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HARMONIC OSCILLATORS WITH NEUMANN CONDITION ON THE HALF-LINE

Virginie Bonnaillie-Noël

IRMAR, ENS Cachan Bretagne, Univ. Rennes 1, CNRS, UEB
av Robert Schuman, F-35170 Bruz, France

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Abstract. We consider the spectrum of the family of one-dimensional self-adjoint operators $-\mathrm{d}^2/\mathrm{d}t^2+(t-\zeta)^2$, $\zeta\in\mathbb{R}$ on the half-line with Neumann boundary condition. It is well known that the first eigenvalue $\mu(\zeta)$ of this family of harmonic oscillators has a unique minimum when $\zeta\in\mathbb{R}$. This paper is devoted to the accurate computations of this minimum Θ_0 and $\Phi(0)$ where Φ is the associated positive normalized eigenfunction. We propose an algorithm based on finite element method to determine this minimum and we give a sharp estimate of the numerical accuracy. We compare these results with a finite element method.

1. Introduction.

1.1. Notation.

In this paper, we are interested in accurate estimates of some spectral quantities of the family of one-dimensional harmonic oscillators with Neumann boundary condition. Let us define this family. For any $\zeta\in\mathbb{R}$, we consider the operator $-\mathrm{d}^2/\mathrm{d}t^2+(t-\zeta)^2$ on $(0,+\infty)$. Its Friedrichs extension from $C_0^\infty([0,+\infty))$ is denoted by $H(\zeta)$ and defined on

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

Thus we notice that the family $H(\zeta)$, $\zeta\in\mathbb{R}$, has a common Neumann domain. We denote by $\mu_k(\zeta)$ the k-th eigenvalue of the harmonic oscillator $H(\zeta)$ arranged in the ascending order with the multiplicity taken into account. The spectral properties of this family of operators have been studied in [12]. Let us recall some of them in the following proposition.

Proposition 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 eigenfunction associated with $\mu_1(\zeta_0)$, then*

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

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

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1.2. **Motivation .** Even if an accurate computation of the spectral quantities of the family of harmonic oscillators $H(\zeta)$, $\zeta \in \mathbb{R}$, can be interessant by itself, the parameters Θ_0 and $\Phi(0)$ appear frequently in the analysis of the superconductivity modelled by Ginzburg-Landau theory. Let us recall now some results in this way. Let $\Omega \subset \mathbb{R}^2$ be a bounded simply-connected domain with Lipschitz boundary. The Ginzburg-Landau functional involves a wave function ψ and a magnetic potential $\mathcal{A}$ and reads

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

for any $(\psi,\mathcal{A}) \in W^{1,2}(\Omega;\mathbb{C}) \times \{\mathcal{A} = \mathcal{A}_0 + \tilde{\mathcal{A}} \text{ with } \tilde{\mathcal{A}} \in \dot{H}^1(\mathbb{R}^2,\mathbb{R}^2), \mathrm{div}\,\tilde{\mathcal{A}} = 0\}$, where $\mathcal{A}_0(x) = 1/2(-x_2,x_1)$. We use the notation $\dot{H}^1(\mathbb{R}^2)$ for the homogeneous Sobolev spaces. The function ψ is called the order parameter and its modulus informs us about the localization of the superconductivity. The parameter κ is a characteristic of the material and we only consider superconductors of type II for which κ is large. The physical interessant states are the minimizers of the functional $\mathcal{E}_{\kappa,H}$ and they satisfy the Euler-Lagrange equation. When H is very large, the unique minimizer is the trivial state $(0,\mathcal{A}_0)$, called the normal state, and there is no superconduting property for the sample in this case. Decreasing the applied magnetic field, the sample becomes superconducting. Thus 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 first rigorous definition of the critical field H_{C_3} appeared in [28]. 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 (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*

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

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 3 (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 4 (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 $(i\nabla + \mathcal{A}_0)^2$ 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 5 (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 exists $(m_j^{(n)})_{j\geq 1}$ such that $\mu^{(n)}(h)$ admits the following asymptotic expansion (for $h \to 0$):*

$$\mu^{(n)}(h) \sim h\Lambda_n + h\sum_{j=1}^{\infty} m_j^{(n)} h^{j/2}.$$

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

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

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 6 (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*

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

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 $\theta \neq 0$, 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 eigenfunctions. They also analyze the asymptotics when $\theta \to 0$. In particular, they prove the following result:

Proposition 7. *We have the following upper-bound for the* n*-th eigenvalue* $\sigma_n(\theta)$ *of* $\mathcal{L}_\theta$*:*

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

For all $n \geq 1$*, there exists a sequence* $(\beta_j^{(n)})_{j\geq 0}$ *such that* $\sigma_n(\theta)$ *is an eigenvalue for* θ *small enough and admits the following asymptotic expansion (for* $\theta \to 0$*):*

$$\sigma_n(\theta) \sim \Theta_0 - (2n-1)\sqrt{\frac{\mu''(\zeta_0)}{2}}\theta + \theta^2\sum_{j=0}^{\infty}\beta_j^{(n)}\theta^j. \tag{2}$$

If we denote by $n(\theta)$ the number of eigenvalues of $\mathcal{L}_\theta$ below the essential spectrum, we have with (1):

$$n(\theta) \geq \frac{1 - \Theta_0\cos\theta}{2\sin\theta} + \frac{1}{2}. \tag{3}$$

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.

