	6.395e-01	8.826e-02	0.893963619858	-2.029e-02	0.788090937531
0.765	0.601304928182	3.144e-01	7.585e-02	0.891237476384	-1.608e-02	0.784814703651
0.766	0.598417489656	5.889e-01	6.162e-02	0.888054169479	-1.166e-02	0.781071024723
0.767	0.595197681398	4.774e-01	4.408e-02	0.884029104176	-6.909e-03	0.776482855100
0.768	0.591201356836	1.450e-01	1.618e-02	0.877276976649	-1.377e-03	0.769255459845
0.769	0.592445239556	3.394e+03	-6.828e+04	0.873788252239	-1.084e-03	0.766599011697
0.7681	0.590667836454	7.786e-02	1.065e-02	0.875868144705	-6.902e-04	0.767846770648
0.7682	0.590132204890	1.014e+02	-1.375e+03	0.873060748639	-9.649e-07	0.765212036038
0.76811	0.590609794273	1.296e-01	9.960e-03	0.875688760473	-6.168e-04	0.767670649972
0.76812	0.590550467623	1.188e-01	9.220e-03	0.875497050852	-5.421e-04	0.767483313548
0.76813	0.590489644618	7.154e-02	8.424e-03	0.875290014381	-4.659e-04	0.767282062448
0.76814	0.590427028617	6.304e-02	7.555e-03	0.875063164549	-3.880e-04	0.767062868811
0.76815	0.590362189929	6.035e-02	6.587e-03	0.874809289953	-3.078e-04	0.766819273601
0.76816	0.590294414679	1.028e-01	5.472e-03	0.874515187142	-2.246e-04	0.766539474233
0.76817	0.590222359089	4.568e-02	4.101e-03	0.874151227495	-1.372e-04	0.766197068734
0.76818	0.590142134621	3.433e-02	2.059e-03	0.873603510214	-4.162e-05	0.765690971474
0.76819	0.590133901819	4.380e+02	-5.339e+02	0.873050162751	-1.803e-05	0.765203307905
0.768181	0.590133151271	2.157e-02	1.743e-03	0.873518100671	-3.110e-05	0.765613198575
0.768182	0.590123767394	2.354e-02	1.362e-03	0.873415004924	-2.018e-05	0.765519794934
0.768183	0.590113720068	1.926e-02	8.410e-04	0.873273226533	-8.599e-06	0.765392272906
0.768184	0.590107683499	1.044e+02	-2.922e+01	0.873043549605	-1.026e-06	0.765189012531
0.7681831	0.590112657421	1.844e-02	7.719e-04	0.873254392844	-7.382e-06	0.765375421300
0.7681832	0.590111566559	1.475e-02	6.959e-04	0.873233650004	-6.138e-06	0.765356887258
0.7681833	0.590110458701	9.661e-03	6.117e-04	0.873210676290	-4.876e-06	0.765336392445
0.7681834	0.590109315459	9.490e-03	5.146e-04	0.873184139830	-3.579e-06	0.765312763566
0.7681835	0.590108138271	9.388e-03	3.972e-04	0.873152039956	-2.249e-06	0.765284247584
0.7681836	0.590106879933	3.373e-03	2.296e-04	0.873106158483	-8.366e-07	0.765243626286
0.7681837	0.590106497981	5.655e+01	-3.973e+00	0.873043196601	-3.010e-07	0.765188318823
0.76818361	0.590106749563	4.694e-03	2.067e-04	0.873099863951	-6.909e-07	0.765238067107
0.76818362	0.590106611147	3.686e-03	1.799e-04	0.873092510715	-5.371e-07	0.765231577409
0.76818363	0.590106470242	2.554e-03	1.488e-04	0.873083997748	-3.808e-07	0.765224070445
0.76818364	0.590106331385	2.147e-03	1.120e-04	0.873073906942	-2.266e-07	0.765215181231
0.76818365	0.590106179248	1.028e-03	5.386e-05	0.873057934293	-5.912e-08	0.765201132509
0.76818366	0.590106139402	6.353e+00	-5.838e-01	0.873043147328	-3.912e-09	0.765188159395
0.768183651	0.590106163301	1.082e-03	4.455e-05	0.873055377601	-4.164e-08	0.765198886499
0.768183652	0.590106145104	9.452e-04	3.139e-05	0.873051762303	-2.190e-08	0.765195711932
0.768183653	0.590106127974	4.699e-04	1.125e-05	0.873046229081	-3.238e-09	0.765190856726
0.768183654	0.590106128318	4.673e+00	-7.211e-02	0.873043139630	-2.045e-09	0.765188149055
0.7681836531	0.590106125876	1.536e-04	5.953e-06	0.873044774598	-9.864e-10	0.765189581249
0.7681836532	0.590106125048	5.487e-01	-3.761e-03	0.873043138584	-4.328e-12	0.765188147079

Table 1: Results obtained with Algorithm 4.2.

