Harmonic oscillators with Neumann condition on the half-line

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Numerical estimates of characteristic parameters Θ_0 and $\Phi(0)$ for superconductivity

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Abstract

This paper is devoted to the computation of the bottom Θ_0 of the spectrum for the Neumann realization of the Schrödinger operator with constant magnetic field in the half-plane. We propose an algorithm to determine Θ_0 and we estimate the accuracy of these computations.

1 Introduction

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

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

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, [10]):

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 $[\Theta_0,+\infty)$. Furthermore, if Φ denotes a normalized eigenvector associated with $\mu_1(\zeta_0)$, then*

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

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

These parameters Θ_0 and $\Phi(0)$ appear naturally when we analyze the emergence of the superconductivity. We state in Section 2 some results concerning the localization of the superconductivity based. This analysis is based on those of the low-lying eigenmodes for the Schrödinger operator with magnetic field (see [7, 8] and Propositions 2.2, 2.3, 2.4). Motivated by the fact the Θ_0 and $\Phi(0)$ appear repeatingly in the analysis of superconductivity (see Propositions 2.1, 2.5), we aim to construct quasi-mode to approximate the eigenfunction Φ. Its energy would be an approximation of Θ_0. Before dealing with this construction,

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Section 3 is devoted to error estimates on eigenmodes: Theorem 3.1 quantifies the gap between the eigenvalue Θ_0 and the energy associated with a quasi-mode for the operator $H(\zeta)$. In Theorem 3.2, 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 3.4 a local 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.

$$|\Theta_0 - 0.590106122| \leq 2 \times 10^{-9} \qquad \textit{and} \qquad |\Phi(0) - 0.8730| \leq 10^{-4}.$$

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 sufficently strong external magnetic field. This transition takes place for a value H_{C_3}[1] of the field which apperas 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

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

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 [18, 2, 21, 22, 23, 19, 11, 12, 13]). In the recent works [11, 12, 13], the defintion 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 [13]] 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 [22].

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 [12]:

Proposition 2.2 (see [12]). *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 exists $h_0 > 0$ 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 the localization of $\mu_k(\alpha)$ according to Θ_0 and then of an accurate estimate of Θ_0. It is also natural to wonder for each 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 improved 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 [9])**.** *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 $\Sigma'=\{\mathsf{s}\in\Sigma|\mu_1(\alpha)\le\mu\}$. There exist constants κ_0, M, C, $\varepsilon>0$ such that if $\kappa\ge\kappa_0$, $H/\kappa\ge\mu^{-1}$, and $(\psi,\mathcal{A})$ is a minimizer of $\mathcal{E}_{\kappa,H}$, then

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

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.

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 $H(\zeta)$.

Theorem 3.1. *Let $\zeta\in\mathbb{R}$ and φ_ζ be a normalized function of $\mathcal{D}$. We assume that*

$$H(\zeta)\varphi_\zeta = \Theta_\zeta\varphi_\zeta + r_\zeta \qquad \text{with} \qquad \langle r_\zeta,\varphi_\zeta\rangle = 0 \qquad \text{and} \qquad (\sqrt{\Theta_\zeta}+|\zeta-\zeta_0|)^2\le\mu_2(\zeta_0).$$

Then we can compare Θ_0 and Θ_ζ:

$$(\sqrt{\Theta_\zeta}-|\zeta-\zeta_0|)^2 - \frac{\left(\|r_\zeta\|_{L^2(\mathbb{R}^+)}+2\sqrt{\Theta_\zeta}|\zeta-\zeta_0|\right)^2+12\Theta_\zeta(\zeta-\zeta_0)^2}{\mu_2(\zeta_0)-(\sqrt{\Theta_\zeta}+|\zeta-\zeta_0|)^2} \le \Theta_0\le\Theta_\zeta\ .$$

Proof. The upper-bound is trivial: by assumptions, we have $\Theta_\zeta=\langle H(\zeta)\varphi_\zeta,\varphi_\zeta\rangle$. Since $\mu_1(\zeta)$ is the bottom of the spectrum of $H(\zeta)$ and is bounded from below by $\Theta_0=\mu_1(\zeta_0)$, we deduce:

$$\Theta_\zeta\ge\mu_1(\zeta)\ge\mu_1(\zeta_0)=\Theta_0.$$

To prove the lower-bound, we bring to mind the Temple inequality (see [20], [15, Theorem 1.15]): Let A be self-adjoint and $\Psi\in\mathcal{D}(A)$, $\|\Psi\|=1$. Suppose that λ is the only 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

$$\eta-\frac{\varepsilon^2}{\beta-\eta}\le\lambda\le\eta+\frac{\varepsilon^2}{\eta-\alpha}. \tag{1}$$