1.3. **Main results.** 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 finite element methods.

To estimate the numerical accuracy, we first establish in Section 2 error estimates on eigenmodes: Theorem 2.1 quantifies the gap between the eigenvalue Θ_0 and the energy associated with a quasi-mode for the operator $H(\zeta)$. In Theorem 2.2, 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 2.3 an estimate of $\Phi(0)$. In Section 3, 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 3.5 and obtain an accurate approximation of Θ_0 and $\Phi(0)$:

Theorem 1.1.

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

Section 4 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 $-\mathrm{d}^2/\mathrm{d}t^2 + (t-\zeta)^2$ on a symmetric interval using a finite difference method.

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

$$q_1^\zeta(u) = \int_{\mathbb{R}^+} (t-\zeta)|u(t)|^2 \,\mathrm{d}t, \qquad q_2^\zeta(u) = \int_{\mathbb{R}^+} (t-\zeta)^2|u(t)|^2 \,\mathrm{d}t. \tag{4}$$

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

$$\eta_\zeta = \breve{\mu}(\zeta) + 2(\zeta-\zeta_0)q_1^\zeta(\varphi_\zeta) + (\zeta-\zeta_0)^2, \tag{5}$$

$$a_\zeta = \left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2|\zeta-\zeta_0|\sqrt{q_2^\zeta(\varphi_\zeta)}\right)^2. \tag{6}$$

With these Notation 2, 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 2.1. *Let $\zeta \in \mathbb{R}$ and φ_ζ be a normalized positive function of $\mathcal{D}$. With Notation 2, we assume*

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

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

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

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

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

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

$$\eta - \frac{\varepsilon^2}{\beta-\eta} \leq \lambda \leq \eta + \frac{\varepsilon^2}{\eta-\alpha}. \tag{7}$$

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 (5). The assumption $\varepsilon^2 < (\beta-\eta)(\eta-\alpha)$ is then obviously fulfilled. Consider now ε^2.

$$\begin{aligned}
\varepsilon^2 &= \int_{\mathbb{R}^+} \left| r_\zeta(t) + 2(\zeta-\zeta_0)(t-\zeta)\varphi_\zeta(t) - 2(\zeta-\zeta_0) q_1^\zeta(\varphi_\zeta)\varphi_\zeta(t) \right|^2 \mathrm{d}t \\
&\leq \left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2|\zeta-\zeta_0| \sqrt{q_2^\zeta(\varphi_\zeta)} \right)^2 - 4(\zeta-\zeta_0)^2 q_1^\zeta(\varphi_\zeta)^2.
\end{aligned} \tag{8}$$

Temple inequality (7) 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 2.2. *Let $\zeta \in \mathbb{R}$ and φ_ζ be a normalized and positive function of $\mathcal{D}$. With Notation 2, 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 8. *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. Theorem 2.2 We apply Proposition 8 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

$$d(E,F) = ||\varphi_\zeta - \langle\varphi_\zeta,\Phi\rangle\Phi||_{L^2(\mathbb{R}^+)} = \sqrt{1-|\langle\varphi_\zeta,\Phi\rangle|^2} \geq \frac{1}{\sqrt{2}}\|\varphi_\zeta - \Phi\|_{L^2(\mathbb{R}^+)}. \quad (9)$$

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 $\langle r_\zeta, \varphi_\zeta\rangle = 0$:

$$\begin{aligned} ||\tilde{r}_\zeta||^2_{L^2(\mathbb{R}^+)} &= \int_{\mathbb{R}^+} \left|2(\zeta-\zeta_0)(t-\zeta)\varphi_\zeta(t) + (\zeta-\zeta_0)^2\varphi_\zeta(t) + r_\zeta(t)\right|^2 \,\mathrm{d}t \\ &\leq a_\zeta + (\zeta-\zeta_0)^3\left(\zeta - \zeta_0 + 4q_1^\zeta(\varphi_\zeta)\right). \end{aligned} \quad (10)$$

Relations (9), (10) and Proposition 8 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:

$$\langle H(\zeta_0)(\Phi-\varphi_\zeta), \Phi - \varphi_\zeta\rangle_{L^2(\mathbb{R}^+)} \geq \|\Phi' - \varphi'_\zeta\|^2_{L^2(\mathbb{R}^+)}. \quad (11)$$

