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Breaking a magnetic zero locus: model operators and numerical approach

V. Bonnaillie-Noël*, N. Raymond†

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Abstract

This paper is devoted to the spectral analysis of a Schrödinger operator in presence of a vanishing magnetic field. The influence of the smoothness of the magnetic zeros locus is studied. In particular, it is proved that breaking the magnetic zero locus induces discrete spectrum below the essential spectrum. Numerical simulations illustrate the theoretical results.

Keywords. Schrödinger operator, magnetic, spectrum, singular zero locus.

Classification MSC. 35P15, 81Q10

1 Introduction and results

1.1 Montgomery operator

This paper is motivated by the analysis of R. Montgomery performed in [18] where the problem is to investigate the semiclassical limit in presence of vanishing magnetic fields. Without going into the details let us explain which model operator is introduced in [18]. Montgomery was concerned by the magnetic Laplacian $(-ih\nabla + \mathbf{A})^2$ on $L^2(\mathbb{R}^2)$ in the case when the magnetic field $\beta = \nabla \times \mathbf{A}$ vanishes along a smooth curve Γ . Assuming that the magnetic field non degenerately vanishes, he was led to consider the self-adjoint realization on $L^2(\mathbb{R}^2)$ of:

$$\mathfrak{L} = D_t^2 + (D_s - st)^2.$$

In this case the magnetic field is given by $\beta(s, t) = s$ so that the zero locus of β is the line $s = 0$. Let us write the following change of gauge:

$$\mathfrak{L}^{\text{Mo}} = e^{-i\frac{s^2 t}{2}} \mathfrak{L} e^{i\frac{s^2 t}{2}} = D_s^2 + \left(D_t + \frac{s^2}{2}\right)^2.$$

The Fourier transform (after changing ξ in $-\xi$) with respect to t gives the direct integral:

$$\mathfrak{L}^{\text{Mo}} = \int^{\oplus} \mathfrak{L}_{\xi}^{\text{Mo}} d\xi, \quad \text{where} \quad \mathfrak{L}_{\xi}^{\text{Mo}} = D_s^2 + \left(-\xi + \frac{s^2}{2}\right)^2.$$

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From this representation, we deduce that:

$$\mathfrak{s}(\mathfrak{L}) = \mathfrak{s}_{\text{ess}}(\mathfrak{L}) = [\mu_{\text{Mo}}, +\infty), \quad (1.1)$$

where μ_{Mo} is defined as:

$$\mu_{\text{Mo}} = \inf_{\xi \in \mathbb{R}} \mu_1^{\text{Mo}}(\xi),$$

where $\mu_1^{\text{Mo}}(\xi)$ denotes the first eigenvalue of $\mathfrak{L}_\xi^{\text{Mo}}$. Let us recall a few important properties of $\mu_1^{\text{Mo}}(\xi)$ (for the proofs, see [19, 10, 14]).

Proposition 1.1 *The following properties hold:*

1. For all $\xi \in \mathbb{R}$, $\mu_1^{\text{Mo}}(\xi)$ is simple.
2. The function $\xi \mapsto \mu_1^{\text{Mo}}(\xi)$ is analytic.
3. We have: $\lim_{|\xi| \rightarrow +\infty} \mu_1^{\text{Mo}}(\xi) = +\infty$.
4. The function $\xi \mapsto \mu_1^{\text{Mo}}(\xi)$ admits a unique minimum at a point ξ_0 and it is non degenerate.

Conjecture 1.2 *We have: $\mu_{\text{Mo}} \geq 0.5$.*

With a finite element method and Dirichlet condition on the artificial boundary, we are able to give an upper-bound of the minimum and our numerical simulations provide $\mu_{\text{Mo}} \simeq 0.5698$ reached for $\xi_{\text{Mo}} \simeq 0.3467$ with a discretization step at 10^{-4} for the parameter ξ . This numerical estimate is already mentioned in [18].

If we consider the Neumann realization $\mathfrak{L}_\xi^{\text{Mo},+}$ of $D_t^2 + \left(-\xi + \frac{t^2}{2}\right)^2$ on \mathbb{R}^+ , then, by symmetry, the bottom of the spectrum of this operator is linked to the Montgomery operator:

Proposition 1.3 *If we denote by $\mu_1^{\text{Mo},+}(\xi)$ the bottom of the spectrum of $\mathfrak{L}_\xi^{\text{Mo},+}$ and $\mu_{\text{Mo},+} = \inf_{\xi \in \mathbb{R}} \mu_1^{\text{Mo},+}(\xi)$, then*

$$\mu_1^{\text{Mo},+}(\xi) = \mu_1^{\text{Mo}}(\xi) \quad \text{and} \quad \mu_{\text{Mo},+} = \mu_{\text{Mo}}.$$

Let us emphasize that the results of Proposition 1.1 were used to investigate the eigenvalues of $(-ih\nabla + \mathbf{A})^2$ in the limit $h \rightarrow 0$ in [19, 13, 11, 12, 8].

1.2 Breaking the Montgomery operator

1.2.1 Heuristics and motivation

As mentioned above, the bottom of the spectrum of \mathfrak{L} is essential. This fact is due to the translation invariance along the zero locus of β . This situation reminds what happens in the waveguides framework (see [9]). The general philosophy developed by Duclos and Exner (see also for instance [3, 4, 15]) establishes that eliminating the translation invariance induces discrete spectrum below the essential spectrum. More recently, waveguides with corners are considered in [6, 7] where it is enlightened that breaking the translation invariance by adding a corner creates bound states having nice structures (see also [2]).

Guided by the ideas developed for the waveguides, we aim at analyzing the effect of breaking the zero locus of β . Introducing the “breaking parameter” $\theta \in (-\pi, \pi]$, we will break the invariance of the zero locus in three different ways:

1. Case with Dirichlet boundary: $\mathfrak{L}_\theta^{\text{Dir}}$. We let $\mathbb{R}_+^2 = \{(s, t) \in \mathbb{R}^2, t > 0\}$ and consider $\mathfrak{L}_\theta^{\text{Dir}}$ the Dirichlet realization, defined as a Friedrichs extension, on $L^2(\mathbb{R}_+^2)$ of:

$$D_t^2 + \left(D_s + \frac{t^2}{2} \cos \theta - st \sin \theta \right)^2.$$

2. Case with Neumann boundary: $\mathfrak{L}_\theta^{\text{Neu}}$. We consider $\mathfrak{L}_\theta^{\text{Neu}}$ the Neumann realization, defined as a Friedrichs extension, on $L^2(\mathbb{R}_+^2)$ of:

$$D_t^2 + \left(D_s + \frac{t^2}{2} \cos \theta - st \sin \theta \right)^2.$$

The corresponding magnetic field is $\beta(s, t) = t \cos \theta - s \sin \theta$. It cancels along the half-line $t = s \tan \theta$.

3. Magnetic broken line: \mathfrak{L}_θ . We consider \mathfrak{L}_θ the Friedrichs extension on $L^2(\mathbb{R}^2)$ of:

$$D_t^2 + \left(D_s + \text{sgn}(t) \frac{t^2}{2} \cos \theta - st \sin \theta \right)^2.$$

The corresponding magnetic field is $\beta(s, t) = |t| \cos \theta - s \sin \theta$; it is a continuous function which cancels along the broken line $|t| = s \tan \theta$.

Notation 1.4 We use the notation $\mathfrak{L}_\theta^\bullet$ where \bullet can be Dir, Neu or \emptyset .

1.2.2 Properties of the spectra

Let us analyze the dependence of the spectra of $\mathfrak{L}_\theta^\bullet$ on the parameter θ .

Symmetries Denoting by S the axial symmetry $(s, t) \mapsto (-s, t)$, we get:

$$\mathfrak{L}_{-\theta}^\bullet = S \overline{\mathfrak{L}_\theta^\bullet} S,$$

where the line denotes the complex conjugation. Then, we notice that $\mathfrak{L}_\theta^\bullet$ and $\overline{\mathfrak{L}_\theta^\bullet}$ are isospectral. Therefore, the analysis is reduced to $\theta \in [0, \pi)$. Moreover, we get:

$$S \mathfrak{L}_\theta^\bullet S = \mathfrak{L}_{\pi-\theta}^\bullet.$$

The study is reduced to $\theta \in [0, \frac{\pi}{2}]$.

Analyticity We observe that at $\theta = 0$ and $\theta = \frac{\pi}{2}$ the domain of $\mathfrak{L}_\theta^\bullet$ is not continuous.

Lemma 1.5 The family $(\mathfrak{L}_\theta^\bullet)_{\theta \in (0, \frac{\pi}{2})}$ is analytic.

Proof: For $\theta \in (0, \frac{\pi}{2})$, we perform the scaling:

$$t = \left(\frac{\sin \theta}{\cos^2 \theta} \right)^{1/3} \tau, \quad s = \left(\frac{\cos \theta}{\sin^2 \theta} \right)^{1/3} \sigma,$$

so that $\mathfrak{L}_\theta^\bullet$ becomes:

$$\widetilde{\mathfrak{L}}_\theta^\bullet = \left(\frac{\cos^2 \theta}{\sin \theta} \right)^{2/3} D_\tau^2 + \left(\frac{\sin^2 \theta}{\cos \theta} \right)^{1/3} \left(D_\sigma + \text{sgn}(\tau) \frac{\tau^2}{2} - \sigma \tau \right)^2,$$

whose form domain does not depend on θ . ■

Essential spectra The following proposition states that the essential spectrum is the same for $\mathfrak{L}_\theta^{\text{Dir}}$, $\mathfrak{L}_\theta^{\text{Neu}}$ and \mathfrak{L}_θ .

Proposition 1.6 For $\theta \in (0, \frac{\pi}{2})$, we have $\mathfrak{s}_{\text{ess}}(\mathfrak{L}_\theta^\bullet) = [\mu_{\mathbf{M}_\bullet}, +\infty)$.

In the Dirichlet case, the spectrum is essential:

Proposition 1.7 For all $\theta \in (0, \frac{\pi}{2})$, we have $\mathfrak{s}(\mathfrak{L}_\theta^{\text{Dir}}) = [\mu_{\mathbf{M}_\bullet}, +\infty)$.

Propositions 1.6 and 1.7 will be proved in Subsection 2.1.

Discrete spectra From now we assume that $\bullet = \text{Neu}, \emptyset$.

Notation 1.8 Let us denote by $\lambda_n^\bullet(\theta)$ the n -th Rayleigh quotient of $\mathfrak{L}_\theta^\bullet$.

The two following propositions are Agmon type estimates and give the exponential decay of the eigenfunctions. \mathbb{R}_\bullet^2 denotes $\mathbb{R}_+^2, \mathbb{R}^2$ when $\bullet = \text{Neu}, \emptyset$ respectively.