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 formulate $H(\zeta_0)$ 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

$$\eta = \Theta_\zeta + 2(\zeta - \zeta_0) \int_{\mathbb{R}^+} (t - \zeta) |\varphi_\zeta(t)|^2 \, dt + (\zeta - \zeta_0)^2.$$

Cauchy-Schwarz inequality leads to

$$(\sqrt{\Theta_\zeta} - |\zeta - \zeta_0|)^2 \leq \eta \leq (\sqrt{\Theta_\zeta} + |\zeta - \zeta_0|)^2 \, . \tag{2}$$

The assumption $\varepsilon^2 < (\beta - \eta)(\eta - \alpha)$ is then obviously fulfilled. Consider now ε^2. Using (2) and orthogonality relation $\langle r_\zeta, \varphi_\zeta \rangle = 0$, we get

$$\begin{aligned} \varepsilon^2 &= \int_{\mathbb{R}^+} \left| r_\zeta(t) + 2(\zeta - \zeta_0)(t - \zeta)\varphi_\zeta(t) + \left[(\zeta - \zeta_0)^2 + (\Theta_\zeta - \eta) \right] \varphi_\zeta(t) \right|^2 \, dt \\ &\leq \left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2\sqrt{\Theta_\zeta} |\zeta - \zeta_0| \right)^2 + 12\Theta_\zeta |\zeta - \zeta_0|^2. \end{aligned} \tag{3}$$

Temple inequality (1) gives

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

Combining this last lower-bound of $\Theta_0 = \mu_1(\zeta_0)$ with the upper-bound (3) of ε^2 and the lower-bound (2) of η achieves the proof. □

Let us now prove an estimate on the eigenfunction.

Theorem 3.2. *Let $\zeta \in \mathbb{R}$ and φ_ζ be normalized in $\mathcal{D}$. We assume that*

$$H(\zeta)\varphi_\zeta = \Theta_\zeta \varphi_\zeta + r_\zeta \qquad \textit{with} \qquad \langle r_\zeta, \varphi_\zeta \rangle = 0 \qquad \textit{and} \qquad (\sqrt{\Theta_\zeta} + |\zeta - \zeta_0|)^2 \leq \mu_2(\zeta_0).$$

Then

$$\|\varphi_\zeta - \Phi\|_{L^2(\mathbb{R}^+)} \leq 2\sqrt{2} \frac{\left[\left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2\sqrt{\Theta_\zeta} |\zeta - \zeta_0| \right)^2 + |\zeta - \zeta_0|^3 \left(|\zeta - \zeta_0| + 4\sqrt{\Theta_\zeta} \right) \right]^{1/2}}{\mu_2(\zeta_0) - \Theta_\zeta},$$

and

$$\begin{aligned} \|\varphi_\zeta' - \Phi'\|_{L^2(\mathbb{R}^+)} &\leq (\sqrt{\Theta_\zeta} + |\zeta - \zeta_0|)^2 - \Theta_0 + 2\Theta_0 \|\Phi - \varphi_\zeta\|_{L^2(\mathbb{R}^+)} \\ &\leq 4\sqrt{\Theta_\zeta} |\zeta - \zeta_0| + \frac{\left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2\sqrt{\Theta_\zeta} |\zeta - \zeta_0| \right)^2 + 12\Theta_\zeta (\zeta - \zeta_0)^2}{\mu_2(\zeta_0) - \Theta_\zeta} + 2\Theta_\zeta \|\Phi - \varphi_\zeta\|_{L^2(\mathbb{R}^+)}. \end{aligned}$$

To prove this result, we use an estimate of quasi-modes established in [17, Proposition 4.1.1, p. 30] :