On the other hand,

$$\begin{aligned} \langle H(\zeta_0)(\varphi_\zeta - \Phi), \varphi_\zeta - \Phi\rangle_{L^2(\mathbb{R}^+)} &= \langle H(\zeta_0)\varphi_\zeta, \varphi_\zeta\rangle_{L^2(\mathbb{R}^+)} - 2\Theta_0\langle\Phi,\varphi_\zeta\rangle_{L^2(\mathbb{R}^+)} + \Theta_0 \\ &= \eta_\zeta - \Theta_0 + \Theta_0\|\Phi - \varphi_\zeta\|^2_{L^2(\mathbb{R}^+)}. \end{aligned} \quad (12)$$

We deduce from (11), (12) and Theorem 2.1 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 2.3. *Using the same notation and assumptions as Theorem 2.2, we have*

$$|\Phi(0) - \varphi_\zeta(0)|^2 \leq 2\|\Phi - \varphi_\zeta\|_{L^2(\mathbb{R}^+)}\, \|\Phi' - \varphi'_\zeta\|_{L^2(\mathbb{R}^+)}. \quad (13)$$

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

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

We conclude with the Cauchy-Schwarz inequality. □

3. **Construction of a quasi-mode by a finite difference method.** Theorem 2.1 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. Comparaison with problem on 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.

3.1. **Comparaison with problem on a finite interval.** Numerically, we have to work on a finite interval. Let us compare the fundamental energy on a finite interval and Θ_0.

Lemma 3.1. *Let $L > 0$. We denote by $\mu^{N,N}(\zeta, L)$ and $\mu^{N,D}(\zeta, L)$ the smallest eigenvalue of $-\mathrm{d}^2/\mathrm{d}t^2 + (t-\zeta)^2$ 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 $L > 0$,

$$\mu^{N,D}(\zeta, L) \geq \mu_1(\zeta) \geq \Theta_0. \tag{14}$$

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

$$\mu^{N,N}(\zeta, L) \leq \mu_1(\zeta). \tag{15}$$

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:

$$\partial_L \mu^{N,N}(\zeta, L) = ((L-\zeta)^2 - \mu^{N,N}(\zeta, L))|u_{\zeta,L}(L)|^2, \tag{16}$$

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

3.2. **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:

$$\left\{ \begin{array}{rcl} H(\zeta_0)\Phi(t) & = & \zeta_0^2 \Phi(t), \quad \forall t > 0, \\ \Phi(0) & = & 1, \\ \Phi'(0) & = & 0. \end{array} \right. \tag{17}$$

Varying parameter ζ_0, it is natural to look for a function φ_ζ and satisfying:

$$\left\{ \begin{array}{rcl} H(\zeta)\varphi_\zeta(t) & = & \zeta^2 \varphi_\zeta(t), \quad \forall t > 0, \\ \varphi_\zeta(0) & = & 1, \\ \varphi'_\zeta(0) & = & 0. \end{array} \right. \tag{18}$$

The system (18) is numerically solved by a finite difference scheme. Let h be step of discretization. We determine recursively an approximation $\tilde{\varphi}_j^\zeta$ of $\varphi_\zeta(jh)$ for any integer $j \geq 0$. 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 $(\tilde{\varphi}_j^\zeta)_{j \geq 0}$:

$$\left\{ \begin{array}{rcl} \tilde{\varphi}_0^\zeta & = & 1, \\ \tilde{\varphi}_1^\zeta & = & 1, \\ \tilde{\varphi}_{j+1}^\zeta & = & (2 + jh^3(jh - 2\zeta))\tilde{\varphi}_j^\zeta - \tilde{\varphi}_{j-1}^\zeta, \quad \forall j \geq 1. \end{array} \right. \tag{19}$$

3.3. **Dependence on ζ of the sequence $(\tilde\varphi_j^\zeta)$.** The change of variables $x = t - \zeta$ in the eigenmode equation leads to the second order differential equation:

$$u''(x) - x^2 u(x) - \zeta^2 u(x) = 0. \tag{20}$$

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 (18) 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:

$$\varphi_\zeta = a_\zeta f_\zeta^- + b_\zeta f_\zeta^+. \tag{21}$$

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 eigenfunction 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 (21) 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 $\zeta < \zeta_0$.

3.4. **Construction of quasi-modes.** Discretization (19) 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:

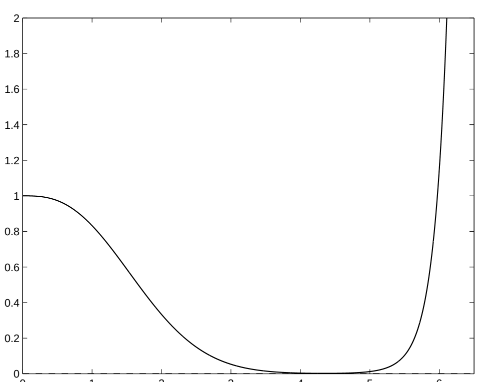

FIGURE 1. $(\tilde\varphi_j^\zeta)_j$ for $\zeta = 0.76818$.