4.6 Estimates of the second eigenvalue

To apply Theorem 3.2, we need an estimate of the second eigenvalue $\mu_2(\zeta_0)$ of $H(\zeta_0)$. For this point, we do not need to be very accurate and so we consider the matrix A^ζ defined by the discretization of $H(\zeta)$ for $\zeta \in [0.76818, 076819]$. If we denote by $A^\zeta_{i,j}$ the coefficients of the matrix A^ζ, we have:

$$\begin{cases} A^\zeta_{1,1} = \dfrac{1}{h^2} + \zeta^2, \quad A^\zeta_{1,2} = -\frac{1}{2}, \\ A^\zeta_{j,j-1} = -\frac{1}{h^2}, \quad A^\zeta_{j,j} = \frac{2}{h^2} + ((j-1)h - \zeta)^2, \quad A^\zeta_{j,j+1} = -\frac{1}{h^2}, \quad \text{for } j = 1, \dots, n-1, \\ A^\zeta_{n,n-1} = -\frac{1}{h^2}, \quad A^\zeta_{n,n} = \frac{1}{h^2} + ((n-1)h - \zeta)^2, \\ A^\zeta_{i,j} = 0 \qquad \text{elsewhere.} \end{cases}$$

We compute the second eigenvalue and obtain $\mu_2(\zeta_0) \geq 3.315$. Theoretically, we can bound from above $\mu_2(\zeta_0)$ by the smallest first eigenvalue of the Dirichlet realization of $D_t^2 + (t-\zeta)^2$ on the half-line. We obtain $\mu_2(\zeta_0) \geq 1$.

4.7 Accurate estimate for Θ_0 and $\Phi(0)$

Lemma 4.3. *We have this first coarse bound:*

$$0.5 \leq \Theta_0 = \zeta_0^2 \leq 1.$$

Proof. The upper-bound was proved in [12] and recalled in Proposition 1.1. Let us prove the lower-bound. For any $\zeta \in \mathbb{R}$, we write

$$1 = \mu_1(\zeta) \leq \langle H(\zeta)\Phi, \Phi\rangle = \langle H(\zeta_0)\Phi, \Phi\rangle + 2(\zeta_0 - \zeta)\int_{\mathbb{R}^+} (t-\zeta_0)|\Phi(t)|^2 dt + (\zeta_0 - \zeta)^2.$$

Choosing $\zeta = 0$ and using Proposition 1.1, we deduce the lower-bound. □

We apply Algorithm 4.2 for h such that $1/h \in \{100 \times k, k = 10, \dots, 40\}$ and for $L = 7, 8, 9, 10$. For each value, we obtain characteristic values as in Table 1 and we complete this table by computing the lower-bound of Θ_0 given by Theorem 3.2, a lower-bound and a upper-bound for $\Phi(0)$ given in Theorem 3.5. To make these computations, we need a lower-bound of $|\zeta - \zeta_0|$. We start with the coarse estimate of Lemma 4.3 and we improve this estimate at each step of the algorithm with the new bounds of Θ_0. Using the upper-bound $\mu_2(\zeta_0) \geq 3.315$, we obtain

Proposition 4.4.

$$0.590106124587 \leq \Theta_0 \leq 0.590106124951,$$

$$0.872997 \leq \Phi(0) \leq 0.873090.$$

This proposition estimates $\Theta_0 \simeq 0.590106125$ with an error less than 10^{-9} and of $\Phi(0) \simeq 0.87304$ at 5×10^{-4}.

5 Finite element method

In this section, we use a finite element method to analyze the dependence of $\mu_k(\zeta)$ with ζ. We compute the eigenvalues of the operator $D_t^2 + (t-\zeta)^2$ on $[0, L]$ with Dirichlet condition on $t = L$ and Neumann condition on $t = 0$. The computed eigenvalues $\breve{\mu}_k(\zeta)$ give a upper-bound of $\mu_k(\zeta)$.
Figure 3 illustrates the fact that the minimum of $\zeta \mapsto \mu_k(\zeta)$ is achieved on the curve $\zeta \mapsto \zeta^2$. We observe also the convergence of $\zeta \mapsto \mu_k(\zeta)$ to $2k-1$ as $\zeta \to +\infty$. For these computations, we use a finite element method with 10 elements of degree $\mathbb{Q}_{10}$ on $[0, 10]$.