Proposition 1.9 There exist $\varepsilon_0, C > 0$ such that for all $\theta \in (0, \frac{\pi}{2})$ and all eigenpair (λ, ψ) of $\mathfrak{L}_\theta^\bullet$ such that $\lambda < \mu_{\mathbf{M}_\bullet}$, we have:

$$\int_{\mathbb{R}_\bullet^2} e^{2\varepsilon_0|t|\sqrt{\mu_{\mathbf{M}_\bullet}-\lambda}}|\psi|^2 dt \leq C(\mu_{\mathbf{M}_\bullet} - \lambda)^{-1}\|\psi\|^2.$$

Proposition 1.10 There exist $\varepsilon_0, C > 0$ such that for all $\theta \in (0, \frac{\pi}{2})$ and all eigenpair (λ, ψ) of $\mathfrak{L}_\theta^\bullet$ such that $\lambda < \mu_{\mathbf{M}_\bullet}$, we have:

$$\int_{\mathbb{R}_\bullet^2} e^{2\varepsilon_0|s|\sin\theta\sqrt{\mu_{\mathbf{M}_\bullet}-\lambda}}|\psi|^2 dt \leq C(\mu_{\mathbf{M}_\bullet} - \lambda)^{-1}\|\psi\|^2.$$

Propositions 1.9 and 1.10 will be proved in Subsections 2.2.1 and 2.2.2 respectively.

The following proposition (the proof of which can be found in [19]) states that $\mathfrak{L}_\theta^{\text{Neu}}$ admits an eigenvalue below its essential spectrum when $\theta \in (0, \frac{\pi}{2})$.

Proposition 1.11 For all $\theta \in (0, \frac{\pi}{2}]$, $\lambda_1^{\text{Neu}}(\theta) < \mu_{\mathbf{M}_\bullet}$.

Remark 1.12 The situation seems to be different for \mathfrak{L}_θ . According to numerical simulations with finite element method, there exists $\theta_0 \in (\frac{\pi}{4}, \frac{\pi}{2})$ such that $\lambda_1(\theta) < \mu_{\mathbf{M}_\bullet}$ for all $\theta \in (0, \theta_0)$ and $\lambda_1(\theta) = \mu_{\mathbf{M}_\bullet}$ for all $\theta \in [\theta_0, \frac{\pi}{2})$.

1.3 Singular limit $\theta \rightarrow 0$

1.3.1 Renormalization

Thanks to Proposition 1.11, one knows that breaking the invariance of the zero locus of the magnetic field with a Neumann boundary creates a bound state. We also would like to tackle this question for \mathfrak{L}_θ and in any case to estimate more quantitatively this effect. A way to do this is to consider the limit $\theta \rightarrow 0$. First, we perform a scaling:

$$s = (\cos\theta)^{-1/3}\hat{s}, \quad t = (\cos\theta)^{-1/3}\hat{t}. \quad (1.2)$$

The operator $\mathfrak{L}_\theta^\bullet$ is thus unitarily equivalent to $(\cos\theta)^{2/3}\hat{\mathfrak{L}}_{\tan\theta}^\bullet$, where the expression of $\hat{\mathfrak{L}}_{\tan\theta}^\bullet$ is given by:

$$D_{\hat{t}}^2 + \left(D_{\hat{s}} + \text{sgn}(\hat{t})\frac{\hat{t}^2}{2} - \hat{s}\hat{t}\tan\theta \right)^2.$$

Notation 1.13 We let $\varepsilon = \tan \theta$.

For $(\alpha, \xi) \in \mathbb{R}^2$ and $\varepsilon > 0$, we introduce the unitary transform:

$$V_{\varepsilon, \alpha, \xi} \psi(\hat{s}, \hat{t}) = e^{-i\xi \hat{s}} \psi\left(\hat{s} - \frac{\alpha}{\varepsilon}, \hat{t}\right),$$

and the conjugate operator:

$$\hat{\mathfrak{L}}_{\varepsilon, \alpha, \xi}^{\bullet} = V_{\varepsilon, \alpha, \xi}^{-1} \hat{\mathfrak{L}}_{\varepsilon}^{\bullet} V_{\varepsilon, \alpha, \xi}.$$

Its expression is given by:

$$\hat{\mathfrak{L}}_{\varepsilon, \alpha, \xi}^{\bullet} = D_{\hat{t}}^2 + \left(-\xi - \alpha \hat{t} + \operatorname{sgn}(\hat{t}) \frac{\hat{t}^2}{2} + D_s - \varepsilon \hat{s} \hat{t} \right)^2.$$

Let us introduce the rescaled variable:

$$\hat{s} = \varepsilon^{-1/2} \hat{\sigma}. \quad (1.3)$$

Therefore $\hat{\mathfrak{L}}_{\varepsilon, \alpha, \xi}^{\bullet}$ is unitarily equivalent to $\mathfrak{M}_{\varepsilon, \alpha, \xi}^{\bullet}$ whose expression is given by:

$$\mathfrak{M}_{\varepsilon, \alpha, \xi}^{\bullet} = D_{\hat{t}}^2 + \left(-\xi - \alpha \hat{t} + \operatorname{sgn}(\hat{t}) \frac{\hat{t}^2}{2} + \varepsilon^{1/2} D_{\hat{\sigma}} - \varepsilon^{1/2} \hat{\sigma} \hat{t} \right)^2. \quad (1.4)$$

1.3.2 New model operators

By taking formally $\varepsilon = 0$ in (1.4) we are led to two families of one dimensional operators on $L^2(\mathbb{R}_{\bullet}^2)$ with two parameters $(\alpha, \xi) \in \mathbb{R}^2$:

$$\mathcal{M}_{\alpha, \xi}^{\bullet} = D_{\hat{t}}^2 + \left(-\xi - \alpha \hat{t} + \operatorname{sgn}(\hat{t}) \frac{\hat{t}^2}{2} \right)^2.$$

These operators have compact resolvents and are analytic families with respect to $(\alpha, \xi) \in \mathbb{R}^2$.

Notation 1.14 We denote by $\mu_n^{\bullet}(\alpha, \xi)$ the n -th eigenvalue of $\mathcal{M}_{\alpha, \xi}^{\bullet}$.

Roughly speaking $\mathcal{M}_{\alpha, \xi}^{\bullet}$ is the operator valued symbol of (1.4), so that we expect that the behavior of the so-called ‘‘band function’’ $(\alpha, \xi) \mapsto \mu_1^{\bullet}(\alpha, \xi)$ determines the structure of the low lying spectrum of $\mathfrak{M}_{\varepsilon, \alpha, \xi}^{\bullet}$ in the limit $\varepsilon \rightarrow 0$.

The two following theorems state that the band functions admit a minimum (see Section 3 for the proofs and numerical simulations).

Theorem 1.15 The function $\mathbb{R} \times \mathbb{R} \ni (\alpha, \xi) \mapsto \mu_1^{\text{Neu}}(\alpha, \xi)$ admits a minimum denoted by $\underline{\mu}_1^{\text{Neu}}$. Moreover we have:

$$\liminf_{|\alpha|+|\xi| \rightarrow +\infty} \mu_1^{\text{Neu}}(\alpha, \xi) \geq \mu_{\text{Mo}} > \min_{(\alpha, \xi) \in \mathbb{R}^2} \mu_1^{\text{Neu}}(\alpha, \xi) = \underline{\mu}_1^{\text{Neu}}.$$

Theorem 1.16 Under Conjecture 1.2, the function $\mathbb{R} \times \mathbb{R} \ni (\alpha, \xi) \mapsto \mu_1(\alpha, \xi)$ admits a minimum denoted by $\underline{\mu}_1$. Moreover we have:

$$\liminf_{|\alpha|+|\xi| \rightarrow +\infty} \mu_1(\alpha, \xi) \geq \mu_{\text{Mo}} > \min_{(\alpha, \xi) \in \mathbb{R}^2} \mu_1(\alpha, \xi) = \underline{\mu}_1.$$

Remark 1.17 *We have:*

$$\underline{\mu}_1^{\text{Neu}} \leq \underline{\mu}_1. \quad (1.5)$$

Our numerical experiments lead to the following conjecture.

Conjecture 1.18 – *The inequality (1.5) is strict.*

– *The minimum $\underline{\mu}_1^\bullet$ is unique and non-degenerate.*

Under this conjecture one can provide an asymptotic expansion of the eigenvalues (see [21]).

Theorem 1.19 *If Conjecture 1.18 is true, then we have, for all $n \geq 1$:*

$$\lambda_n^\bullet(\theta) = \underline{\mu}_1^\bullet + (2n - 1)\theta (\det \underline{\text{Hess}}^\bullet)^{1/2} + o(\theta), \quad (1.6)$$

where $\underline{\text{Hess}}^\bullet$ denotes the Hessian matrix of μ^\bullet at the point where the minimum $\underline{\mu}_1^\bullet$ is reached. In particular, if Conjecture 1.2 is true, we infer that $\lambda_n(\theta)$ is an eigenvalue when θ is small enough.

This theorem is illustrated and confirmed by our numerical simulations in Section 4. In particular we can even provide approximations of $(\det \underline{\text{Hess}}^\bullet)^{1/2}$.

2 Rough localization near the “corner”

2.1 Estimate of the essential spectrum

Let us first prove a weaker version of Proposition 1.7:

Lemma 2.1 *For all $\theta \in (0, \frac{\pi}{2})$, we have $\mathfrak{s}(\mathfrak{L}_\theta^{\text{Dir}}) \subset [\mu_{\text{Mo}}, +\infty)$.*

Proof: By the min-max principle, we have:

$$\inf \mathfrak{s} \left(\mathfrak{L}_\theta^{\text{Dir}} \right) \geq \inf \mathfrak{s}(M_\theta),$$

where M_θ is the Friedrichs extension on $L^2(\mathbb{R}^2)$ of:

$$D_t^2 + \left(D_s + \frac{t^2}{2} \cos \theta - st \sin \theta \right)^2.$$

By using the rotation of angle $\frac{\pi}{2} - \theta$ and a change of gauge we are reduced to the operator:

$$D_t^2 + (D_s - st)^2.$$

From (1.1), we have $\mathfrak{s}(M_{\frac{\pi}{2}}) = [\mu_{\text{Mo}}, +\infty)$. The conclusion follows. \blacksquare

Let us now prove Proposition 1.6.

Proof: For this, we use the Persson’s lemma [20]:

Lemma 2.2 *Let Ω be an unbounded domain of \mathbb{R}^2 with Lipschitzian boundary. Then the bottom of the essential spectrum of the Neumann realization P of the Schrödinger operator $-\Delta_{\mathbf{A}} := (-i\nabla + \mathbf{A})^2$ is given by*

$$\inf \text{sp}_{\text{ess}}(P) = \lim_{R \rightarrow \infty} \Sigma(-\Delta_{\mathbf{A}}, R),$$

with

$$\Sigma(-\Delta_{\mathbf{A}}, R) = \inf_{\psi \in C_0^\infty(\overline{\Omega} \cap \mathcal{B}_R)} \frac{\int_{\mathbb{R}_\bullet^2} |(-i\nabla + \mathbf{A})\psi|^2}{\int_{\Omega} |\psi|^2},$$

where \mathcal{B}_R denotes the ball of radius R (for any norm) centered at the origin and $\mathcal{CB}_R = \Omega \setminus \mathcal{B}_R$.

