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Original article

A model of sheared nanoribbons

Ph. Briet

Aix Marseille Université, Université de Toulon, CNRS, CPT, Marseille France

briet@univ-tln.fr

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ABSTRACT In this note, we investigate the spectral properties of the Dirichlet Laplacian defined on an infinite band subject to a "shearing". We give conditions for which the shear does not produce discret eigenvalue. In a second part we discuss the existence of discrete spectrum.

KEYWORDS Quantum waveguide, sheared band, Hardy inequality

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1. Introduction

The purpose of this note is to describe some unexpected spectral properties due to geometric shearing in a two dimensional quantum waveguide. To this end, we introduce the following model. Let $f:\ \mathbb{R} \to \mathbb{R}$ such that:
(**h**) *the derivative* $f' \in L^\infty_{loc}(\mathbb{R})$ *and has a limit* β *at infinity:* $f'(s) \to \beta$ *as* $|s| \to \infty$, $\beta \in \mathbb{R} \cup \{\pm\infty\}$.
If $\beta \in \mathbb{R}$, the deviation is denoted by $\varepsilon := f'(s) - \beta$. Let $d > 0$. Consider the domain in $\mathbb{R}^2$:

$$\Omega = \{(x,y) \in \mathbb{R}^2; x \in \mathbb{R}, f(x) < y < f(x) + d\}$$

The straight tube is denoted as $\Omega_0 = \mathbb{R} \times (0,d)$ $(f = 0)$.

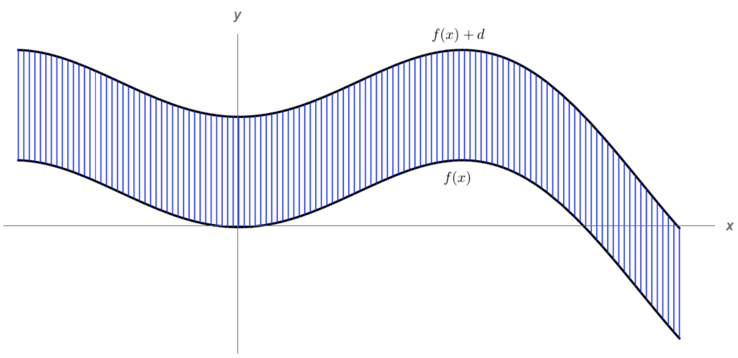

FIG. 1. Sheared nanoribbon

We are focusing on the spectral analysis of the "Dirichlet Laplacian" denoted by $-\Delta_D$ in $\mathrm{L}^2(\Omega)$ i.e. the self-adjoint operator in $\mathrm{L}^2(\Omega)$ defined from the quadratic form

$$\mathcal{Q}_D[\psi] = \int_\Omega |\nabla\psi(x,y)|^2 dxdy, \quad \psi \in \mathrm{H}^1_0(\Omega).$$

Here, we use standard notation for Sobolev space e.g. $\mathrm{H}^1_0(\Omega)$: H^1-norm closure of $C^\infty_0(\Omega)$, the H^1 norm is denoted by $\|\cdot\|_1$. For finite β it is convenient to use an appropriate change of variables:

$$(s,t) \in \Omega_0 \longrightarrow \mathcal{L}(s,t) = (s, f(s) + t) \in \Omega$$

The Laplace operator in the curvilinear coordinates $(s,t) \in \mathbb{R} \times (0,d)$ is given by:

$$H_f = -(\partial_s - f'\partial_t)^2 - \partial_t^2.$$

It is associated to the following quadratic form:

$$q[\varphi] = \|(\partial_s - f'\partial_t)\varphi\|^2 + \|\partial_t\varphi\|^2; \varphi \in \mathrm{Dom}(q) \tag{1}$$

By direct calculation or by using the following inequalities, [1]:

$$c_1\|\varphi\|_1^2 \leq q[\varphi] \leq c_2\|\varphi\|_1^2, \varphi \in C_0^\infty(\Omega_0), \tag{2}$$

for two constants $c_1, c_2 > 0$ we see that q is closed on $\mathrm{Dom}(q) = H_0^1(\Omega_0)$.