Proposition 3.3. *Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Let $I \subset \mathbb{R}$ be a compact interval, $\Psi_1, \dots, \Psi_N \in \mathcal{H}$ linearly independent in $\mathcal{D}(A)$ and $\mu_1, \dots, \mu_N \in I$ 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 $\Psi_1, \dots, \Psi_N$ 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 3.2. We apply Proposition 3.3 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

$$d(E, F) = ||\varphi_\zeta - \langle \varphi_\zeta, \Phi \rangle \Phi||_{L^2(\mathbb{R}^+)} = \sqrt{1 - |\langle \varphi_\zeta, \Phi \rangle|^2} = \frac{1}{\sqrt{2}} \|\varphi_\zeta - \Phi\|_{L^2(\mathbb{R}^+)}. \tag{4}$$

Writing

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

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

$$\begin{aligned} ||\tilde{r}_\zeta||^2_{L^2(\mathbb{R}^+)} &= \int_{\mathbb{R}^+} \left| 2(\zeta - \zeta_0)(t - \zeta)\varphi_\zeta(t) + (\zeta - \zeta_0)^2 \varphi_\zeta(t) + r_\zeta(t) \right|^2 dt \\ &\leq \left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2\sqrt{\Theta_\zeta}\, |\zeta - \zeta_0| \right)^2 + |\zeta - \zeta_0|^3 \left(|\zeta - \zeta_0| + 4\sqrt{\Theta_\zeta} \right). \end{aligned} \tag{5}$$

Relations (4), (5) and Proposition 3.3 with $a = (\mu_2(\zeta_0) - \Theta_\zeta)/2$ give the L^2-estimate on $(\varphi_\zeta - \Phi)$. This estimate makes appear Θ_0 which can be bounded thanks to Theorem 3.1.
Let us now estimate the L^2-norm of $(\varphi'_\zeta - \Phi')$. An integration by parts gives:

$$\langle H(\zeta_0)(\Phi - \varphi_\zeta), \Phi - \varphi_\zeta \rangle_{L^2(\mathbb{R}^+)} = \|\Phi' - \varphi'_\zeta\|^2_{L^2(\mathbb{R}^+)} + \int_0^\infty (t - \zeta_0)^2 |\Phi - \varphi_\zeta|^2(t)\, dt \geq \|\Phi' - \varphi'_\zeta\|^2_{L^2(\mathbb{R}^+)}. \tag{6}$$

On the other hand,

$$\begin{aligned} \langle H(\zeta_0)(\varphi_\zeta - \Phi), \varphi_\zeta - \Phi \rangle_{L^2(\mathbb{R}^+)} &= \langle H(\zeta_0)\varphi_\zeta, \varphi_\zeta \rangle_{L^2(\mathbb{R}^+)} - \Theta_0 + 2\Theta_0 \langle \varphi_\zeta, \varphi_\zeta - \Phi \rangle_{L^2(\mathbb{R}^+)} \\ &\leq \langle H(\zeta_0)\varphi_\zeta, \varphi_\zeta \rangle_{L^2(\mathbb{R}^+)} - \Theta_0 + 2\Theta_0 \|\varphi_\zeta - \Phi\|_{L^2(\mathbb{R}^+)}. \end{aligned} \tag{7}$$

With the notation $\eta = \langle H(\zeta_0)\varphi_\zeta, \varphi_\zeta \rangle_{L^2(\mathbb{R}^+)}$, we deduce from (6), (7), (2) and Theorem 3.1 a upper-bound for the L^2-norm of $\Phi' - \varphi'_\zeta$:

$$\begin{aligned} \|\Phi' - \varphi'_\zeta\|^2_{L^2(\mathbb{R}^+)} &\leq \eta - \Theta_0 + 2\Theta_0 \|\Phi - \varphi_\zeta\|_{L^2(\mathbb{R}^+)} \\ &\leq 4\sqrt{\Theta_\zeta}|\zeta - \zeta_0| + \frac{\left(\|r_\zeta\|_{L^2(\mathbb{R}^+)} + 2\sqrt{\Theta_\zeta}|\zeta - \zeta_0| \right)^2 + 12\Theta_\zeta(\zeta - \zeta_0)^2}{\mu_2(\zeta_0) - (\sqrt{\Theta_\zeta} + |\zeta - \zeta_0|)^2} + 2\Theta_\zeta \|\Phi - \varphi_\zeta\|_{L^2(\mathbb{R}^+)}. \end{aligned}$$

