EIGENPAIRS OF A MODEL SCHRÖDINGER OPERATOR WITH NEUMANN BOUNDARY CONDITIONS

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Talk Abstract

The considered Schrödinger operator has a quadratic potential which is degenerate in the sense that it reaches its minimum all along a line which makes the angle θ with the boundary of the half-plane where the problem is set. We exhibit localization properties for the eigenfunctions associated with its lowest eigenvalues below its essential spectrum. We investigate the densification and the asymptotics of the eigenvalues below the essential spectrum in the limit $\theta \to 0$.

1 Introduction

This note is devoted to the investigation of the ground states of the Schrödinger operator

$$\mathcal{L}_\theta = -\Delta_{s,t} + (t\cos\theta - s\sin\theta)^2 \qquad (1)$$

defined for (s,t) in the half-space $\Omega = \mathbb{R}_s \times \mathbb{R}_t^+$. More precisely, $\mathcal{L}_\theta$ denotes the self-adjoint Neumann realization on Ω. The parameter $\theta \in [0,\pi]$ is the angle between the boundary of Ω and the line $t\cos\theta = s\sin\theta$ which is the set where the potential $(t\cos\theta - s\sin\theta)^2$ reaches its minimum. Thus the potential is quadratic and degenerate. When $\theta = 0$, $\frac{\pi}{2}$ or π, it is easy to see by an even reflection through the boundary $t = 0$ that the spectrum $\mathrm{sp}(\mathcal{L}_\theta)$ of $\mathcal{L}_\theta$ coincides with the spectrum of the operator $\mathcal{A} := -\Delta_{y,z} + y^2$ on the whole space $\mathbb{R}^2$. Since $\mathcal{A}$ is the sum of the harmonic oscillator on $\mathbb{R}$ and of $-\partial_z^2$, we find

$$\text{For } \theta \in \{0, \tfrac{\pi}{2}, \pi\}, \quad \mathrm{sp}(\mathcal{L}_\theta) = [1, +\infty). \qquad (2)$$

In these cases, $\mathrm{sp}(\mathcal{L}_\theta)$ coincides with the essential spectrum $\mathrm{sp}_{\mathrm{ess}}(\mathcal{L}_\theta)$. In fact $\mathrm{sp}_{\mathrm{ess}}(\mathcal{L}_\theta)$ does not depend on θ, [5]:

$$\text{For } \theta \in [0, \pi], \quad \mathrm{sp}_{\mathrm{ess}}(\mathcal{L}_\theta) = [1, +\infty). \qquad (3)$$

For any positive integer n we define $\sigma_n(\theta)$ as the n-th Rayleigh quotient associated with $\mathcal{L}_\theta$. Then if $\sigma_n(\theta)$ is strictly less than 1, it is an eigenvalue, and, conversely, the n-th eigenvalue of $\mathcal{L}_\theta$ ordered in increasing order and counted with multiplicity, is $\sigma_n(\theta)$. It is proved in [5] that for any n the function $(0, \frac{\pi}{2}] \ni \theta \mapsto \sigma_n(\theta)$ is non decreasing. Concerning the ground state, it is proved in [6, Lemma 3.6] that $(0, \frac{\pi}{2}) \ni \theta \mapsto \sigma_1(\theta)$ is increasing, $\sigma_1(\theta) < 1$ and corresponds to a simple eigenvalue.

2 Lower and upper bounds for eigenvalues

The operator $\mathcal{L}_\theta$ is the sum of the two operators $\mathcal{A}_s$ and $\mathcal{A}_t$:

$$\begin{aligned} \mathcal{A}_s &= -\partial_s^2 + (\sin\theta)^2 (t\cos\theta - s\sin\theta)^2 \\ \mathcal{A}_t &= -\partial_t^2 + (\cos\theta)^2 (t\cos\theta - s\sin\theta)^2. \end{aligned} \qquad (4)$$

The change of variables $\tilde{t} = t\cos\theta$ shows that $\mathcal{A}_t$ is isospectral with the operator $(\cos\theta)^2 H_{s\sin\theta}(\tilde{t}; \partial_{\tilde{t}})$ where $H_\zeta(z; \partial_z) := -\partial_z^2 + (z - \zeta)^2$ denotes the de Gennes operator of order $k = 1$ defined on the half-line $\mathbb{R}_+$ with Neumann condition on $z = 0$. The first eigenvalue $\mu(\zeta)$ of H_ζ is a smooth function of ζ which has a unique minimum denoted Θ_0, non degenerate, attained for the value $\zeta = \zeta_0 = \sqrt{\Theta_0}$, see [3, Theorem 4.3]. A 9-digit numerical approximation of Θ_0 is 0.590106125 [1]. A consequence of the above decomposition of $\mathcal{L}_\theta$ is the lower bound for its first eigenvalue, [4, Lemma 6.2.2]

$$\sigma_1(\theta) \geq (\cos\theta)^2 \Theta_0 + (\sin\theta)^2, \quad \theta \in (0, \tfrac{\pi}{2}). \qquad (5)$$