We recall that \mathbb{R}_\bullet^2 denotes \mathbb{R}^2 when $\bullet = \emptyset$ and \mathbb{R}_\pm^2 if $\bullet = \text{Dir}$ or Neu . Let us denote by $\mathfrak{Q}_\theta^\bullet$ the quadratic form associated with $\mathfrak{L}_\theta^\bullet$.

Lower bound We introduce

$$\Omega_{R,\theta} = \{(s, t) \in \mathbb{R}_\bullet^2 : |s| \leq R(\sin \theta)^{-1}, |t| \leq R\}.$$

Let $\psi \in C^\infty(\Omega_{\theta,R}^c)$ and (χ_0, χ_1) be a partition of unity such that

$$\chi_0(t) = \begin{cases} 1 & \text{for } |t| \leq \frac{1}{2}, \\ 0 & \text{for } |t| \geq 1. \end{cases}$$

For $j = 0, 1$, we let:

$$\chi_{j,R}(t) = \chi_j(R^{-1}t),$$

so that:

$$\chi_{0,R}^2 + \chi_{1,R}^2 = 1.$$

The ‘‘IMS’’ formula gives:

$$\mathfrak{Q}_\theta^\bullet(\psi) \geq \mathfrak{Q}_\theta^\bullet(\chi_{0,R}\psi) + \mathfrak{Q}_\theta^\bullet(\chi_{1,R}\psi) - CR^{-2}\|\psi\|^2.$$

Using Lemma 2.1, we have:

$$\mathfrak{Q}_\theta^\bullet(\chi_{1,R}\psi) \geq \mu_{\text{Mo}}\|\chi_{1,R}\psi\|^2.$$

Moreover, using that $\mathfrak{Q}_\theta^\bullet(v) \geq \left| \int_{\mathbb{R}_\bullet^2} \beta(s, t) |v|^2 \, ds \, dt \right|$, we have on the support of $\chi_{0,R}\psi$:

$$\mathfrak{Q}_\theta^\bullet(\chi_{0,R}\psi) \geq \int_{\mathbb{R}_\bullet^2} ||t| \cos \theta - s \sin \theta| |\chi_{0,R}\psi|^2 \, ds \, dt.$$

On the support of $\chi_{0,R}\psi$, we have:

$$||t| \cos \theta - s \sin \theta| \geq R(1 - \cos \theta).$$

It follows that:

$$\mathfrak{Q}_\theta^\bullet(\psi) \geq (\min(\mu_{\text{Mo}}, R(1 - \cos \theta)) - CR^{-2}) \|\psi\|^2.$$

Consequently, we deduce

$$\Sigma(\mathfrak{L}_\theta^\bullet, R) \geq \min(\mu_{\text{Mo}}, R(1 - \cos \theta)) - CR^{-2}.$$

Thus

$$\inf \text{sp}_{\text{ess}}(\mathfrak{L}_\theta^\bullet) \geq \mu_{\text{Mo}}.$$

Upper bound Using the operator \mathfrak{L} or $\mathfrak{L}^{\mathbf{M}_0}$, we can realize a rotation and adaptative gauge transform to deal with the realization on \mathbb{R}^2 of $D_t^2 + (D_s + \frac{t^2}{2} \cos \theta - st \sin \theta)^2$ whose bottom of the spectrum equals $\mu_{\mathbf{M}_0}$. For any $\varepsilon > 0$, there exists a L^2 -normalized function $u \in \mathcal{C}_0^\infty(\mathbb{R}^2)$ such that

$$\mu_{\mathbf{M}_0} \leq \int_{\mathbb{R}^2} |D_t u|^2 + \left| \left(D_s + \frac{t^2}{2} \cos \theta - st \sin \theta \right) u \right|^2 ds dt \leq \mu_{\mathbf{M}_0} + \varepsilon.$$

There exists $\ell > 0$ such that $\text{supp } u \subset [-\ell, \ell]^2$. Let $R > 0$ be fixed. After a translation and gauge transform, we can construct a function ψ whose support is included in $[R, R + 2\ell]^2$ such that:

$$\begin{aligned} \mu_{\mathbf{M}_0} + \varepsilon &\geq \int_{[R, R+2\ell]^2} |D_t \psi|^2 + \left| \left(D_s + \frac{t^2}{2} \cos \theta - st \sin \theta \right) \psi \right|^2 ds dt \\ &= \int_{[R, R+2\ell]^2} |D_t \psi|^2 + \left| \left(D_s + \frac{t^2}{2} \cos \theta - st \sin \theta \right) \psi \right|^2 ds dt \\ &= \mathfrak{Q}_\theta^\bullet(\psi). \end{aligned}$$

Thus

$$\Sigma(\mathfrak{L}_\theta^\bullet, R) \leq \mu_{\mathbf{M}_0} + \varepsilon.$$

Using the Persson's lemma and taking $\varepsilon \rightarrow 0$, we deduce $\inf \text{sp}_{\text{ess}}(\mathfrak{L}_\theta^\bullet) \leq \mu_{\mathbf{M}_0}$. \blacksquare

Combining Lemma 2.1 and Proposition 1.6, we deduce Proposition 1.7.

2.2 Agmon estimates

In this section we aim at establishing Propositions 1.9 and 1.10.

2.2.1 Agmon estimates with respect to t

Let us fix $m \geq 1$ and $\varepsilon > 0$. We let $\Phi_m(t) = |t| \chi_m(t) \sqrt{\varepsilon} \sqrt{\mu_{\mathbf{M}_0} - \lambda}$, where χ_m is a $\mathcal{C}^\infty(\mathbb{R})$ cut-off function such that

$$\chi_m(t) = \chi_0\left(\frac{t}{m}\right). \quad (2.1)$$

For shortness, we denote $\tilde{\psi}_m = e^{\Phi_m} \psi$. We have:

$$\mathfrak{Q}_\theta^\bullet(\chi_{0,R} \tilde{\psi}_m) + \mathfrak{Q}_\theta^\bullet(\chi_{1,R} \tilde{\psi}_m) - CR^{-2} \|\tilde{\psi}_m\|^2 \leq \lambda \|\tilde{\psi}_m\|^2 + \|\nabla \Phi_m \tilde{\psi}_m\|^2.$$

Let $\tilde{C} > 0$ be independent of m and such that $\|\nabla \Phi_m\|_\infty^2 \leq \varepsilon \tilde{C} (\mu_{\mathbf{M}_0} - \lambda)$. We have:

$$\mathfrak{Q}_\theta^\bullet(\chi_{1,R} \tilde{\psi}_m) \geq \mu_{\mathbf{M}_0} \|\chi_{1,R} \tilde{\psi}_m\|^2, \quad (2.2)$$

so that:

$$(\mu_{\mathbf{M}_0} - \lambda - CR^{-2} - \varepsilon \tilde{C} (\mu_{\mathbf{M}_0} - \lambda)) \|\chi_{1,R} \tilde{\psi}_m\|^2 \leq (\lambda + CR^{-2} + \varepsilon \tilde{C} (\mu_{\mathbf{M}_0} - \lambda)) \|\chi_{0,R} \tilde{\psi}_m\|^2.$$

We choose $\varepsilon \leq \frac{1}{2\tilde{C}}$ and $R \geq \frac{2\sqrt{\tilde{C}}}{\sqrt{\mu_{\mathbf{M}_0} - \lambda}}$ so that:

$$(\mu_{\mathbf{M}_0} - \lambda) \|\chi_{1,R} \tilde{\psi}_m\|^2 \leq \hat{C} \|\chi_{0,R} \tilde{\psi}_m\|^2 \leq C \|\psi\|^2.$$

It follows that:

$$(\mu_{\mathbf{M}_0} - \lambda) \|\tilde{\psi}_m\|^2 \leq C \|\psi\|^2.$$

Then, we take the limit $m \rightarrow +\infty$.

2.2.2 Rough Agmon estimates with respect to s

Let us fix $m \geq 1$ and $\varepsilon > 0$. We let $\Phi_m(s) = |s| \sin \theta \chi_m(s) \sqrt{\varepsilon} \sqrt{\mu_{\mathbf{M}_0} - \lambda}$. For shortness, we let $\tilde{\psi}_m = e^{\Phi_m} \psi$. We have:

$$\mathfrak{Q}_\theta^\bullet(\chi_{0,R}(t)\tilde{\psi}_m) + \mathfrak{Q}_\theta^\bullet(\chi_{1,R}(t)\tilde{\psi}_m) - CR^{-2}\|\tilde{\psi}_m\|^2 \leq \lambda\|\tilde{\psi}_m\|^2 + \|\nabla\Phi_m\tilde{\psi}_m\|^2.$$

As in the proof of Proposition 1.9, upper-bound (2.2) is still available and we choose $\varepsilon \leq \frac{1}{2\hat{C}}$ and $R \geq \frac{2\sqrt{\hat{C}}}{\sqrt{\mu_{\mathbf{M}_0} - \lambda}}$ so that:

$$(\mu_{\mathbf{M}_0} - \lambda)\|\chi_{1,R}\tilde{\psi}_m\|^2 \leq \hat{C}\|\chi_{0,R}\tilde{\psi}_m\|^2.$$

Thus, we deduce:

$$\mathfrak{Q}_\theta^\bullet(\chi_{0,R}(t)\tilde{\psi}_m) \leq (\lambda + CR^{-2})\|\chi_{0,R}(t)\tilde{\psi}_m\|^2 + \|\nabla\Phi_m\chi_{0,R}(t)\tilde{\psi}_m\|^2.$$

Let us now use a partition of unity with respect to s :

$$\chi_{0,R,\theta}^2 + \chi_{1,R,\theta}^2 = 1,$$

where $\chi_{j,R,\theta}(s) = \chi_j(s(2R)^{-1} \sin \theta)$. We have:

$$\sum_{j=1}^2 \mathfrak{Q}_\theta^\bullet(\chi_{j,R,\theta}(s)\chi_{0,R}(t)\tilde{\psi}_m) \leq (\lambda + \hat{C}R^{-2})\|\chi_{0,R}(t)\tilde{\psi}_m\|^2 + \|\nabla\Phi_m\chi_{0,R}(t)\tilde{\psi}_m\|^2.$$

We get:

$$\mathfrak{Q}_\theta^\bullet(\chi_{1,R,\theta}(s)\chi_{0,R}(t)\tilde{\psi}_m) \geq R \left(1 - \frac{\cos \theta}{2}\right) \|\chi_{1,R,\theta}(s)\chi_{0,R}(t)\tilde{\psi}_m\|^2.$$

We infer that:

$$\begin{aligned} & \left(R \left(1 - \frac{\cos \theta}{2}\right) - \lambda - \hat{C}R^{-2} - \tilde{C}\varepsilon(\mu_{\mathbf{M}_0} - \lambda) \right) \|\chi_{1,R,\theta}(s)\chi_{0,R}(t)\tilde{\psi}_m\|^2 \\ & \leq (\lambda + \hat{C}R^{-2} + \tilde{C}\varepsilon(\mu_{\mathbf{M}_0} - \lambda))\|\chi_{0,R,\theta}(s)\chi_{0,R}(t)\tilde{\psi}_m\|^2 \leq c\|\chi_{0,R}(t)\psi\|^2, \end{aligned}$$

so that:

$$\|\chi_{0,R}(t)\tilde{\psi}_m\|^2 \leq c\|\chi_{0,R}(t)\psi\|^2.$$

We infer that:

$$\|e^{\Phi_m}\psi\| \leq C((\mu_{\mathbf{M}_0} - \lambda)^{-1} + 1)\|\psi\|.$$

It remains to take the limit $m \rightarrow +\infty$.