□

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

Theorem 3.4. *Using the same notation and assumptions as Theorem 3.2, we have*

$$|\Phi(0) - \varphi_\zeta(0)|^2 \leq 2\|\Phi - \varphi_\zeta\|_{L^2(\mathbb{R}^+)} \, \|\Phi' - \varphi'_\zeta\|_{L^2(\mathbb{R}^+)}. \tag{8}$$

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

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

We conclude with the Cauchy-Schwarz inequality. □

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

Theorem 3.1 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. 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 intervall $[0, L]$: 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 $L > 0$,

$$\int_a^\infty |\varphi_\zeta(t)|^2 dt \leq 2\frac{C}{L}\int_L^\infty te^{-t^2} \, dt = \frac{Ce^{-L^2}}{L}. \tag{9}$$

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

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

It is equivalent to find L such that $L^2 + \ln L \geq N \ln 10 + \ln C$.
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 $L > 0$,*

$$\mu^{N,D}(\zeta, L) \geq \mu_1(\zeta) \geq \Theta_0. \tag{10}$$

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

$$\mu^{N,N}(\zeta, L) \leq \mu_1(\zeta). \tag{11}$$

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:

$$\partial_L \mu^{N,N}(\zeta, L) = ((L-\zeta)^2 - \mu^{N,N}(\zeta, L))|u_{\zeta,L}(L)|^2, \tag{12}$$

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:

$$\left\{ \begin{array}{rcl} H(\zeta_0)\Phi(t) & = & \zeta_0^2 \Phi(t), \quad \forall t > 0, \\ \Phi(0) & = & 1, \\ \Phi'(0) & = & 0. \end{array} \right. \tag{13}$$

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:

$$\left\{ \begin{array}{rcl} H(\zeta)\varphi_\zeta(t) & = & \zeta^2 \varphi_\zeta(t), \quad \forall t \in (0, L), \\ \varphi_\zeta(0) & = & 1, \\ \varphi'_\zeta(0) & = & 0. \end{array} \right. \tag{14}$$

The system (14) 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 $j \in \{0, \ldots, n\}$. 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 $(\tilde{\varphi}_j^\zeta)_{j=0,\ldots,n}$:

$$\left\{ \begin{array}{rcl} \tilde{\varphi}_0^\zeta & = & 1, \\ \tilde{\varphi}_1^\zeta & = & 1, \\ \tilde{\varphi}_{j+1}^\zeta & = & (2 + jh^3(jh - 2\zeta))\tilde{\varphi}_j^\zeta - \tilde{\varphi}_{j-1}^\zeta, \ \forall j = 1, \ldots, n-1. \end{array} \right. \tag{15}$$

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

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

$$u''(x) - x^2 u(x) - \zeta^2 u(x) = 0. \tag{16}$$

The Sturm-Liouville equation (cf [14, 16, 25, 10]) 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 (14) 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:

$$\varphi_\zeta = a_\zeta f_\zeta^- + b_\zeta f_\zeta^+. \tag{17}$$

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 "does not explode". 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 (17) 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 (15) 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:

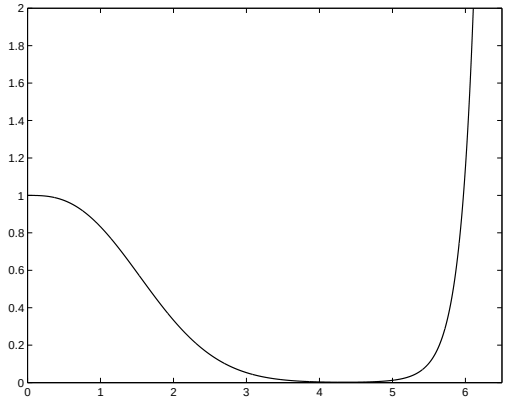

Figure 1: $(\tilde{\varphi}_j^\zeta)_j$ for $\zeta = 0.76818$.