Let v_{ζ_0} be an eigenvector associated with the first eigenvalue Θ_0 of the operator H_{ζ_0}, and let ψ_j be the j-th Hermite function with the "physicists" convention ($j \geq 0$). Let us use the following rescaling and translation:

$$y = s\sqrt{\sin\theta} - \frac{\zeta_0}{\sqrt{\tan\theta}} \quad \text{and} \quad z = t\sqrt{\cos\theta}\,. \qquad (6)$$

Considering the orthogonal functions $(s,t) \mapsto \psi_j(y)\, v_{\zeta_0}(z)$ in the Rayleigh quotients of $\mathcal{L}_\theta$, we prove [2, §3] the following generalization to $n > 1$ of [4, Lemma 6.2.2]

$$\sigma_n(\theta) \leq \Theta_0 \cos\theta + (2n-1)\sin\theta, \qquad n \geq 1, \quad \theta \in (0, \tfrac{\pi}{2}). \qquad (7)$$

Therefore, the number of eigenvalues tends to infinity as the angle θ tends to 0. We also have a densification of the spectrum in the following sense: For all $\lambda_0 \in (\Theta_0, 1)$ and for all $\varepsilon > 0$, there exists $\theta_0 > 0$ small enough so that for all $\theta \in (0, \theta_0]$ the distance of λ_0 to $\mathrm{sp}(\mathcal{L}_\theta)$ is less than ε.

3 Exponential decay of eigenvectors

Numerical simulation of the ground state for different values of θ by the finite element method using [7] are shown in Figure 1. The computational domain is $[-5,15]\times[0,75]$ for the first 4 values of θ and $[-15,25]\times[0,15]$ for the last 3 ones.

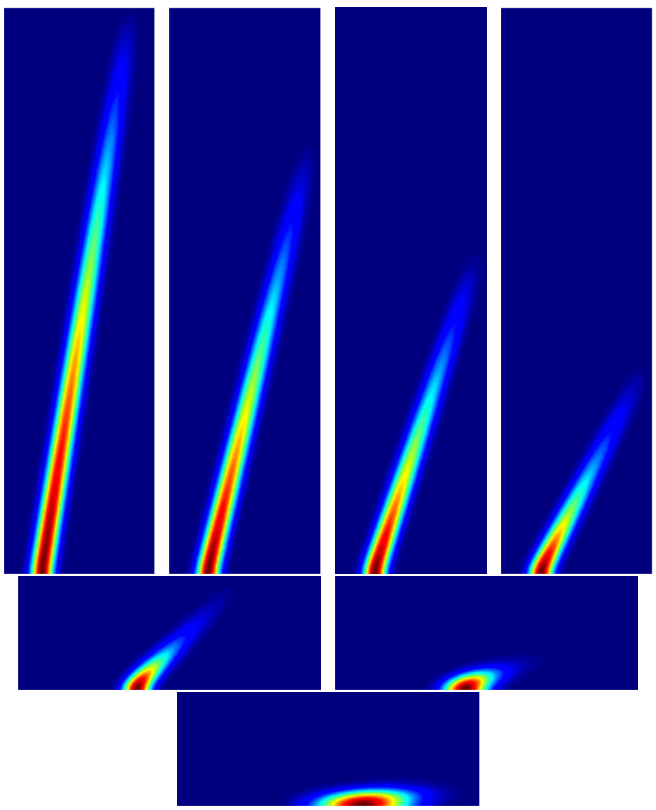

Figure 1: First eigenvector of $\mathcal{L}_\theta$ for $\theta = \vartheta\pi/2$ with $\vartheta = 0.9, 0.85, 0.8, 0.7, 0.5, 0.2$, and 0.05, and computed eigenvalues 1.0001, 0.9998, 0.9991, 0.9945, 0.9611, 0.7950, and 0.6481, respectively.