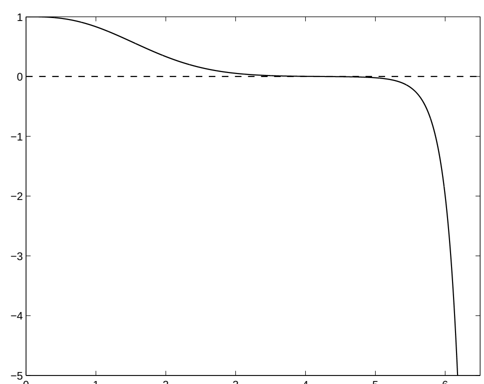

FIGURE 2. $(\tilde\varphi_j^\zeta)_j$ for $\zeta = 0.76819$.

- The sequence $(\tilde\varphi_j^\zeta)_j$ remains positive (see Figure 1). We determine n the smallest integer where the sequence $(\tilde\varphi_j^\zeta)_j$ reaches its minimum and we denote $L = nh$. The restriction of $\tilde\varphi_\zeta$ on $(0, L)$ makes a better quasi-mode and we have $\mu^{N,N}(\zeta, L) \le \tilde\mu(\zeta, L)$ with $\tilde\mu(\zeta, L)$ the energy of $(\tilde\varphi_j^\zeta)_j$ computed on $[0, L]$. Nevertheless, as we can not compare $\mu^{N,N}(\zeta, L)$ 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:

$$\varphi_j^\zeta = \begin{cases} \dfrac{\tilde{\varphi}_j^\zeta - \tilde{\varphi}_n^\zeta}{\tilde{\varphi}_1^\zeta - \tilde{\varphi}_n^\zeta} & \text{for } j = 1, \dots, n-1, \\ 0 & \text{for } j \geq n. \end{cases} \tag{22}$$

The energy associated with a regular interpolation of $(\varphi_j^\zeta)_j$ gives a upper-bound of Θ_0 according to Lemma 3.1. The initial sequence (see Figure 1) corresponds to $b_\zeta > 0$ in the decomposition (21).

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

$$\varphi_j^\zeta = \begin{cases} \tilde{\varphi}_j^\zeta & \text{for } j = 1, \dots, n-1, \\ 0 & \text{for } j \geq n. \end{cases} \tag{23}$$

Lemma 3.1 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 (21).

We would like to find a sequence such that $b_\zeta = 0$ and our algorithm could then be seen as a shooting method.

Let us now be more explicit about the interpolation of the sequence $(\varphi_j^\zeta)_j$ to construct the quasi-mode φ_ζ. We denote by $L = nh$. 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 necessarly 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:

$$\forall j = 0, \dots, n-1, \ \forall t \in [jh, (j+1)h], \quad \varphi_\zeta(t) = \alpha_j (t - jh)^2 + \tau_j (t - jh) + \varphi_j^\zeta, \tag{24}$$

with $\tau_0 = 0$ and for $j = 0, \dots, n-1$:

$$\begin{cases} \tau_{j+1} &= 2\dfrac{\varphi_{j+1}^\zeta - \varphi_j^\zeta}{h} - \tau_j, \\ \alpha_j &= \dfrac{\varphi_{j+1}^\zeta - \varphi_j^\zeta}{h^2} - \dfrac{\tau_j}{h}. \end{cases} \tag{25}$$

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:

$$\begin{aligned} ||\varphi_\zeta||^2_{L^2(\mathbb{R}^+)} &= \sum_{j=0}^{n-1} \int_0^h |\alpha_j x^2 + \tau_j x + \varphi_j^\zeta|^2 \, \mathrm{d}x \\ &= h \sum_{j=0}^{n-1} \left(\frac{h^4}{5} \alpha_j^2 + \frac{h^3}{2} \alpha_j \tau_j + \frac{h^2}{3} (\tau_j^2 + 2\alpha_j \varphi_j^\zeta) + h \tau_j \varphi_j^\zeta + (\varphi_j^\zeta)^2 \right). \end{aligned} \tag{26}$$

Let us compute the energy of φ_ζ:

$$||\varphi_\zeta'||^2_{L^2(\mathbb{R}^+)} = \sum_{j=0}^{n-1} \int_0^h |2\alpha_j x + \tau_j|^2 \, \mathrm{d}x = h \sum_{j=0}^{n-1} \left(\frac{4}{3} h^2 \alpha_j^2 + 2h \alpha_j \tau_j + \tau_j^2 \right). \tag{27}$$