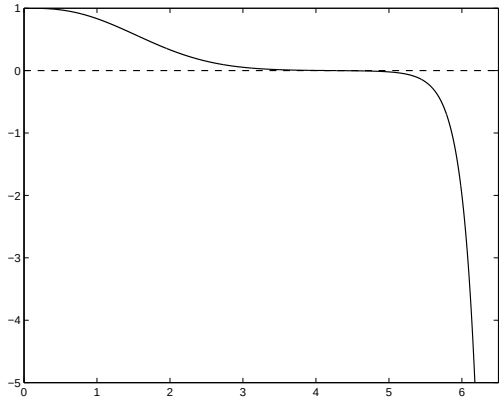

Figure 2: $(\tilde{\varphi}_j^\zeta)_j$ for $\zeta = 0.76819$.

- The sequence $(\tilde{\varphi}_j^\zeta)_j$ remains positive (see Figure 1). We determine 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 $\mu^{N,N}(\zeta, L') \leq \tilde{\Theta}_\zeta$ with $\tilde{\Theta}_\zeta$ the energy of $\tilde{\varphi}_j^\zeta$ 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:

$$\varphi_j^\zeta = \begin{cases} \dfrac{\tilde{\varphi}_j^\zeta - \tilde{\varphi}_{j_0}^\zeta}{\tilde{\varphi}_1^\zeta - \tilde{\varphi}_{j_0}^\zeta} & \text{for } j = 1, \ldots, j_0 - 1, \\ 0 & \text{for } j = j_0, \ldots, n. \end{cases} \tag{18}$$

The energy associated with a regular interpolation of $(\varphi_j^\zeta)_j$ gives a upper-bound of Θ_0 according to Lemma 4.1. Figure 3 plots the new sequence constructed with (15) for $\zeta = 0.76818$. The initial sequence (see Figure 1) corresponds to $b_\zeta > 0$ in the decomposition (17).

- 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

$$\varphi_j^\zeta = \begin{cases} \tilde{\varphi}_j^\zeta & \text{for } j = 1, \ldots, j_0 - 1, \\ 0 & \text{for } j = j_0, \ldots, n. \end{cases} \tag{19}$$

Lemma 4.1 bounds from above Θ_0 by the energy of the function constructed from $(\varphi_j^\zeta)_j$. Figure 4 draws the sequence deduced with (19) for $\zeta = 0.76819$ (see Figure 2). For the intital sequence, $b_\zeta < 0$ in the decomposition (17).

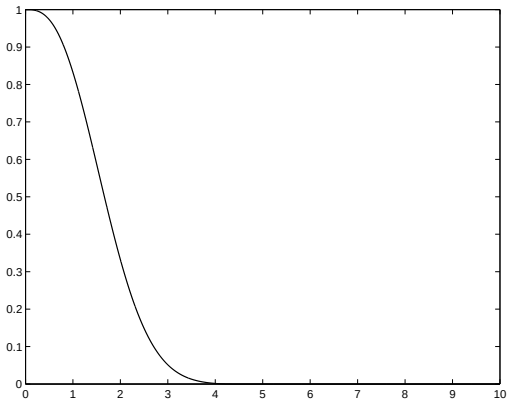

Figure 3: Sequence $(\varphi_j^\zeta)_j$ constructed with (18) for $\zeta = 0.76818$.

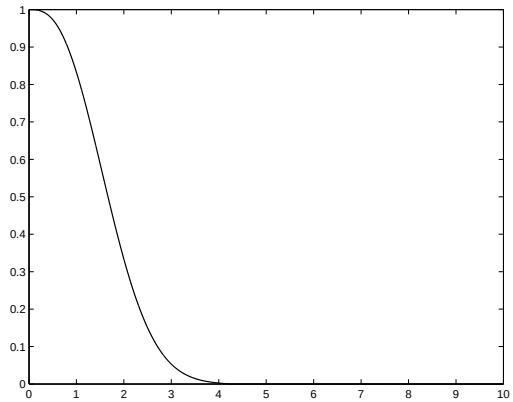

Figure 4: Sequence $(\varphi_j^\zeta)_j$ constructed with (19) for $\zeta = 0.76819$.