1.1. Related model

Our motivation for this work comes mainly from recent results about the spectral analysis of the Dirichlet Laplacian defined on a twisting tube in $\mathbb{R}^3$, [2]. Let $\omega \in \mathbb{R}^2$ an open bounded set of $\mathbb{R}^2$ and $\mathbf{\Omega_0} = \{(s, t_1, t_2) \in \mathbb{R}^3, s \in \mathbb{R}; (t_1, t_2) \in \omega\}$ the straight tube of section ω. Denoting by $\theta = \theta(s)$ the angle-rotation of ω at s around the longitudinal axis. In this natural coordinate system, the Laplace operator on $L^2(\mathbf{\Omega_0})$ reads as:

$$H_{\theta'} := -(\partial_s + \theta'(s)\partial_\varphi)^2 - \Delta_t,$$

where $\Delta_t := \partial_{t_1}^2 + \partial_{t_2}^2$, $\partial_\varphi := t_1\partial_{t_2} - t_2\partial_{t_1}$. The function θ is supposed to have a finite limit β at infinity, let $\varepsilon(s) := \theta'(s) - \beta$ be the deviation. For this model, if ε has a definite sign, the existence of discrete eigenvalues is implied by the condition $\beta\varepsilon < 0$, see [2,3]. On the other hand it is proved in [4] that $H_{\theta'}$ has no discrete spectrum if $\beta\varepsilon \geq 0$. This last result is proved for some β and ε but it is conjectured to be true for every $\beta \in \mathbb{R}$ and deviation ϵ s.t. $\beta\varepsilon \geq 0$, see [4]. This then leads us to introduce the following terminology, we will talk about *repulsive twisting* if $\beta\varepsilon \geq 0$ and the other cases as e.g. $\beta\varepsilon < 0$ correspond to *attractive twisting*. For related works see [5].

Similary in this note if β is finite, *repulsive shearing* means $\beta\varepsilon \geq 0$, while *attractive shearing* means $\beta\varepsilon < 0$.

The issues we address here are the following. We study first the localisation of the essential spectrum in section 2, this allows us to show that the spectrum is purely discrete for $\beta = \mp\infty$. Then in section 3 we prove the absence of discrete spectrum for repulsive shearing. Finally, we discuss the case of attractive shearing and the existence of discrete eigenvalues in the last section.

2. Essential spectrum

2.1. Finite limit

Let $E_1(\beta) = (1 + \beta^2)\, E_1$, where $E_1 = \left(\frac{\pi}{d}\right)^2$ is the first transverse mode: $-\partial_t^2\chi(t) = E_1\chi(t), \|\chi\|_{L^2(0,d)} = 1$. In fact $\chi(t) = \sqrt{\frac{2}{d}}\sin(\frac{\pi t}{d})$.

Theorem 2.1. *Suppose that* $\varepsilon(s) \to 0$ *as* $|s| \to \infty$. *Then*

$$\sigma_{ess}(H_f) = [E_1(\beta), +\infty]$$

To prove the Theorem 2.1 we use the following Weyl Criteria in a suitable form sense. We denote by $\mathrm{Dom}(q)^*$ the dual space equipped with the norm:

$$\|\cdot\|_{-1} := \sup_{\varphi\in\mathrm{Dom}(q), \|\varphi\|_1=1} |(\cdot, \varphi)| = \|(H_f + 1)^{-1/2} \cdot \|.$$

Then

Proposition 2.1. *Then* $\lambda \in \sigma_{ess}(H_f)$ *iff there exists* $(\varphi_n)_{n\in\mathbb{N}} \in C_0^\infty(\Omega_0), \|\varphi_n\| = 1$, *s.t. the following conditions hold:*

i) $supp\varphi_n \subset \Omega_0 \setminus (-n, n) \times (0, d), \forall n \geq 1$

ii) $\|(H_f - \lambda)\varphi_n\|_{-1} \to 0$

For the proof of this proposition, see [1], we noticed that this type of result is reminiscent of the spectral analysis of N-body quantum systems see e.g. [6] and conversely in the context of multistratified media [7]. It is worth noting that here the smoothness of the deviation ε is not required.