3 Montgomery operator with two parameters

We will see that the properties of $\mathcal{M}_{\alpha,\xi}^{\text{Neu}}$ be can used to investigate those of $\mathcal{M}_{\alpha,\xi}$. Therefore we begin by analyzing the family of operators $\mathcal{M}_{\alpha,\xi}^{\text{Neu}}$ and we prove Theorem 1.15 and apply it to prove Theorem 1.16.

3.1 Analysis of $\mathcal{M}_{\alpha,\xi}^{\text{Neu}}$

3.1.1 Existence of a minimum for $\mu_1^{\text{Neu}}(\alpha, \xi)$

To analyze the family of operators $\mathcal{M}_{\alpha,\xi}^{\text{Neu}}$ depending on parameters (α, ξ) , we introduce the new parameters (α, δ) using a change of variables. Let us introduce the following change of parameters:

$$\mathcal{P}(\alpha, \xi) = (\alpha, \delta) = \left(\alpha, \xi + \frac{\alpha^2}{2} \right).$$

A straight forward computation provides that $\mathcal{P} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ is a C^∞ -diffeomorphism such that:

$$|\alpha| + |\xi| \rightarrow +\infty \Leftrightarrow |\mathcal{P}(\alpha, \xi)| \rightarrow +\infty.$$

We have $\mathcal{M}_{\alpha,\xi}^{\text{Neu}} = \mathcal{N}_{\alpha,\delta}^{\text{Neu}}$, where:

$$\mathcal{N}_{\alpha,\delta}^{\text{Neu}} = D_t^2 + \left(\frac{(t-\alpha)^2}{2} - \delta \right)^2,$$

with Neumann condition on $t = 0$. Let us denote by $\nu_1^{\text{Neu}}(\alpha, \delta)$ the lowest eigenvalue of $\mathcal{N}_{\alpha,\delta}^{\text{Neu}}$, so that:

$$\mu_1^{\text{Neu}}(\alpha, \xi) = \nu_1^{\text{Neu}}(\alpha, \delta) = \nu_1^{\text{Neu}}(\mathcal{P}(\alpha, \xi)).$$

We denote by $\text{Dom}(\mathcal{Q}_{\alpha,\delta}^{\text{Neu}})$ the domain of the operator and by $\mathcal{Q}_{\alpha,\delta}^{\text{Neu}}$ the associated quadratic form. To prove Theorem 1.15, we establish the following result:

Theorem 3.1 *The function $\mathbb{R} \times \mathbb{R} \ni (\alpha, \delta) \mapsto \nu_1^{\text{Neu}}(\alpha, \delta)$ admits a minimum. Moreover we have:*

$$\liminf_{|\alpha|+|\delta| \rightarrow +\infty} \nu_1^{\text{Neu}}(\alpha, \delta) \geq \mu_{\text{Mo}} > \min_{(\alpha,\delta) \in \mathbb{R}^2} \nu_1^{\text{Neu}}(\alpha, \delta).$$

To prove this result, we decompose the plane in subdomains (see Figure 1) and analyze in each part. It is too higher when parameters (α, δ) are in some areas.

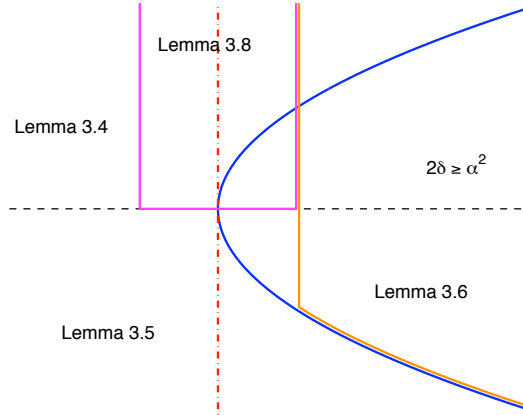


Figure 1: Illustration of the partition of \mathbb{R}^2 to localize the minimizer of $\mathcal{N}_{\alpha,\delta}^{\text{Neu}}$

Lemma 3.2 *For all $(\alpha, \delta) \in \mathbb{R}^2$ such that $\delta \geq \frac{\alpha^2}{2}$, we have:*

$$-\partial_\alpha \nu_1^{\text{Neu}}(\alpha, \delta) + \sqrt{2\delta} \partial_\delta \nu_1^{\text{Neu}}(\alpha, \delta) > 0.$$

Thus there is no critical point in the area $\{\delta \geq \frac{\alpha^2}{2}\}$.

Proof: The Feynman-Hellmann formulas provide:

$$\partial_\alpha \nu_1^{\text{Neu}}(\alpha, \delta) = -2 \int_0^{+\infty} \left(\frac{(t-\alpha)^2}{2} - \delta \right) (t-\alpha) u_{\alpha, \delta}^2(t) dt,$$

$$\partial_\delta \nu_1^{\text{Neu}}(\alpha, \delta) = -2 \int_0^{+\infty} \left(\frac{(t-\alpha)^2}{2} - \delta \right) u_{\alpha, \delta}^2(t) dt.$$

We infer:

$$-\partial_\alpha \nu_1^{\text{Neu}}(\alpha, \delta) + \sqrt{2\delta} \partial_\delta \nu_1^{\text{Neu}}(\alpha, \delta) = \int_0^{+\infty} (t-\alpha-\sqrt{2\delta})(t-\alpha+\sqrt{2\delta})(t-\alpha-\sqrt{2\delta}) u_{\alpha, \delta}^2(t) dt.$$

We have:

$$\int_0^{+\infty} (t-\alpha-\sqrt{2\delta})^2 (t-\alpha+\sqrt{2\delta}) u_{\alpha, \delta}^2(t) dt > 0.$$

■

Lemma 3.3 *We have:*

$$\inf_{(\alpha, \delta) \in \mathbb{R}^2} \nu_1^{\text{Neu}}(\alpha, \delta) < \mu_{\text{Mo}}.$$

Proof: We apply Lemma 3.2 at $\alpha = 0$ and $\delta = \delta_{\text{Mo}}$ to deduce that:

$$\partial_\alpha \nu_1^{\text{Neu}}(0, \delta_{\text{Mo}}) < 0.$$

■

The following lemma is obvious:

Lemma 3.4 *For all $\delta \leq 0$, we have:*

$$\nu_1^{\text{Neu}}(\alpha, \delta) \geq \delta^2.$$

In particular, we have

$$\nu_1^{\text{Neu}}(\alpha, \delta) > \mu_{\text{Mo}}, \quad \forall \delta < -\sqrt{\mu_{\text{Mo}}}.$$

Lemma 3.5 *For $\alpha \leq 0$ and $\delta \leq \frac{\alpha^2}{2}$, we have:*

$$\nu_1^{\text{Neu}}(\alpha, \delta) \geq \mu_1^{\text{Mo}}(0) > \mu_{\text{Mo}}.$$

Proof: We have, for all $\psi \in \text{Dom}(\mathcal{Q}_{\alpha, \delta}^{\text{Neu}})$:

$$\mathcal{Q}_{\alpha, \delta}^{\text{Neu}}(\psi) = \int_{\mathbb{R}_+} |D_t \psi|^2 + \left(\frac{(t-\alpha)^2}{2} - \delta \right)^2 |\psi|^2 dt$$

and

$$\left(\frac{(t-\alpha)^2}{2} - \delta \right)^2 \geq \left(\frac{t^2}{2} - \alpha t + \frac{\alpha^2}{2} - \delta \right)^2 \geq \frac{t^4}{4}.$$

The min-max principle provides:

$$\nu_1^{\text{Neu}}(\alpha, \delta) \geq \mu_1^{\text{Mo}}(0).$$

Moreover, thanks to the Feynman-Hellmann theorem, we get:

$$\left(\partial_\delta \mu_1^{\text{Mo}}(\delta) \right)_{\delta=0} = - \int_{\mathbb{R}_+} t^2 u_0(t)^2 dt < 0.$$

■

Lemma 3.6 *There exist $C, D > 0$ such that for all $\alpha \in \mathbb{R}$ and $\delta \geq D$ such that $\frac{\alpha}{\sqrt{\delta}} \geq -1$:*

$$\nu_1^{\text{Neu}}(\alpha, \delta) \geq C\delta^{1/2}.$$

Proof: For $\alpha \in \mathbb{R}$ and $\delta > 0$, we can perform the change of variable:

$$\tau = \frac{t - \alpha}{\sqrt{\delta}}.$$

The operator $\delta^{-2}\mathcal{N}_{\alpha, \delta}^{\text{Neu}}$ is unitarily equivalent to:

$$\hat{\mathcal{N}}_{\hat{\alpha}, h}^{\text{Neu}} = h^2 D_\tau^2 + \left(\frac{\tau^2}{2} - 1 \right)^2,$$

on $L^2((-\hat{\alpha}, +\infty))$, with $\hat{\alpha} = \frac{\alpha}{\sqrt{\delta}}$ and $h = \delta^{-3/2}$. We denote by $\hat{\nu}_1^{\text{Neu}}(\hat{\alpha}, h)$ the lowest eigenvalue of $\hat{\mathcal{N}}_{\hat{\alpha}, h}^{\text{Neu}}$. We aim at establishing a uniform lower with respect to $\hat{\alpha}$ of $\hat{\nu}_1^{\text{Neu}}(\hat{\alpha}, h)$ when $h \rightarrow 0$. We have to be careful with the dependence on $\hat{\alpha}$.