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

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

Consequently

$$\begin{aligned}\int_{\mathbb{R}^+}(t-\zeta)|\varphi_\zeta(t)|^2\,\mathrm{d}t \quad &= \quad h\sum_{j=0}^{n-1}\Big(\frac{h^5}{6}\alpha_j^2+\frac{h^4}{5}\alpha_j(2\tau_j+\alpha_j\delta_j)\\ &\quad +\frac{h^3}{4}(\tau_j^2+2\alpha_j\varphi_j^\zeta+2\alpha_j\tau_j\delta_j)\\ &\quad +\frac{h^2}{3}(2\tau_j\varphi_j^\zeta+2\alpha_j\varphi_j^\zeta\delta_j+\tau_j^2\delta_j)\\ &\quad +\frac{h}{2}((\varphi_j^\zeta)^2+2\tau_j\delta_j\varphi_j^\zeta)+(\varphi_j^\zeta)^2\delta_j\Big).\end{aligned} \tag{28}$$

$$\begin{aligned}||(t-\zeta)\varphi_\zeta||^2_{L^2(\mathbb{R}^+)} \quad &= \quad h\sum_{j=0}^{n-1}\Big(\frac{h^6}{7}\alpha_j^2+\frac{h^5}{3}\alpha_j(\tau_j+\alpha_j\delta_j)\\ &\quad +\frac{h^4}{5}((\tau_j+\alpha_j\delta_j)^2+2\alpha_j(\varphi_j^\zeta+\tau_j\delta_j))\\ &\quad +\frac{h^3}{2}(\alpha_j\varphi_j^\zeta\delta_j+(\tau_j+\alpha_j\delta_j)(\varphi_j^\zeta+\tau_j\delta_j))\\ &\quad +\frac{h^2}{3}((\varphi_j^\zeta+\tau_j\delta_j)^2+2\varphi_j^\zeta\delta_j(\tau_j+\alpha_j\delta_j))\\ &\quad +h\varphi_j^\zeta\delta_j(\varphi_j^\zeta+\tau_j\delta_j)+(\varphi_j^\zeta)^2\delta_j^2\Big).\end{aligned} \tag{29}$$

Expressions (26), (27) and (29) present the main advantage to be exact. Let $\breve{\mu}(\zeta)$ be the Rayleigh quotient of φ_ζ:

$$\breve{\mu}(\zeta) = \frac{||\varphi'_\zeta||^2_{L^2(\mathbb{R}^+)}+||(t-\zeta)\varphi_\zeta||^2_{L^2(\mathbb{R}^+)}}{||\varphi_\zeta||^2_{L^2(\mathbb{R}^+)}}. \tag{30}$$

To apply Theorem 2.1, 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 (26), (27) and (29), the computation of $\|r_\zeta\|_{L^2(\mathbb{R}^+)}$ is explicit. For $j = 0,\dots,n-1$, we define:

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

A change of variables gives:

$$\begin{aligned}||r_\zeta||^2_{L^2(\mathbb{R}^+)} = h\sum_{j=0}^{n-1}\Big(&\frac{h^8}{9}\alpha_j^2 + \frac{h^7}{4}\alpha_j r_{3,j} + \frac{h^6}{7}(2\alpha_j r_{2,j} + r_{3,j}^2)\\ &+\frac{h^5}{3}(\alpha_j r_{1,j} + r_{3,j}r_{2,j}) + \frac{h^4}{5}(2\alpha_j r_{0,j} + 2r_{3,j}r_{1,j} + r_{2,j}^2)\\ &+\frac{h^3}{2}(r_{3,j}r_{0,j} + r_{2,j}r_{1,j}) + \frac{h^2}{3}(2r_{2,j}r_{0,j} + r_{1,j}^2) + hr_{1,j}r_{0,j} + r_{0,j}^2\Big). \quad (31)\end{aligned}$$

3.5. **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.

Algorithm 3.2.

1. We choose 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 $(\varphi_j^\zeta)_j$ by (19).
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 (22).
5. While $(\varphi_j^\zeta)_j$ has only positive coefficients,
   (a) we define the function φ_ζ by relations (24) and (25),
   (b) we compute the L^2-norm of φ_ζ thanks to (26) 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 (26), (27), (29) and (30),
   (d) we estimate the residus $\|r_\zeta\|_{L^2(\mathbb{R}^+)} = ||(H(\zeta) - \breve{\mu}(\zeta))\varphi_\zeta||_{L^2(\mathbb{R}^+)}$ with relation (31),
   (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 $h = 1/26000$. In each part, results given at the last line correspond to a function φ_ζ which takes negative values and for which $b_\zeta < 0$ in decomposition (21). The normalized eigenfunction Φ is such that $b_\zeta = 0$, but it is impossible to recover a quasi-mode with $b_\zeta = 0$. Our method consists then to detect the transition $b_\zeta > 0$ to $b_\zeta < 0$ when ζ is increasing. This transition means that we go from $\zeta < \zeta_0$ to $\zeta > \zeta_0$. We observe that the gap $\zeta^2 - \breve{\mu}(\zeta)$ becomes smaller and smaller when ζ is close to ζ_0. This is coherent since $\zeta_0^2 = \mu(\zeta_0)$. Table 1 gives also the behavior of $\varphi_j^\zeta(0)$ when ζ become close to ζ_0. 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).
Of course, a dichotomy method should be faster but we aim at determining decimals step by step.