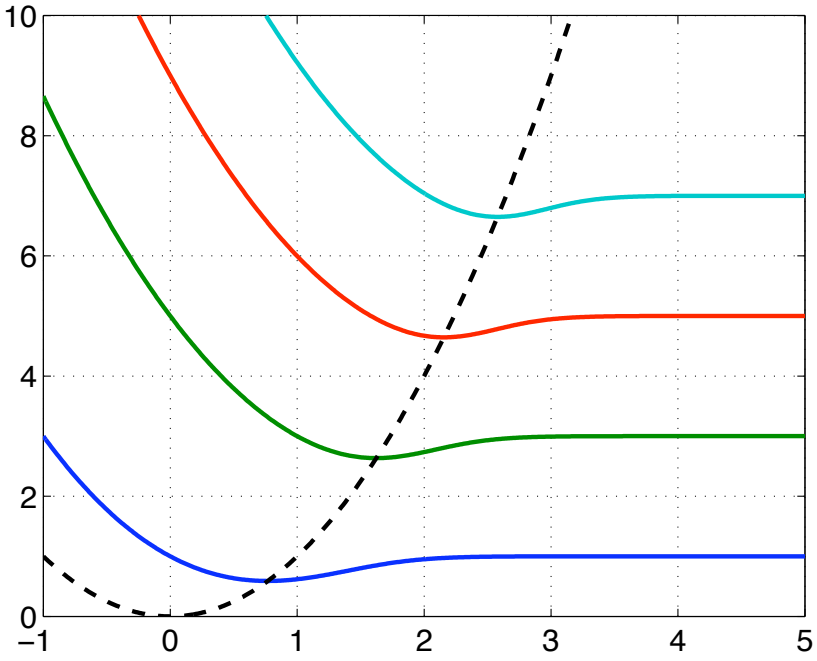

Figure 3: $\mu_k(\zeta)$ for $\zeta \in [-1, 5]$, $k = 1, \ldots, 4$ and curve $\zeta \mapsto \zeta^2$ in dashed line.

Let us now use the finite element method to approximate Θ_0 and Φ_0. With this method, we do not have exact estimate of the error but only a upper-bound for Θ_0. To determine accurately ζ_0, we use a finite element method of degree $\mathbb{Q}_8$ or $\mathbb{Q}_{10}$ and $nbel$ elements. The computational domain is $[0, L]$ and we impose Dirichlet condition on $t = L$. We compute the first eigenvalue $\breve{\mu}(\zeta)$ and compare it with ζ^2. These computations give also an accurate value for $\Phi(0)$ and a_1. Let $\breve{\varphi}_\zeta$ be the computed normalized positive eigenvector associated with $\breve{\mu}(\zeta)$. Then, we compute $\breve{a}_1 = \sqrt{\zeta}\breve{\varphi}_\zeta(0)$. Table 2 gives the results of these computations. In particular we obtain approximation for Θ_0, $\Phi(0)$ and a_1:

$$\breve{\Theta}_0 = 0.590106125, \qquad \breve{\Phi}(0) = 0.873043139, \qquad \breve{a}_1 = 0.765188147.$$

Notice that computed values $\breve{\mu}(\zeta)$ in Table 2 provide better upper-bounds for Θ_0 than in Proposition 4.4.

L	nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
7	70	8	0.768183653140	0.590106124950497	1.0e-12	0.873043138513904	0.765188146985675
7	70	8	0.768183653141	0.590106124949945	3.1e-12	0.873043138513613	0.765188146985918
7	70	10	0.768183653140	0.590106124952671	-1.2e-12	0.873043138513392	0.765188146985226
7	70	10	0.768183653141	0.590106124952394	6.6e-13	0.873043138513095	0.765188146985464
8	100	8	0.768183653140	0.590106124949903	1.6e-12	0.873043138513603	0.765188146985411
8	100	8	0.768183653141	0.590106124949336	3.7e-12	0.873043138513245	0.765188146985595
8	100	10	0.768183653140	0.590106124952819	-1.3e-12	0.873043138513197	0.765188146985055
8	100	10	0.768183653141	0.590106124952989	6.3e-14	0.873043138512816	0.765188146985219
9	90	8	0.768183653140	0.590106124950496	1.0e-12	0.873043138513906	0.765188146985677
9	90	8	0.768183653141	0.590106124949943	3.1e-12	0.873043138513614	0.765188146985919
9	90	10	0.768183653140	0.590106124952671	-1.2e-12	0.873043138513392	0.765188146985226
9	90	10	0.768183653141	0.590106124952389	6.6e-13	0.873043138513095	0.765188146985464
10	100	8	0.768183653140	0.590106124950496	1.0e-12	0.873043138513906	0.765188146985677
10	100	8	0.768183653141	0.590106124949948	3.1e-12	0.873043138513614	0.765188146985919
10	100	10	0.768183653140	0.590106124952670	-1.2e-12	0.873043138513391	0.765188146985225
10	100	10	0.768183653141	0.590106124952392	7e-13	0.873043138513095	0.765188146985464
12	110	8	0.768183653140	0.590106124948481	3.0e-12	0.873043138514059	0.765188146985811
12	110	8	0.768183653141	0.590106124948091	5.0e-12	0.873043138513689	0.765188146985984
12	110	10	0.768183653140	0.590106124949202	2.3e-12	0.873043138513313	0.765188146985156
12	110	10	0.768183653141	0.590106124949127	3.9e-12	0.873043138513068	0.765188146985440
15	200	8	0.768183653140	0.590106124951757	-2e-13	0.873043138513820	0.765188146985601
15	200	8	0.768183653141	0.590106124951625	1.4e-12	0.873043138513444	0.765188146985769
15	200	10	0.768183653140	0.590106124949226	2.3e-12	0.873043138513258	0.765188146985109
15	200	10	0.768183653141	0.590106124949262	3.8e-12	0.873043138512969	0.765188146985353

Table 2: Computation with the finite element method.

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