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:

$$\forall j = 0, \ldots, n-1, \ \forall t \in [jh, (j+1)h], \quad \varphi_\zeta(t) = \alpha_j (t - jh)^2 + \tau_j (t - jh) + \varphi_j^\zeta, \tag{20}$$

with $\tau_0 = 0$ and

$$\begin{cases} \tau_{j+1} &= 2\dfrac{\varphi_{j+1}^\zeta - \varphi_j^\zeta}{h} - \tau_j, \\ \alpha_j &= \dfrac{\varphi_{j+1}^\zeta - \varphi_j^\zeta}{h^2} - \dfrac{\tau_j}{h}. \end{cases} \tag{21}$$

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

$j = 0, \ldots, n-1$. Furthermore, any computations (norm, energy, ...) are explicit. With the change of variables $x = t - jh$, we have:

$$\begin{aligned} ||\varphi_\zeta||^2_{L^2(\mathbb{R}^+)} &= \sum_{j=0}^{n-1} \int_0^h |\alpha_j x^2 + \tau_j x + \varphi_j^\zeta|^2 \, dx \\ &= h \sum_{j=0}^{n-1} \left(\frac{h^4}{5}\alpha_j^2 + \frac{h^3}{2}\alpha_j\tau_j + \frac{h^2}{3}(\tau_j^2 + 2\alpha_j\varphi_j^\zeta) + h\tau_j\varphi_j^\zeta + (\varphi_j^\zeta)^2 \right). \end{aligned} \tag{22}$$

Let us compute the energy of φ_ζ:

$$||\varphi_\zeta'||^2_{L^2(\mathbb{R}^+)} = \sum_{j=0}^{n-1} \int_0^h |2\alpha_j x + \tau_j|^2 \, dx = h \sum_{j=0}^{n-1} \left(\frac{4}{3}h^2\alpha_j^2 + 2h\alpha_j\tau_j + \tau_j^2 \right). \tag{23}$$

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

$$\begin{aligned} ||(t-\zeta)\varphi_\zeta||^2_{L^2(\mathbb{R}^+)} &= \sum_{j=0}^{n-1} \int_0^h |(x+\delta_j)(\alpha_j x^2 + \tau_j x + \varphi_j^\zeta|^2 \, dx \\ &= h \sum_{j=0}^{n-1} \left(\frac{h^6}{7}\alpha_j^2 + \frac{h^5}{3}\alpha_j(\tau_j + \alpha_j\delta_j) + \frac{h^4}{5}((\tau_j + \alpha_j\delta_j)^2 + 2\alpha_j(\varphi_j^\zeta + \tau_j\delta_j)) \right. \\ &\quad + \frac{h^3}{2}(\alpha_j\varphi_j^\zeta\delta_j + (\tau_j + \alpha_j\delta_j)(\varphi_j^\zeta + \tau_j\delta_j)) \\ &\quad \left. + \frac{h^2}{3}((\varphi_j^\zeta + \tau_j\delta_j)^2 + 2\varphi_j^\zeta\delta_j(\tau_j + \alpha_j\delta_j)) + h\varphi_j^\zeta\delta_j(\varphi_j^\zeta + \tau_j\delta_j) + (\varphi_j^\zeta)^2\delta_j^2 \right). \end{aligned} \tag{24}$$

Expressions (22), (23) and (24) present the main advantage to be exact. If we choose ζ to be a rational number, then the computation of these three expressions still gives a rational number.
Let Θ_ζ be the Rayleigh quotient of φ_ζ:

$$\Theta_\zeta = \frac{||\varphi_\zeta'||^2_{L^2(\mathbb{R}^+)} + ||(t-\zeta)\varphi_\zeta||^2_{L^2(\mathbb{R}^+)}}{||\varphi_\zeta||^2_{L^2(\mathbb{R}^+)}}. \tag{25}$$

To apply Theorem 3.1, we have to estimate the residus $\|r_\zeta\|^2_{L^2(\mathbb{R}^+)}$ with $r_\zeta := (H(\zeta) - \Theta_\zeta)\varphi_\zeta$. 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 $j = 0, \ldots, n-1$ and $t \in [jh, (j+1)h]$, we get:

$$r_\zeta(t) = -2\alpha_j + ((t-\zeta)^2 - \Theta_\zeta)(\alpha_j(t-jh)^2 + \tau_j(t-jh) + \varphi_j^\zeta). \tag{26}$$

As in (22), (23) and (24), the computation of $\|r_\zeta\|_{L^2(0,a)}$ is explicit. For $j = 0, \ldots, n-1$, we define:

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

A change of variables gives:

$$||r_\zeta||^2_{L^2(\mathbb{R}^+)} = h\sum_{j=0}^{n-1}\left(\frac{h^8}{9}\alpha_j^2 + \frac{h^7}{4}\alpha_j r_{3,j} + \frac{h^6}{7}(2\alpha_j r_{2,j} + r_{3,j}^2) + \frac{h^5}{3}(\alpha_j r_{1,j} + r_{3,j}r_{2,j})\right.$$
$$\left. + \frac{h^4}{5}(2\alpha_j r_{0,j} + 2r_{3,j}r_{1,j} + r_{2,j}^2) + \frac{h^3}{2}(r_{3,j}r_{0,j} + r_{2,j}r_{1,j}) + \frac{h^2}{3}(2r_{2,j}r_{0,j} + r_{1,j}^2) + hr_{1,j}r_{0,j} + r_{0,j}^2\right). \tag{27}$$

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* (15)*.*
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* (18)*.*
5. *While $(\varphi_j^\zeta)_j$ has only positive coefficients,*
   (a) *we define the function φ_ζ by relations* (20) *and* (21)*,*
   (b) *we compute the L^2-norm of φ_ζ thanks to* (22) *and deduce the value of $\varphi_\zeta(0)$ after normalization,*
   (c) *we compute the energy Θ_ζ associated with φ_ζ thanks to relations* (22)*,* (23)*,* (24) *and* (25)*,*
   (d) *we estimate the residus $\|r_\zeta\|_{L^2(\mathbb{R}^+)} = ||(H(\zeta) - \Theta_\zeta)\varphi_\zeta||_{L^2(\mathbb{R}^+)}$ with relation* (27)*,*
   (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 termes.*

Table 1 sums up the results obtained by application of the algorithm: we choose $h = 1/22700$ and $L = 7$. In each part, results given at the last line correspond to a function φ_ζ constructed from sequence with negative coefficients.

4.6 Estimates of the second eigenvalue

To apply Theorem 3.1, 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

ζ	Θ_ζ	$\|r_\zeta\|_{L^2(\mathbb{R}^+)}$	$\min_j \tilde{\varphi}_j^\zeta$	$\varphi_j^\zeta(0)$	L^2 bound	H^1 bound
0.76811	0.590609794	1.24e-01	9.96e-03	0.875688761	4.04e-01	1.29e-01
0.76812	0.590550468	7.09e-02	9.22e-03	0.875497052	2.29e-01	7.37e-02
0.76813	0.590489644	6.38e-02	8.42e-03	0.875290012	2.06e-01	6.63e-02
0.76814	0.590427030	1.14e-01	7.55e-03	0.875063169	3.69e-01	1.18e-01
0.76815	0.590362191	1.15e-01	6.59e-03	0.874809295	3.75e-01	1.20e-01
0.76816	0.590294421	4.68e-02	5.47e-03	0.874515214	1.51e-01	4.86e-02
0.76817	0.590222360	3.69e-02	4.10e-03	0.874151234	1.18e-01	3.83e-02
0.76818	0.590142138	2.97e-02	2.06e-03	0.873603539	9.51e-02	3.08e-02
0.76819	0.590142240	4.62e+02	-5.34e+02	0.873050163	1.74e+04	4.80e+02
0.768181	0.590133151	1.91e-02	1.74e-03	0.873518103	6.10e-02	1.98e-02
0.768182	0.590123772	1.48e-02	1.36e-03	0.873415060	4.74e-02	1.54e-02
0.768183	0.590113724	1.15e-02	8.41e-04	0.873273295	3.69e-02	1.20e-02
0.768184	0.590108700	1.29e+02	-2.92e+01	0.873043549	2.58e+03	1.34e+02
0.7681831	0.590112653	1.01e-02	7.72e-04	0.873254315	3.23e-02	1.05e-02
0.7681832	0.590111566	1.38e-02	6.96e-04	0.873233646	4.42e-02	1.43e-02
0.7681833	0.590110455	8.01e-03	6.11e-04	0.873210604	2.56e-02	8.31e-03
0.7681834	0.590109318	8.42e-03	5.15e-04	0.873184197	2.69e-02	8.74e-03
0.7681835	0.590108136	5.45e-03	3.97e-04	0.873151984	1.74e-02	5.65e-03
0.7681836	0.590106880	5.47e-03	2.30e-04	0.873106156	1.75e-02	5.68e-03
0.7681837	0.590106199	3.63e+00	-3.95e+00	0.873043196	1.67e+01	3.77e+00
0.76818361	0.590106747	3.08e-03	2.06e-04	0.873099730	9.85e-03	3.20e-03
0.76818362	0.590106610	2.87e-03	1.80e-04	0.873092435	9.16e-03	2.98e-03
0.76818363	0.590106472	3.73e-03	1.49e-04	0.873084081	1.19e-02	3.87e-03
0.76818364	0.590106327	3.07e-03	1.11e-04	0.873073561	9.82e-03	3.19e-03
0.76818365	0.590106176	1.62e-03	5.24e-05	0.873057522	5.17e-03	1.68e-03
0.76818366	0.590106138	3.59e+00	-6.03e-01	0.873043148	1.65e+01	3.72e+00
0.768183651	0.590106159	8.42e-04	4.21e-05	0.873054696	2.70e-03	8.77e-04
0.768183652	0.590106143	8.63e-04	2.98e-05	0.873051330	2.77e-03	8.99e-04
0.768183653	0.590106126	1.79e-04	6.65e-06	0.873044968	5.86e-04	1.88e-04
0.768183654	0.590106128	4.14e+00	-7.38e-02	0.873043140	1.97e+01	4.29e+00