We introduce a partition of unity on \mathbb{R} with balls of size $r > 0$ and centers τ_j and such that:

$$\sum_j \chi_{j,r}^2 = 1, \quad \sum_j \chi_{j,r}^2 \leq Cr^{-2}.$$

We can assume that there exist j_- and j_+ such that $\tau_{j_-} = -\sqrt{2}$ and $\tau_{j_+} = \sqrt{2}$. The ‘‘IMS’’ formula provides:

$$\hat{\mathcal{Q}}_{\hat{\alpha}, h}^{\text{Neu}}(\psi) \geq \sum_j \hat{\mathcal{Q}}_{\hat{\alpha}, h}^{\text{Neu}}(\chi_{j,r}\psi) - Ch^2 r^{-2} \|\psi\|^2.$$

We let $V(\tau) = \left(\frac{\tau^2}{2} - 1 \right)^2$. Let us fix ε_0 such that

$$V(\tau) \geq \frac{V''(\tau_{j_\pm})}{4} (\tau - \tau_{j_\pm})^2 \quad \text{if} \quad |\tau - \tau_{j_\pm}| \leq \varepsilon_0. \quad (3.1)$$

There exists $\eta_0 > 0$ such that

$$V(\tau) \geq \eta_0 \quad \text{if} \quad |\tau - \tau_{j_\pm}| > \frac{\varepsilon_0}{4}. \quad (3.2)$$

Let us consider j such that $j = j_-$ or $j = j_+$. We can write the Taylor expansion:

$$V(\tau) = \frac{V''(\tau_{j_\pm})}{2} (\tau - \tau_{j_\pm})^2 + \mathcal{O}(|\tau - \tau_{j_\pm}|^3) = 2(\tau - \tau_{j_\pm})^2 + \mathcal{O}(|\tau - \tau_{j_\pm}|^3). \quad (3.3)$$

We have:

$$\hat{\mathcal{Q}}_{\hat{\alpha}, h}^{\text{Neu}}(\chi_{j,r}\psi) \geq \sqrt{2}\Theta_0 h \|\chi_{j,r}\psi\|^2 - Cr^3 \|\chi_{j,r}\psi\|^2, \quad (3.4)$$

where $\Theta_0 > 0$ is the infimum of the bottom of the spectrum for the ξ -dependent family of de Gennes operators $D_\tau^2 + (\tau - \xi)^2$ on \mathbb{R}_+ with Neumann boundary condition ([5, 1]). We are led to choose $r = h^{2/5}$.

We consider now the other balls: $j \neq j_-$ and $j \neq j_+$. If the center τ_j satisfies $|\tau_j - \tau_{j_\pm}| \leq \varepsilon_0/2$, then, for all $\tau \in B(\tau_j, h^{2/5})$, we have for h small enough:

$$|\tau - \tau_{j_\pm}| \leq h^{2/5} + \frac{\varepsilon_0}{2} \leq \varepsilon_0.$$

If $|\tau_j - \tau_{j\pm}| \leq 2h^{2/5}$, then for $\tau \in B(\tau_j, h^{2/5})$, we have $|\tau - \tau_{j\pm}| \leq 3h^{2/5}$ and we can use the Taylor expansion (3.3). Thus (3.4) is still available.

We now assume that $|\tau_j - \tau_{j\pm}| \geq 2h^{2/5}$ so that, on $B(\tau_j, h^{2/5})$, we have:

$$V(\tau) \geq \frac{V''(\tau_{j\pm})}{4} h^{4/5}.$$

If the center τ_j satisfies $|\tau_j - \tau_{j\pm}| > \varepsilon_0/2$, then, for all $\tau \in B(\tau_j, h^{2/5})$, we have $|\tau - \tau_{j\pm}| \geq \varepsilon_0/4$ and thus:

$$V(\tau) \geq \eta_0.$$

Gathering all the contributions, we find:

$$\hat{Q}_{\hat{\alpha}, h}^{\text{Neu}}(\psi) \geq (\sqrt{2}\Theta_0 h - Ch^{6/5}) \|\psi\|^2.$$

We infer, using the min-max principle:

$$\nu_1^{\text{Neu}}(\alpha, \delta) \geq \delta^2 (\sqrt{2}\Theta_0 \delta^{-3/2} - C\delta^{-9/5}) \geq C\delta^{1/2},$$

for δ small enough. ■

Lemma 3.7 *Let u_δ be an eigenfunction associated with the first eigenvalue of $\mathfrak{L}_\delta^{\text{Mo},+}$. Let $D > 0$. There exist $\varepsilon_0, C > 0$ such that, for all δ such that $|\delta| \leq D$, we have:*

$$\int_0^{+\infty} e^{2\varepsilon_0 t^3} |u_\delta|^2 dt \leq C \|u_\delta\|^2.$$

Proof: We let $\Phi_m = \varepsilon \chi_m(t) t^3$. The Agmon identity provides:

$$\int_0^\infty \left(\frac{t^2}{2} - \delta \right)^2 |e^{\Phi_m} u_\delta|^2 dt \leq \mu_1^{\text{Mo}}(\delta) \|e^{\Phi_m} u_\delta\|^2 + \|\nabla \Phi_m e^{\Phi_m} u_\delta\|^2.$$

It follows that:

$$\int_0^\infty \frac{t^4}{8} |e^{\Phi_m} u_\delta|^2 dt \leq (\mu_1^{\text{Mo}}(\delta) + 2\delta^2) \|e^{\Phi_m} u_\delta\|^2 + \|\nabla \Phi_m e^{\Phi_m} u_\delta\|^2.$$

We infer that:

$$\int_0^\infty t^4 |e^{\Phi_m} u_\delta|^2 dt \leq M(D) \|e^{\Phi_m} u_\delta\|^2 + 8 \|\nabla \Phi_m e^{\Phi_m} u_\delta\|^2.$$

With our choice of Φ_m , we have

$$|\nabla \Phi_m|^2 \leq 18\varepsilon^2 \chi_m^2(t) t^4 + 2\varepsilon^2 \chi_m'(t)^2 t^6 \leq 18\varepsilon^2 t^4 + 2\varepsilon^2 \chi_m'(t)^2 t^6 \leq C\varepsilon^2 t^4,$$

since $\chi_m'(t)^2 t^2$ is bounded. For ε fixed small enough, we deduce

$$\int_0^\infty t^4 |e^{\Phi_m} u_\delta|^2 dt \leq \frac{M(D)}{1 - 8C\varepsilon^2} \|e^{\Phi_m} u_\delta\|^2 \leq \tilde{M}(D) \|e^{\Phi_m} u_\delta\|^2.$$

Let us choose $R > 0$ such that: $R^4 - M(D) > 0$. We have:

$$(R^4 - \tilde{M}(D)) \int_R^{+\infty} e^{2\Phi_m} |u_\delta|^2 dt \leq \tilde{M}(D) \int_0^R e^{2\Phi_m} |u_\delta|^2 dy \leq \tilde{M}(D) C(R) \|u_\delta\|^2,$$

and:

$$\int_R^{+\infty} e^{2\Phi_m} |u_\delta|^2 dt \leq C(R, D) \|u_\delta\|^2.$$

We infer:

$$\int_0^{+\infty} e^{2\Phi_m} |u_\delta|^2 dt \leq \tilde{C}(R, D) \|u_\delta\|^2.$$

It remains to take the limit $m \rightarrow +\infty$. ■

Lemma 3.8 *For all $D > 0$, there exist $A > 0$ and $C > 0$ such that for all $|\delta| \leq D$ and $\alpha \geq A$, we have:*

$$\left| \nu_1(\alpha, \delta) - \mu_1^{\text{Mo}}(\delta) \right| \leq C\alpha^{-2}.$$

Proof: We perform the translation $\tau = t - \alpha$, so that $\mathcal{N}_{\alpha, \delta}^{\text{Neu}}$ is unitarily equivalent to:

$$\tilde{\mathcal{N}}_{\alpha, \delta}^{\text{Neu}} = D_\tau^2 + \left(\frac{\tau^2}{2} - \delta \right)^2,$$

on $L^2(-\alpha, +\infty)$. The corresponding quadratic form writes:

$$\tilde{\mathcal{Q}}_{\alpha, \delta}^{\text{Neu}}(\psi) = \int_{-\alpha}^{+\infty} |D_\tau \psi|^2 + \left(\frac{\tau^2}{2} - \delta \right)^2 |\psi|^2 d\tau.$$

Upper bound We take $\psi(\tau) = \chi_0(\alpha^{-1}\tau)u_\delta(\tau)$. The ‘‘IMS’’ formula provides:

$$\tilde{\mathcal{Q}}_{\alpha, \delta}^{\text{Neu}}(\chi_0(\alpha^{-1}\tau)u_\delta(\tau)) = \mu_1^{\text{Mo}}(\delta) \|\chi_0(\alpha^{-1}\tau)u_\delta(\tau)\|^2 + \|(\chi_0(\alpha^{-1}\tau))'u_\delta(\tau)\|^2.$$

Jointly min-max principle with Lemma 3.7, we infer that:

$$\begin{aligned} \nu_1(\alpha, \delta) &\leq \mu_1^{\text{Mo}}(\delta) + \frac{\|(\chi_0(\alpha^{-1}\tau))'u_\delta(\tau)\|^2}{\|\chi_0(\alpha^{-1}\tau)u_\delta(\tau)\|^2} \\ &\leq \mu_1^{\text{Mo}}(\delta) + \frac{C\alpha^{-2}}{e^{2c\varepsilon_0\alpha^3}}. \end{aligned}$$

Lower bound Let us now prove the converse inequality. We denote by $\tilde{u}_{\alpha, \delta}$ the positive and L^2 -normalized groundstate of $\tilde{\mathcal{N}}_{\alpha, \delta}^{\text{Neu}}$. On the one hand, with the ‘‘IMS’’ formula, we have:

$$\tilde{\mathcal{Q}}_{\alpha, \delta}^{\text{Neu}}(\chi_0(\alpha^{-1}\tau)\tilde{u}_{\alpha, \delta}) \leq \nu_1(\alpha, \delta) \|\chi_0(\alpha^{-1}\tau)\tilde{u}_{\alpha, \delta}\|^2 + C\alpha^{-2}.$$

On the other hand, we notice that:

$$\int_{-\alpha}^{+\infty} t^4 |\tilde{u}_{\alpha, \delta}|^2 d\tau \leq C, \quad \int_{-\alpha}^{-\frac{\alpha}{2}} t^4 |\tilde{u}_{\alpha, \delta}|^2 d\tau \leq C,$$

and thus:

$$\int_{-\alpha}^{-\frac{\alpha}{2}} |\tilde{u}_{\alpha, \delta}|^2 d\tau \leq \tilde{C}\alpha^{-4}.$$

We infer that:

$$\tilde{\mathcal{Q}}_{\alpha, \delta}^{\text{Neu}}(\chi_0(\alpha^{-1}\tau)\tilde{u}_{\alpha, \delta}) \leq (\nu_1(\alpha, \delta) + C\alpha^{-2}) \|\chi_0(\alpha^{-1}\tau)\tilde{u}_{\alpha, \delta}\|^2.$$

We deduce that:

$$\mu_1^{\text{Mo}}(\delta) \leq \nu_1(\alpha, \delta) + C\alpha^{-2}. ■$$

Proof of Theorem 1.15: Using the decomposition of Figure 1, we proved in Lemmas 3.4-3.6 and 3.8 that the limit inferior of $\nu_1(\alpha, \delta)$ in these areas are not less than μ_{M_0} . Then, we deduce the existence of a minimum with Lemma 3.3. ■

3.1.2 Numerical simulations for $\nu_1^{\text{Neu}}(\alpha, \delta)$

Figure 2 gives numerical estimates of $\nu_1^{\text{Neu}}(\alpha, \delta)$ using a finite differential method to discretize the operator $\mathcal{N}_{\alpha, \delta}^{\text{Neu}}$, for $\alpha \in \{\frac{k}{10}, 0 \leq k \leq 100\}$, $\delta \in \{\frac{k}{10}, 0 \leq k \leq 200\}$. We choose as computed domain $[0, 60]$ with a discretized step of differential method $h = 1/1000$ and Dirichlet condition on the artificial boundary.