3.6. **Estimates of the second eigenvalue.** To apply Theorem 2.1, 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 $A_{i,j}^\zeta$ the coefficients of the matrix

A^ζ, we have:

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

ζ	$\breve{\mu}(\zeta)$	$\Vert r_\zeta \Vert$	$\min_j \tilde{\varphi}^\zeta_j$	$\varphi^\zeta_j(0)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{a}_1$
0.761	0.611266093453	4e-01	1e-01	0.900663817	-3e-02	0.796379904
0.762	0.608936310293	1e+00	1e-01	0.898608815	-3e-02	0.793804657
0.763	0.606516822831	1e+00	1e-01	0.896392500	-2e-02	0.791059093
0.764	0.603984720795	6e-01	9e-02	0.893963620	-2e-02	0.788090938
0.765	0.601304928182	3e-01	8e-02	0.891237476	-2e-02	0.784814707
0.766	0.598417489656	5e-01	6e-02	0.888054169	-1e-02	0.781071025
0.767	0.595197681398	5e-01	4e-02	0.884029104	-7e-03	0.776482855
0.768	0.591201356836	1e-01	2e-02	0.877276977	-1e-03	0.769255460
0.769	0.592445239556	3e+03	-7e+4	0.873788252	-1e-03	0.766599012
0.7681	0.590667836454	8e-02	1e-02	0.875868145	-7e-04	0.767846771
0.7682	0.590132204890	1e+02	-1e+3	0.873060749	-1e-06	0.765212036
0.76811	0.590609794273	1e-01	1e-02	0.875688760	-6e-04	0.767670650
0.76812	0.590550467623	1e-01	9e-03	0.875497051	-5e-04	0.767483314
0.76813	0.590489644618	7e-02	8e-03	0.875290014	-5e-04	0.767282062
0.76814	0.590427028617	6e-02	8e-03	0.875063165	-4e-04	0.767062869
0.76815	0.590362189929	6e-02	7e-03	0.874809290	-3e-04	0.766819274
0.76816	0.590294414679	1e-01	5e-03	0.874515187	-2e-04	0.766539474
0.76817	0.590222359089	5e-02	4e-03	0.874151227	-1e-04	0.766197069
0.76818	0.590142134621	3e-02	2e-03	0.873603510	-4e-05	0.765690971
0.76819	0.590133901819	4e+02	-5e+2	0.873050163	-2e-05	0.765203308
0.768181	0.590133151271	2e-02	2e-03	0.873518101	-3e-05	0.765613199
0.768182	0.590123767394	2e-02	1e-03	0.873415005	-2e-05	0.765519795
0.768183	0.590113720068	2e-02	8e-04	0.873273227	-9e-06	0.765392273
0.768184	0.590107683499	1e+02	-3e+1	0.873043550	-1e-06	0.765189013
0.7681831	0.590112657421	2e-02	8e-04	0.873254393	-7e-06	0.765375421
0.7681832	0.590111566559	1e-02	7e-04	0.873233650	-6e-06	0.765356887
0.7681833	0.590110458701	1e-02	6e-04	0.873210676	-5e-06	0.765336392
0.7681834	0.590109315459	9e-03	5e-04	0.873184140	-4e-06	0.765312764
0.7681835	0.590108138271	9e-03	4e-04	0.873152040	-2e-06	0.765284248
0.7681836	0.590106879933	3e-03	2e-04	0.873106158	-8e-07	0.765243626
0.7681837	0.590106497981	6e+01	-4e+0	0.873043197	-3e-07	0.765188319
0.76818361	0.590106749563	5e-03	2e-04	0.873099864	-7e-07	0.765238067
0.76818362	0.590106611147	4e-03	2e-04	0.873092511	-5e-07	0.765231577
0.76818363	0.590106470242	3e-03	1e-04	0.873083998	-4e-07	0.765224070
0.76818364	0.590106331385	2e-03	1e-04	0.873073907	-2e-07	0.765215181
0.76818365	0.590106179248	1e-03	5e-05	0.873057934	-6e-08	0.765201133
0.76818366	0.590106139402	6e+00	-6e-1	0.873043147	-4e-09	0.765188160
0.768183651	0.590106163301	1e-03	4e-05	0.873055378	-4e-08	0.765198886
0.768183652	0.590106145104	9e-04	3e-05	0.873051762	-2e-08	0.765195712
0.768183653	0.590106127974	5e-04	1e-05	0.873046229	-3e-09	0.765190857
0.768183654	0.590106128318	5e+00	-7e-2	0.873043140	-2e-09	0.765188149
0.7681836531	0.590106125876	2e-04	6e-06	0.873044775	-1e-09	0.765189581
0.7681836532	0.590106125048	5e-01	-4e-3	0.873043139	-4e-12	0.765188147

TABLE 1. Results obtained with Algorithm 3.2.