Table 1: Results obtained by Algorithm 4.2.

$\zeta \in [0.76818, 076819]$. If we denote by $A^{\zeta}_{i,j}$ the coefficients of the matrix A^{ζ}, we have:

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

We compute the second value and obtain $\mu_2(\zeta) \geq 3.315$. Figure 5 draws the second eigenvector.

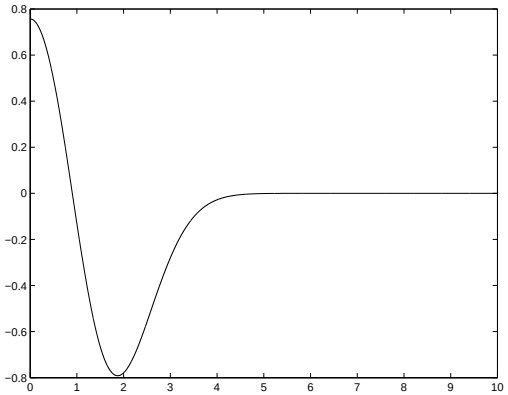

Figure 5: Second eigenvetor of $H(\zeta)$ for ζ close to ζ_0.

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

We apply Algorithm 4.2 for h such that $1/h \in \{100 \times k, k = 10, \ldots, 30000\}$ and for $L = 7, 8, 9, 10$. For each value, we obtain characteritic values as in Table 1 and we complete this table by computing the lower-bound of Θ_0 given by Theorem 3.1, a lower-bound and a upper-bound for $\Phi(0)$ given in Theorem 3.4. To make these computations, we need a lower-bound of $|\zeta - \zeta_0|$. The De Gennes [24] lower-bound of Θ_0 by 0.5901, our upper-bound by Θ_ζ and the monotonicity of the square-root function bound ζ_0 by

$$\sqrt{0.5901} < \zeta_0 < \sqrt{\Theta_\zeta}.$$

We can improve the upper-bound by choosing for Θ_ζ the lowest energy among all the computations and improve the lower-bound by the maximum between $\sqrt{0.5901}$ and the square-root of the lower-bound of Θ_0. We can iterate these computations and combine then to obtain the best result.
To extract the best computations, we collect the largest lower-bound of Θ_0 and $\Phi(0)$, the smallest energy Θ_ζ, the smallest upper-bound of $\Phi(0)$. We obtain:

Proposition 4.3.

$$0.590106122 \leq \Theta_0 \leq 0.590106125,$$
$$0.872991 \leq \Phi(0) \leq 0.873095.$$

This proposition estimates $\Theta_0 \simeq 0.590106123$ with an error less than 2×10^{-9} and of $\Phi(0) \simeq 0.8730$ at 10^{-4}.

5 Conclusion

The parameters Θ_0 and $\Phi(0)$ intervene naturally in the determination of the nucleation of superconductivity. We establish in this paper a very accurate estimate for them. These computations are useful to quantify the location of superconductivity and generate improvement of the numerics in domains with corners.

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