Figure 3 is a zoom for $\alpha \in \{\frac{k}{30}, 0 \leq k \leq 90\}$, $\delta \in \{-1 + \frac{k}{30}, 0 \leq k \leq 30\}$. To have an accurate estimate of the minimum, we make refined computations with a step discretization in (α, ξ) of 10^{-4} . Numerical computations give us that the minimizer is reached for $(\alpha, \delta) \simeq (1.2647, 0.5677)$ and

$$\underline{\mu}_1 \simeq 0.26547.$$

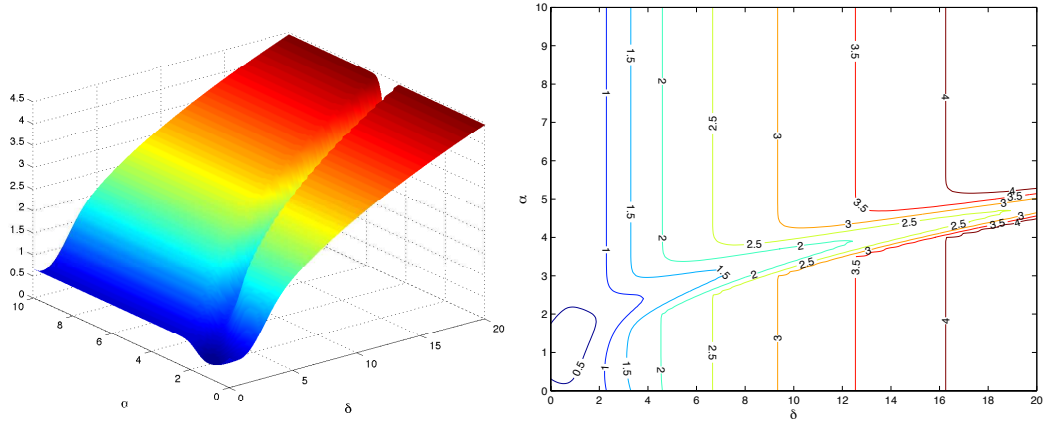


Figure 2: Bottom of the spectrum of $\mathcal{N}_{\alpha, \delta}^{\text{Neu}}$, $(\alpha, \delta) \in [0, 10] \times [0, 20]$

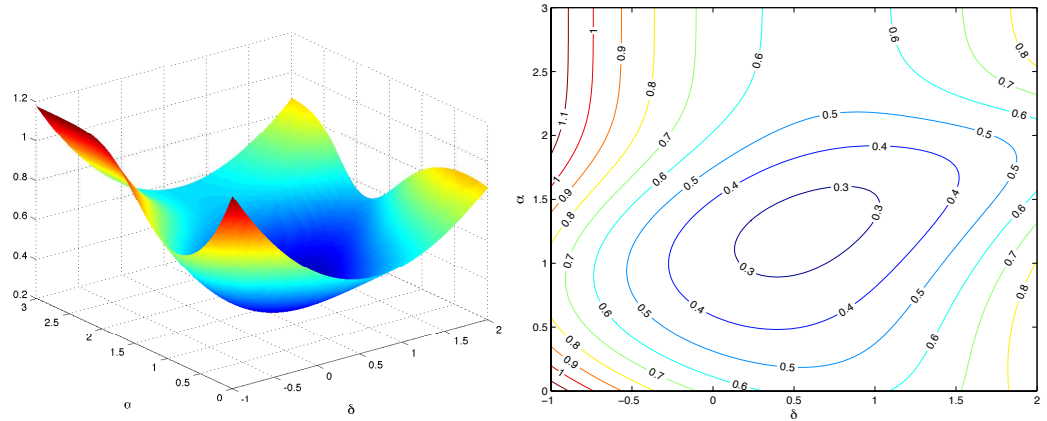


Figure 3: Bottom of the spectrum of $\mathcal{N}_{\alpha, \delta}^{\text{Neu}}$, $(\alpha, \delta) \in [0, 3] \times [-1, 2]$

3.2 Analysis of $\mathcal{M}_{\alpha,\xi}$

3.2.1 Existence of a minimum for $\mu_1(\alpha, \xi)$

Theorem 1.16 is a consequence of the two following lemmas.

Lemma 3.9 *If Conjecture 1.2 is true, we have:*

$$\underline{\mu}_1^{\text{Neu}} < \mu_{\text{Mo}}.$$

Proof: We have

$$\underline{\mu}_1^{\text{Neu}} = \inf_{(\alpha,\xi) \in \mathbb{R}^2} \mu_1(\alpha, \xi) \leq \inf_{\alpha \in \mathbb{R}} \mu_1(\alpha, 0).$$

We use a finite element method, with the Finite Element Library MÉLINA (see [17]), on $[-10, 10]$ with Dirichlet condition on the artificial boundary, with 1000 elements \mathbb{P}_2 . For any α , these computations give an upper-bound of $\mu_1(\alpha, 0)$. We consider a discretized step 10^{-3} for computation for $\alpha \in [0, 2]$. Figure 4 gives the behavior of $\mu_1(\alpha, 0)$ according to α . Numerical computations and Conjecture 1.2 give

$$\inf_{\alpha \in \mathbb{R}} \mu_1(\alpha, 0) \leq 0.33227 < 0.5 < \mu_{\text{Mo}},$$

In fact, numerical simulations suggest that $\inf_{\alpha \in \mathbb{R}} \mu_1(\alpha, 0) \simeq 0.33227$ which is an approximation of the first eigenvalue for $\alpha = 0.827$. ■

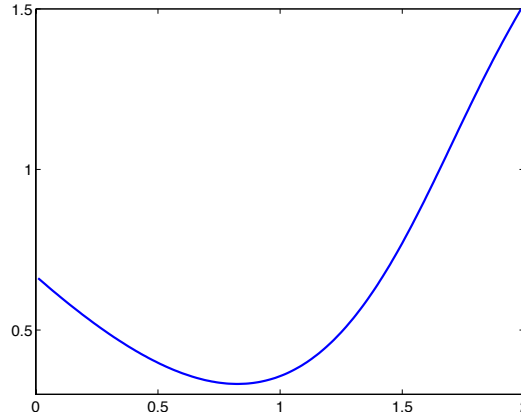


Figure 4: First eigenvalue $\mu_1(\alpha, 0)$ of $\mathcal{M}_{\alpha,0}$ according to α

Lemma 3.10 *For all $(\alpha, \xi) \in \mathbb{R}^2$, we have:*

$$\mu_1(\alpha, \xi) \geq \min(\mu_1^{\text{Neu}}(\alpha, \xi), \mu_1^{\text{Neu}}(\alpha, -\xi)).$$

Proof: Let u be a normalized eigenfunction associated with $\mu_1(\alpha, \xi)$. We can split:

$$\begin{aligned} \mu_1(\alpha, \xi) &= \int_{-\infty}^0 |D_t u|^2 + \left(\frac{t^2}{2} + \alpha t + \xi\right)^2 |u|^2 dt + \int_0^{+\infty} |D_t u|^2 + \left(\frac{t^2}{2} - \alpha t - \xi\right)^2 |u|^2 dt \\ &\geq \mu_1^{\text{Neu}}(\alpha, \xi) \int_{-\infty}^0 |u|^2 dt + \mu_1^{\text{Neu}}(\alpha, -\xi) \int_0^{+\infty} |u|^2 dt \\ &\geq \min(\mu_1^{\text{Neu}}(\alpha, \xi), \mu_1^{\text{Neu}}(\alpha, -\xi)). \end{aligned}$$

■

3.2.2 Numerical simulations for $\mathcal{M}_{\alpha,\xi}$

Figure 5 gives numerical estimates of $\mu_1(\alpha, \xi)$ using a finite differential method to discretize the operator $\mathcal{M}_{\alpha,\xi}$, for $\alpha \in \{-5 + \frac{k}{10}, 0 \leq k \leq 200\}$, $\xi \in \{-20 + \frac{k}{10}, 0 \leq k \leq 400\}$. We choose as computed domain $[-50, 50]$ with a discretized step of differential method $h = 1/1000$ and Dirichlet condition on the artificial boundary. To have an accurate estimate of the minimum, we make refined computations with a step discretization in (α, ξ) of 10^{-4} . Numerical simulations provide that the minimum is reached for $(\alpha, \xi) \simeq (0.8257, 0)$ and

$$\underline{\mu}_1 \simeq 0.33226.$$

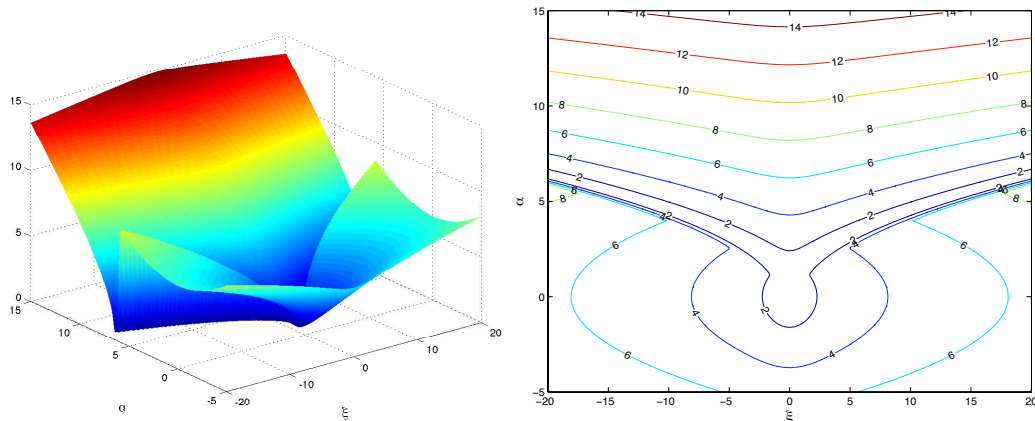


Figure 5: Bottom of the spectrum $\mu_1(\alpha, \xi)$ of $\mathcal{M}_{\alpha,\xi}$ according to $(\alpha, \xi) \in [-5, 15] \times [-20, 20]$