The concentration and decay of the eigenvectors strongly depend on θ. We have isotropic and anisotropic Agmon type estimates [2, §2]:

Theorem 1 *Let $(\sigma(\theta), u_\theta)$ be an eigenpair of $\mathcal{L}_\theta$ with $\sigma(\theta) < 1$. We have the following four estimates:*

$$\forall\alpha\in\left(0,\sqrt{1-\sigma(\theta)}\right),\quad \exists C_1 = C_1(\alpha,\theta) > 0,$$
$$\|\exp\left(\alpha\sqrt{s^2+t^2}\right)u_\theta\|_{L^2(\Omega)} \le C_1\|u_\theta\|_{L^2(\Omega)}. \tag{8}$$

$$\forall\beta\in(0,\tfrac{1}{2}),\quad \exists C_2 = C_2(\beta) > 0,$$
$$\|\exp\left(\beta(t\cos\theta - s\sin\theta)^2\right)u_\theta\|_{L^2(\Omega)} \le C_2\|u_\theta\|_{L^2(\Omega)}. \tag{9}$$

$$\forall\eta<1,\ \forall\gamma\in\left(0,\sqrt{1-\eta}\right),\quad \exists C_3 = C_3(\eta,\gamma),$$
$$\left\{\sigma(\theta)\le\eta \ \Rightarrow\ \|\exp(\gamma t)\,u_\theta\|_{L^2(\Omega)} \le C_3\|u_\theta\|_{L^2(\Omega)}\right\}. \tag{10}$$

$$\exists C_4>0,\ \exists\theta_0>0,\quad \forall\theta\in(0,\theta_0],$$
$$\|\exp\left(s\sqrt{\sin\theta} - \frac{\zeta_0}{\sqrt{\tan\theta}}\right)u_\theta\|_{L^2(\Omega)} \le C_4\|u_\theta\|_{L^2(\Omega)}. \tag{11}$$

The isotropic estimates (8) clearly degenerates as $\sigma(\theta)\to 1$. It is also degenerating as $\theta\to 0$, because the constant $C_1(\alpha,\theta)$ blows up. The three other estimates are stable as $\theta\to 0$: The modes u_θ are uniformly localized in an horizontal layer above the boundary, and they concentrate around the point $(s_0(\theta),0)$ with $s_0(\theta)$ such that $s_0(\theta)\sin\theta = \zeta_0\sqrt{\cos\theta}$. Thus $s_0(\theta)\to\infty$ as $\theta\to 0$, which would contradict uniform estimates.

4 Eigenvalue asymptotics in the small angle limit

We perform the change of variables $(s,t)\mapsto(y,z)$ defined by (6). In the new variables, the operator $\mathcal{L}_\theta$ writes

$$-\sin\theta\,\partial_y^2 - \cos\theta\,\partial_z^2 + \cos\theta(z-\zeta_0-y\sqrt{\tan\theta})^2 =: \cos\theta(\mathfrak{L}_h+\Theta_0),$$

where we have set $h=\tan\theta$ and introduced

$$\mathfrak{L}_h := -h\partial_y^2 - \partial_z^2 + (z-\zeta_0-yh^{1/2})^2 - \Theta_0. \tag{12}$$

We denote by $\mathfrak{s}_n(h)$ the n-th eigenvalue of $\mathfrak{L}_h$. Due to the change of variables, we have

$$\sigma_n(\theta) = \cos\theta\big(\Theta_0 + \mathfrak{s}_n(\tan\theta)\big). \tag{13}$$

The behavior of $\sigma_n(\theta)$ as $\theta\to 0$ is determined by $\mathfrak{s}_n(h)$ as $h\to 0$. Using the de Gennes operator H_ζ, we have

$$\mathfrak{L}_h = -h\partial_y^2 + H_{\zeta_0+y\sqrt{h}}(z;\partial_z) - \Theta_0. \tag{14}$$

The Born-Oppenheimer approximation consists of replacing $H_{\zeta_0+y\sqrt{h}}$ by its ground energy $\mu(\zeta_0+y\sqrt{h})$ and to implement the standard harmonic approximation in the semi-classical limit for the one-dimensional operator:

$$\mathfrak{L}_{h,\mathrm{BO}} := -h\partial_y^2 + \mu(\zeta_0+y\sqrt{h}) - \Theta_0.$$

Indeed, the potential $y\mapsto\mu(\zeta_0+y\sqrt{h})-\Theta_0$ has 0 as non-degenerate minimum in $y=0$ and the n-th eigenvalue of $\mathfrak{L}_{h,\mathrm{BO}}$ has the asymptotics $h(2n-1)\sqrt{\mu''(\zeta_0)/2}$ modulo $h^{3/2}$ as $h\to 0$. In fact, the Born-Oppenheimer approximation does provide the asymptotics of $\mathfrak{s}_n(h)$ and $\sigma_n(\theta)$:

Theorem 2 *For any rank $N \geq 1$, there exist $C(N) > 0$ and $h_0 > 0$ such that for all $n = 1, \ldots, N$*

$$\forall h \in (0, h_0],\qquad \big|\, h(2n-1)\sqrt{\mu''(\zeta_0)/2} - \mathfrak{s}_n(h)\,\big| \leq C(N)\, h^{3/2}, \quad (15)$$

$$\forall \theta \in (0, h_0],\qquad \big|\, \Theta_0 + \theta(2n-1)\sqrt{\mu''(\zeta_0)/2} - \sigma_n(\theta)\,\big| \leq C(N)\, \theta^{3/2}. \quad (16)$$

The proof, see [2, §4], incorporates a construction of quasimodes by an expansion of $\mathfrak{L}_h$ in powers of $h^{1/2}$. These quasimodes are associated with the approximate eigenvalues $h(2n-1)\sqrt{\mu''(\zeta_0)/2}$, $n = 1, \ldots, N$. In the fitted variables (y, z) introduced in (6) they take the form

$$\mathfrak{u}_n(h) = \psi_{n-1}\Big(\Big[\frac{\mu''(\zeta_0)}{2}\Big]^{1/4} y\Big)\, v_{\zeta_0}(z), \quad n = 1, 2, \ldots, \quad (17)$$

where we recall that ψ_j is the j-th Hermite function and v_{ζ_0} an eigenvector of the de Gennes operator associated with the minimal eigenvalue Θ_0, see Section 2.

In order to check that the n-th approximate eigenvalue is the approximation on the n-th eigenvalue, we rely on the Born-Oppenheimer approximation. However $\mathfrak{L}_{h,\mathrm{BO}}$, seen as an operator acting on the domain of $\mathfrak{L}_h$ – i.e. as two-dimensional operator, has eigenvalues of infinite multiplicity, and we cannot use directly the min-max principle to compare its spectrum with the eigenvalues of $\mathfrak{L}_h$. Thus, we justify, through the Agmon estimates (10)–(11) and a Grushin type argument, that the eigenvalues of $\mathfrak{L}_h$ are bounded from below by those of $\mathfrak{L}_{h,\mathrm{BO}}$ seen as one-dimensional operator. Our proof is inspired by the procedure described in [8] for degenerate potentials in $\mathbb{R}^n$.

5 Regularity of the first eigenvalue in function of the angle

Let us consider the question of the regularity of the function $\theta \mapsto \sigma_1(\theta)$ for $\theta \in [0, \pi]$. We have parity with respect to $\frac{\pi}{2}$: $\sigma_1(\frac{\pi}{2} + \theta) = \sigma_1(\frac{\pi}{2} - \theta)$. We recall that we have $\sigma_1(0) = \sigma_1(\frac{\pi}{2}) = \sigma_1(\pi) = 1$. From (5)–(7), we find that σ_1 tends to 1 when θ tends to $\frac{\pi}{2}$. We prove that $\partial_\theta \sigma_1(\theta)$ tends to 0 as θ tends to $\frac{\pi}{2}$. As a consequence of this fact and of Theorem 2, we find

Proposition 3 *The function $\theta \mapsto \sigma_1(\theta)$ is $\mathcal{C}^1$ on $(0, \pi)$. It has a $\mathcal{C}^1$ extension $\bar\sigma_1$ to the closed interval $[0, \pi]$ obtained by setting $\bar\sigma_1(0) = \bar\sigma_1(\pi) = \Theta_0$. The function σ_1 itself is discontinuous at $\theta = 0$ and $\theta = \pi$.*

The discontinuity of σ_1 at $\theta = 0$ is related to the behavior of the ground state as $\theta \to 0$ which is localized around the point $(s_0(\theta), 0)$ with $s_0(\theta) \to \infty$ as $\theta \to 0$, with a localization length which also tends to infinity.

We conclude this note by the graph of $\sigma_1(\theta)$ obtained by a finite element approximation for a sampling of 198 values of θ (the values of θ are $k\pi/200$ with $k = 1, \ldots, 99, 101, \ldots, 199$), see Figure 2.

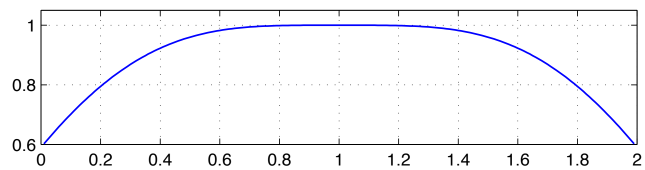

Figure 2: Approximation of σ_1 on $[0, \pi]$

Full proofs and other numerical experimentations can be found in [2].

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