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 $-\mathrm{d}^2/\mathrm{d}t^2 + (t-\zeta)^2$ on the half-line. We obtain $\mu_2(\zeta_0) \geq 1$.

3.7. Accurate estimate for Θ_0 and $\Phi(0)$.

Lemma 3.3. *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. Let us prove the lower-bound. For any $\zeta \in \mathbb{R}$, we write

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

Choosing $\zeta = 0$ and using Proposition 1, we deduce the lower-bound. □

We apply Algorithm 3.2 for h such that $1/h \in \{100 \times k, k = 10, \dots, 40\}$. 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 2.1, a lower-bound and a upper-bound for $\Phi(0)$ given in Theorem 2.3. To make these computations, we need a lower-bound of $|\zeta - \zeta_0|$. We start with the coarse estimate of Lemma 3.3 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 9.

$$0.590106124587 \leq \Theta_0 \leq 0.590106124951,$$
$$0.872997 \leq \Phi(0) \leq 0.873090.$$

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}.

4. 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 $-\mathrm{d}^2/\mathrm{d}t^2 + (t-\zeta)^2$ on $[0, L]$ with Dirichlet condition on $t = L$ and Neumann condition on $t = 0$. Let $\mathcal{V}$ a disrete variational space. We denote by $(\breve{\mu}_k(\zeta), \breve{\varphi}_{k,\zeta})$ the k-th discrete eigenpair of the operator in $\mathcal{V}$:

$$\int_0^L (\breve{\varphi}'_{k,\zeta}(t)v'(t) + (t-\zeta)^2\breve{\varphi}_{k,\zeta}(t)v(t))\,\mathrm{d}t = \breve{\mu}_k(\zeta)\int_0^L \breve{\varphi}_{k,\zeta}(t)v(t)\,\mathrm{d}t, \qquad \forall v \in \mathcal{V}.$$

The computed eigenvalues $\breve{\mu}_k(\zeta)$ give a upper-bound of $\mu_k(\zeta)$. We omit the subscript k when $k = 1$.

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 $[0, 10]$.

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 eigenfunction associated with $\breve{\mu}(\zeta)$. Then, we

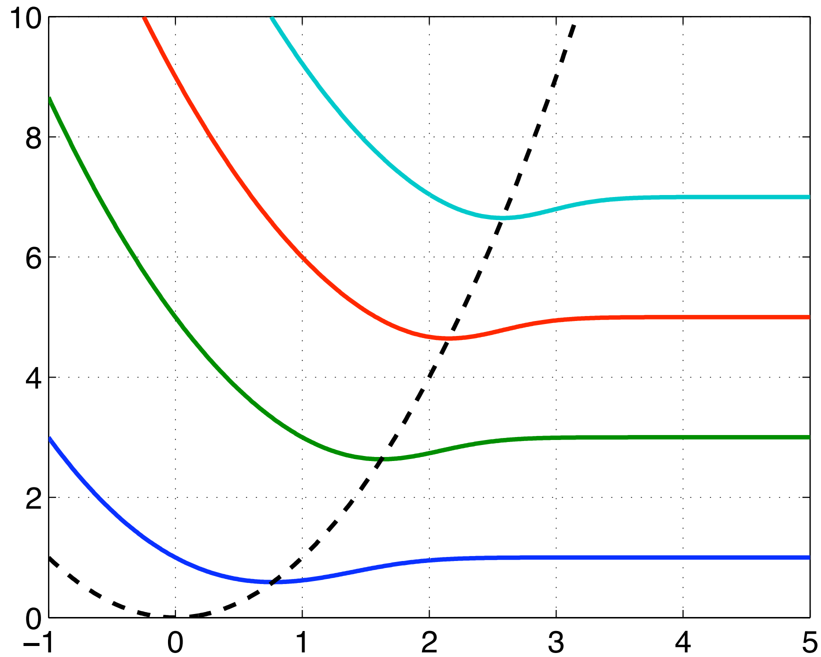

FIGURE 3. $\mu_k(\zeta)$ for $\zeta \in [-1, 5]$, $k = 1, \dots, 4$ and curve $\zeta \mapsto \zeta^2$ in dashed line.

compute $\breve{a}_1 = \sqrt{\zeta}\breve{\varphi}_\zeta(0)$. Tables 2 and 3 give the results of these computations. In particular we obtain approximation for Θ_0, $\Phi(0)$ and a_1:

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

In Table 2, we study the influence of L. As soon L is larger than 7, the cut-off do not interfere the computations which are then satisfactory. In Table 3, we present the computations at a fixed number of degrees of freedom. We observe that the numerical simulations are comparable for degrees larger than 4. Notice that computed values $\breve{\mu}(\zeta)$ in Tables 2 and 3 provide better upper-bounds for Θ_0 than in Proposition 9.