4 Simulations for the eigenpairs of \mathfrak{L}_θ and $\mathfrak{L}_\theta^{\text{Neu}}$

Let us now use the finite element method and the Finite Element Library MÉLINA++, see [16]. To approximate the plane and the half-plane, we use an artificial domain $[a, b] \times [-c, c]$ or $[a, b] \times [0, c]$ respectively and impose Dirichlet condition on the artificial boundaries $x = a$, $x = b$, $y = c$ (and $y = -c$ for \mathfrak{L}_θ). We denote $\lambda_n^\bullet(\theta; a, b, c)$ (with $\bullet = \emptyset, \text{Neu}$) the n -th eigenvalue computed numerically. We have necessarily

$$\lambda_n^\bullet(\theta) \leq \lambda_n^\bullet(\theta; a, b, c).$$

Figures 6 give an approximation of the first eigenvalues of \mathfrak{L}_θ (left) for $\theta \in \{k\pi/60, 1 \leq k \leq 15\}$ and $\mathfrak{L}_\theta^{\text{Neu}}$ (right) for $\theta \in \{k\pi/60, 1 \leq k \leq 30\}$ below the bottom of the essential spectrum equal to $\mu_{M_0} \simeq 0.5698$. Let us notice that the computed eigenvalues $\lambda_n(\theta; a, b, c)$ are larger than μ_{M_0} as soon as $\theta \in \{k\pi/60, 16 \leq k \leq 30\}$ and are consequently not represented in the Figure 6 (left). This is in fact the motivation for Remark 1.12.

Figures 7 give an approximation of $\lambda_n(\theta)$ and $\lambda_n^{\text{Neu}}(\theta)$ for small values of θ . Figure 7(a) gives the eigenvalues $\lambda_n(\theta; -5, 75, 7)$ with 80×7 quadrangular elements of degree \mathbb{Q}_8 for $\theta \in \{k\pi/200, 4 \leq k \leq 20\}$ and $\lambda_n(\theta; -10, 120, 7)$ with 130×7 quadrangular elements of degree \mathbb{Q}_6 for $\theta \in \{k\pi/1000, 4 \leq k \leq 20\}$.

Figure 7(b) gives the eigenvalues $\lambda_n^{\text{Neu}}(\theta; -20, 60, 10)$ with 80×10 quadrangular elements of degree \mathbb{Q}_8 for $\theta \in \{k\pi/200, 4 \leq k \leq 20\}$ and $\lambda_n(\theta; -10, 90, 10)$ with 50×5 quadrangular elements of degree \mathbb{Q}_{10} for $\theta \in \{k\pi/1000, 8 \leq k \leq 20\}$.

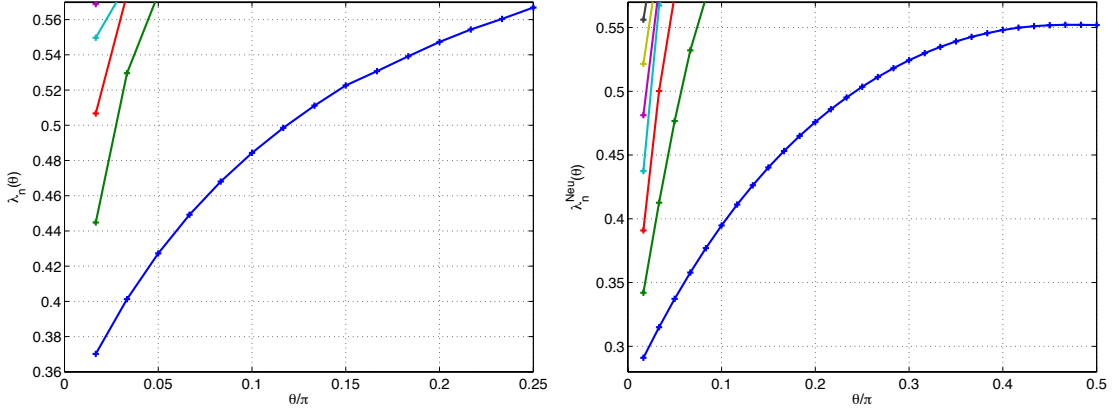
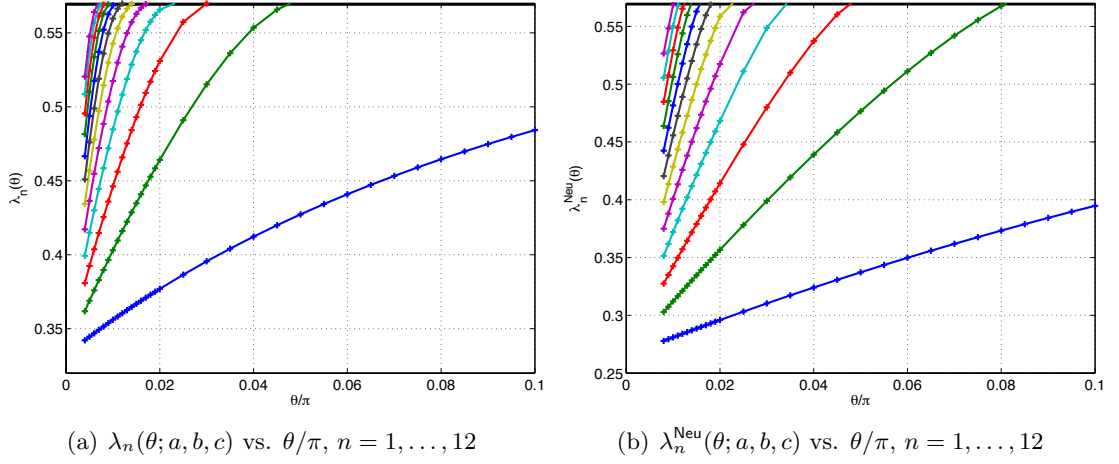


Figure 6: Bottom of the spectrum of \mathfrak{L}_θ (left) and $\mathfrak{L}_\theta^{\text{Neu}}$ (right)



(a) $\lambda_n(\theta; a, b, c)$ vs. θ/π , $n = 1, \dots, 12$

(b) $\lambda_n^{\text{Neu}}(\theta; a, b, c)$ vs. θ/π , $n = 1, \dots, 12$

Figure 7: Low lying eigenvalues of \mathfrak{L}_θ (left) and $\mathfrak{L}_\theta^{\text{Neu}}$ (right)

Let us now illustrate the asymptotic expansion (1.6). In this mind, we define

$$\rho_n^\bullet(\theta) = \frac{\lambda_n^\bullet(\theta) - \underline{\mu}_1^\bullet}{\theta}, \quad \text{with } \bullet = \emptyset, \text{Neu.} \quad (4.1)$$

We use the numerical estimate

$$\underline{\mu}_1 \simeq 0.33226 \quad \text{and} \quad \underline{\mu}_1^{\text{Neu}} \simeq 0.26547. \quad (4.2)$$

If (1.6) is true, we have

$$\frac{\rho_n^\bullet(\theta)}{2n-1} \rightarrow (\det \underline{\text{Hess}}^\bullet)^{1/2} \quad \text{as } \theta \rightarrow 0.$$

Plotting the associated numerical quotient $\rho_n^\bullet(\theta)/(2n-1)$ according to θ as $\theta \rightarrow 0$ (we take $\theta/\pi \in \{2^{-p}, 5 \leq p \leq 11\}$ for our numerical simulations), we deduce the numerical approximations (at 10^{-2})

$$(\det \underline{\text{Hess}})^{1/2} \simeq 0.795, \quad \left(\det \underline{\text{Hess}}^{\text{Neu}} \right)^{1/2} \simeq 0.498.$$

Setting these values for the determinants, Figures 8 give $\rho_n^\bullet(\theta) (\det \underline{\text{Hess}}^\bullet)^{-1/2}$ according to $\theta/\pi \in \{2^{-p}, 5 \leq p \leq 11\}$ and we observe the convergence to the odd numbers $2n - 1$ as $\theta \rightarrow 0$. Table 1 gives the characteristic of the geometric domains for the numerical computations: the artificial domain is $[a, b] \times [-c, c]$ or $[a, b] \times [0, c]$ with nel quadrangular elements of degree \mathbb{Q}_{10} .

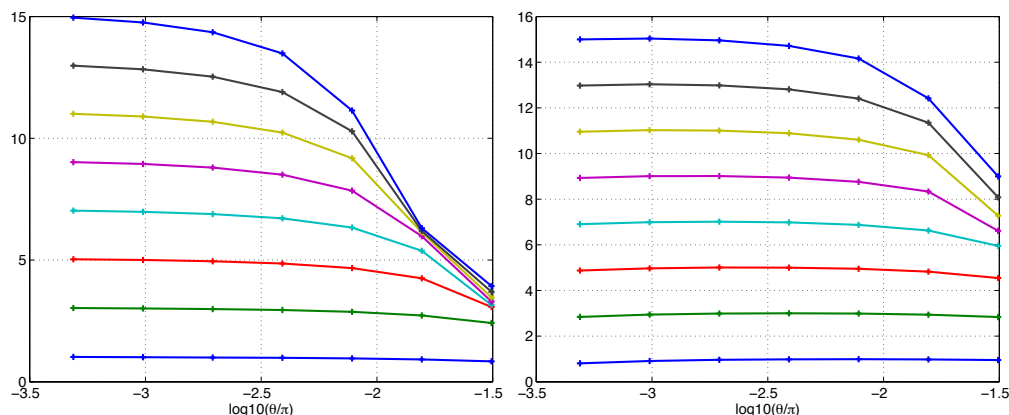


Figure 8: Convergence of $\rho_n(\theta) (\det \underline{\text{Hess}})^{-1/2}$ (left) and $\rho_n^{\text{Neu}}(\theta) (\det \underline{\text{Hess}}^{\text{Neu}})^{1/2}$ (right) as $\theta \rightarrow 0$, $n = 1, \dots, 8$

| $\theta = 2^{-p}$ | $\mathfrak{L}(\theta)$ | | | | $\mathfrak{L}^{\text{Neu}}(\theta)$ | | | |
|-------------------|------------------------|-----|-----|-----------------|-------------------------------------|------|-----|----------------|
| p | a | b | c | nel | a | b | c | nel |
| 5, 6, 7 | -50 | 150 | 10 | 100×10 | -50 | 150 | 10 | 100×5 |
| 8 | 0 | 200 | 10 | 100×10 | 0 | 200 | 10 | 100×5 |
| 9 | 50 | 250 | 10 | 100×10 | 100 | 300 | 10 | 100×5 |
| 10 | 150 | 450 | 5 | 150×5 | 250 | 550 | 5 | 150×5 |
| 11 | 400 | 700 | 5 | 150×5 | 600 | 1000 | 5 | 200×5 |

Table 1: Artificial domains and meshes to compute the eigenvalues for $\theta = 2^{-p}$

Let us now give the first eigenvectors. The geometrical characteristic of the artificial domains are given in Table 2. In Figures 9 and 10, we represent the first eight eigenmodes of the operators \mathfrak{L}_θ and $\mathfrak{L}_\theta^{\text{Neu}}$ respectively for $\theta = \pi/100$. Figures 11 and 12 give the first eigenvalue and the modulus and the phase of the associated eigenvector for $\theta = \pi/4$ for \mathfrak{L}_θ and $\mathfrak{L}_\theta^{\text{Neu}}$. The case $\theta = \pi/2$ is illustrated in Figure 13 for the operator $\mathfrak{L}_\theta^{\text{Neu}}$.

| θ/π | $\mathfrak{L}(\theta)$ | | | | | $\mathfrak{L}^{\text{Neu}}(\theta)$ | | | | |
|--------------|------------------------|-----|-----|----------------|----------------|-------------------------------------|-----|-----|----------------|----------------|
| | a | b | c | nel | \mathbb{Q}_k | a | b | c | nel | \mathbb{Q}_k |
| 1/100 | -5 | 85 | 5 | 90×10 | 8 | -5 | 85 | 5 | 90×5 | 8 |
| 1/4 | -10 | 10 | 10 | 20×20 | 10 | -10 | 10 | 10 | 20×20 | 10 |
| 1/2 | -5 | 5 | 20 | 20×20 | 10 | -5 | 5 | 20 | 20×20 | 10 |

Table 2: Artificial domains and meshes to compute the eigenmodes for $\theta = \frac{\pi}{100}, \frac{\pi}{4}, \frac{\pi}{2}$

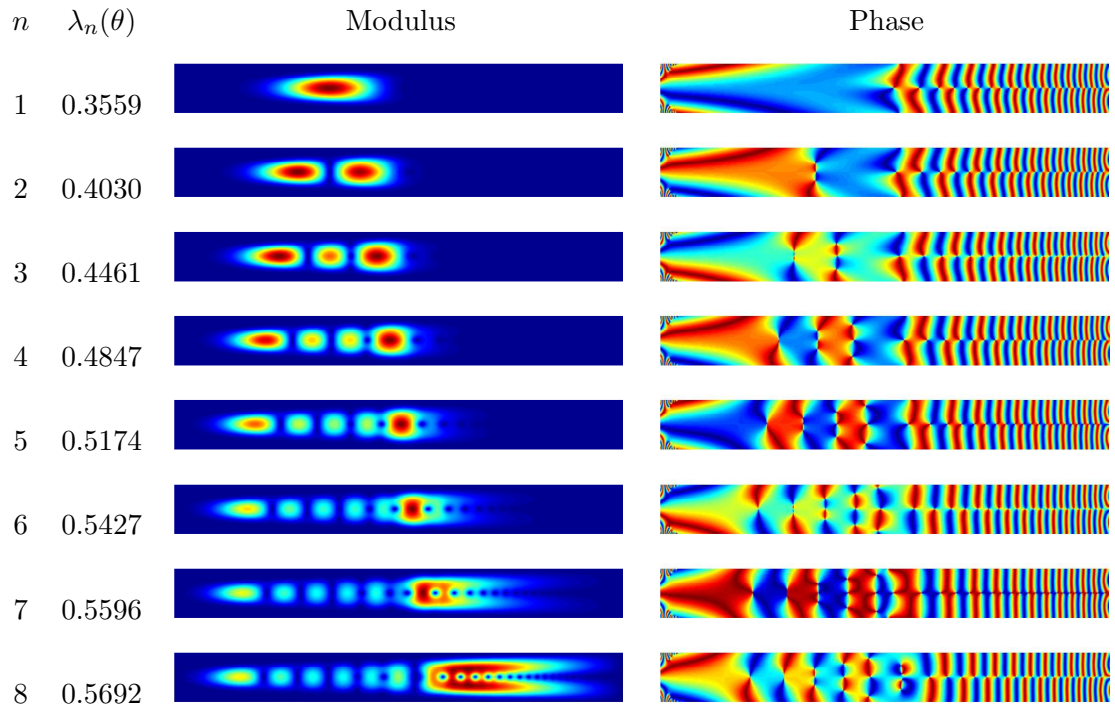


Figure 9: First eight eigenmodes of \mathfrak{L}_θ , $\theta = \frac{\pi}{100}$

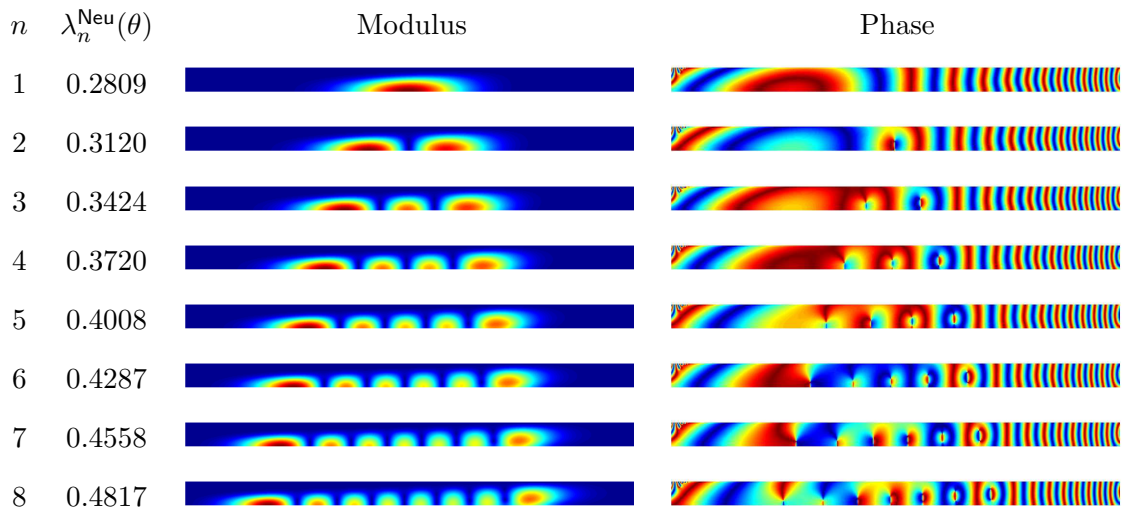


Figure 10: First eight eigenmodes of $\mathfrak{L}_\theta^{\text{Neu}}$, $\theta = \frac{\pi}{100}$

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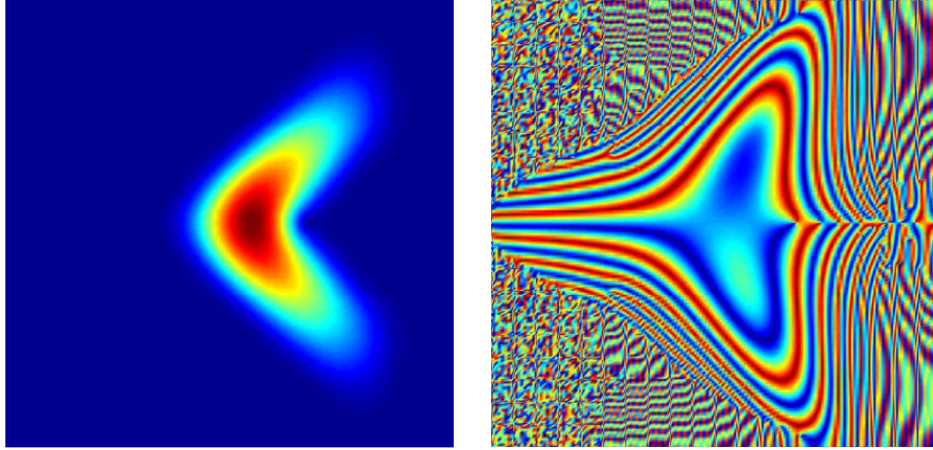


Figure 11: First eight eigenmodes of \mathfrak{L}_θ , $\theta = \frac{\pi}{4}$, $\lambda_1(\theta) = 0.5645$

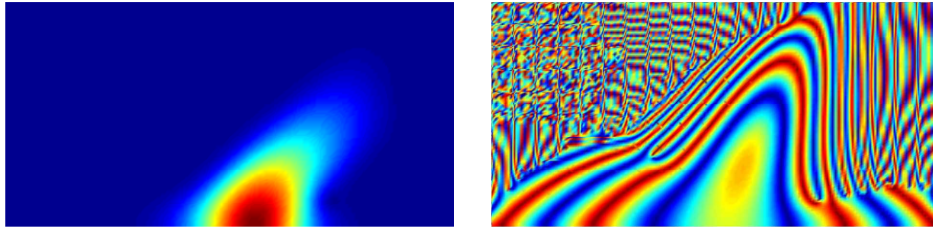


Figure 12: First eight eigenmodes of $\mathfrak{L}_\theta^{\text{Neu}}$, $\theta = \frac{\pi}{4}$, $\lambda_1^{\text{Neu}}(\theta) = 0.5035$

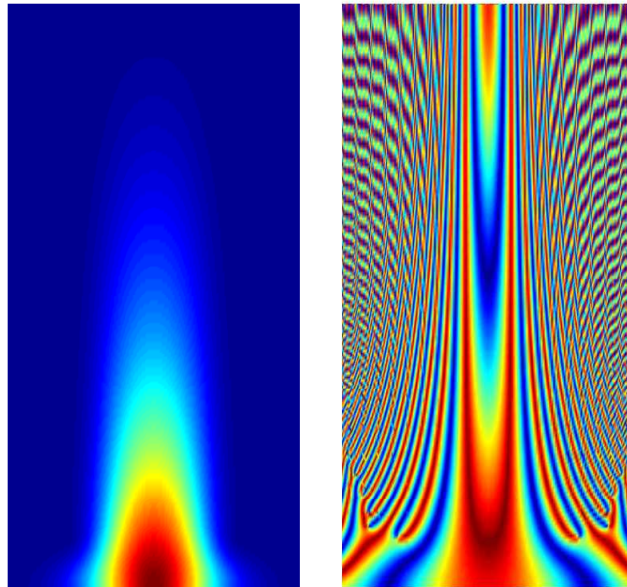


Figure 13: First eight eigenmodes of $\mathfrak{L}_\theta^{\text{Neu}}$, $\theta = \frac{\pi}{2}$, $\lambda_1^{\text{Neu}}(\theta) = 0.5494$

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