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$L = 7$

nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
70	8	ζ_a	0.59010612495049	1.0e-12	0.873043138513904	0.765188146985675
70	8	ζ_b	0.590106124949945	3.1e-12	0.873043138513613	0.765188146985918
70	10	ζ_a	0.590106124952671	-1.2e-12	0.873043138513392	0.765188146985226
70	10	ζ_b	0.590106124952394	6.6e-13	0.873043138513095	0.765188146985464

$L = 8$

nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
100	8	ζ_a	0.590106124949903	1.6e-12	0.873043138513603	0.765188146985411
100	8	ζ_b	0.590106124949336	3.7e-12	0.873043138513245	0.765188146985595
100	10	ζ_a	0.590106124952819	-1.3e-12	0.873043138513197	0.765188146985055
100	10	ζ_b	0.590106124952989	6.3e-14	0.873043138512816	0.765188146985219

$L = 9$

nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
90	8	ζ_a	0.590106124950496	1.0e-12	0.873043138513906	0.765188146985677
90	8	ζ_b	0.590106124949943	3.1e-12	0.873043138513614	0.765188146985919
90	10	ζ_a	0.590106124952671	-1.2e-12	0.873043138513392	0.765188146985226
90	10	ζ_b	0.59010612495238	6.6e-13	0.873043138513095	0.765188146985464

$L = 10$

nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
100	8	ζ_a	0.590106124950496	1.0e-12	0.873043138513906	0.765188146985677
100	8	ζ_b	0.590106124949948	3.1e-12	0.873043138513614	0.765188146985919
100	10	ζ_a	0.590106124952670	-1.2e-12	0.873043138513391	0.765188146985225
100	10	ζ_b	0.590106124952392	7e-13	0.873043138513095	0.765188146985464

$L = 12$

nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
110	8	ζ_a	0.590106124948481	3.0e-12	0.873043138514059	0.765188146985811
110	8	ζ_b	0.590106124948091	5.0e-12	0.873043138513689	0.765188146985984
110	10	ζ_a	0.590106124949202	2.3e-12	0.873043138513313	0.765188146985156
110	10	ζ_b	0.590106124949127	3.9e-12	0.873043138513068	0.765188146985440

$L = 15$

nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
200	8	ζ_a	0.590106124951757	-2e-13	0.873043138513820	0.765188146985601
200	8	ζ_b	0.590106124951625	1.4e-12	0.873043138513444	0.765188146985769
200	10	ζ_a	0.590106124949226	2.3e-12	0.873043138513258	0.765188146985109
200	10	ζ_b	0.590106124949262	3.8e-12	0.873043138512969	0.765188146985353

Table 2. Computation with the finite element method, $\zeta_a = 0.768183653140$ and $\zeta_b = 0.768183653141$.

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nbel	Q	ζ	$\breve{\mu}(\zeta)$	$\zeta^2 - \breve{\mu}(\zeta)$	$\breve{\varphi}_\zeta(0)$	$\breve{a}_1$
1000	1	ζ_a	0.590108508413493	-2.4e-6	0.873045921182187	0.765190585885533
1000	1	ζ_b	0.590108508413308	-2.4e-6	0.873045921181916	0.765190585885794
500	2	ζ_a	0.590106125169424	-2.2e-10	0.873043138593626	0.765188147055548
500	2	ζ_b	0.590106125169391	-2.1e-10	0.873043138593299	0.765188147055759
250	4	ζ_a	0.590106124952589	-1.1e-12	0.873043138513866	0.765188146985642
250	4	ζ_b	0.590106124952587	4.6e-13	0.873043138513550	0.765188146985862
200	5	ζ_a	0.590106124950764	7.5e-13	0.873043138513719	0.765188146985513
200	5	ζ_b	0.590106124950785	2.3e-12	0.873043138513551	0.765188146985863
125	8	ζ_a	0.590106124949906	1.6e-12	0.873043138513603	0.765188146985411
125	8	ζ_b	0.590106124949337	3.7e-12	0.873043138513246	0.765188146985596
100	10	ζ_a	0.590106124952670	-1.2e-2	0.873043138513391	0.765188146985225
100	10	ζ_b	0.590106124952392	6.6e-13	0.873043138513095	0.765188146985464

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E-mail address: `virginie.bonnaillie@bretagne.ens-cachan.fr`