Proof of the Theorem. First, we suppose $f' = \beta \in \mathbb{R}$, denote by H_β the corresponding operator, it is invariant with respect to the longitudinal translation, then by using standard argument of the integral direct decomposition of operators we obtain $\sigma(H_\beta) = \sigma_{ess}(H_\beta) = [E_1(\beta), +\infty]$, [3].

Let us show that $\sigma_{ess}(H_f) = \sigma_{ess}(H_\beta)$. We choose $\lambda \in \sigma_{ess}(H_f)$ and let $(\varphi_n)_{n\in\mathbb{N}}$ be a Weyl sequence in the sense of the proposition 2.1. We have

$$H_\beta\varphi_n = H_f\varphi_n + W\varphi_n;\ W\varphi_n = \big(-\partial_t\varepsilon\partial_s - \partial_s\varepsilon\partial_t + (2\beta\varepsilon + \varepsilon^2)\partial_t^2\big)\varphi_n$$

Then to prove that $\lambda \in \sigma_{ess}(H_\beta)$ it is sufficient to show that $\|W\varphi_n\|_{-1} \to 0$ as $n \to \infty$. Set $\varepsilon_n = esssup\{|\varepsilon(s)|; s \in (-\infty, -n) \cup (n, \infty)\}$. First consider

$$\|\partial_t\varepsilon\partial_s\varphi_n\|_{-1} = \sup_{\varphi\in\mathrm{Dom}(q), \|\varphi\|_1=1} |(\varepsilon\partial_s\varphi_n, \partial_t\varphi)|.$$

We have $\forall\varphi \in \mathrm{Dom}(q), \|\varphi\|_1 = 1$, $|(\varepsilon\partial_s\varphi_n, \partial_t\varphi)| \leq \varepsilon_n\|\partial_s\varphi_n\|\|\partial_t\varphi\|$ and $\|\partial_s\varphi_n\| \leq \|\partial_s(H_f+1)^{-1/2}\|\|(H_f+1)\varphi_n\|_{-1} < c$ for some constant $c > 0$. Therefore $\|\partial_t\varepsilon\partial_s\varphi_n\|_{-1} \to 0$ as $n \to \infty$.
By using the same arguments we also have $\|\partial_s\varepsilon\partial_t\varphi_n\|_{-1}$ and

$$\|\partial_t(2\beta\varepsilon+\varepsilon^2)\partial_t\varphi_n\|_{-1} \leq const.\varepsilon_n\|\partial_t(H_f+1)^{-1/2}\|\|(H_f+1)\varphi_n\|_{-1} \to 0$$

as $n \to \infty$. This implies our claim. The reverse inclusion follows in a similar way. $\square$

2.2. Infinite limit

We prove the following theorem.

Theorem 2.2. *Suppose that $f' \in L^\infty_{loc}(\mathbb{R})$ and $f' \to \pm\infty$. Then $\sigma_{ess}(H) = \emptyset$.*

In this note we give a slightly different proof of this theorem than the one in [1].

Proof. Let $R > 0$ and large, let $\Omega_R^{int} := \{x = (x,y) \in \Omega; |y| < R\}$ and $\Omega_R^{ext} := \{x = (x,y) \in \Omega; |y| > R\}$. Denote by q_{int} (resp. q_{ext}) the following quadratic form. Let $\mathrm{Dom}(q_{int}) = \{\psi = \varphi\lfloor_R^{\Omega_{int}}, \varphi \in \mathrm{Dom}(q)\}$ (resp. $\mathrm{Dom}(q_{ext}) = \{\psi = \varphi\lfloor_{\Omega_R^{ext}}, \varphi \in \mathrm{Dom}(q)\}$)and for $\psi \in \mathrm{Dom}(q_{int})$ (resp. $\psi \in \mathrm{Dom}(q_{ext})$,

$$q_{int}[\psi] = q[\psi](\text{resp. } \mathrm{q_{ext}}[\psi] = \mathrm{q}[\psi]).$$

Then let H_{int} (resp. H_{ext}) be the associated self-adjoint operator in $L^2(\Omega_R^{int})$ (resp. $L^2(\Omega_R^{ext})$), the operator $H_{int} \oplus H_{ext}$ correspond to the operator H but defined by means of Neumann boundary conditions at $(x,y) \in \Omega, y = R$. Then from [8] we know that for every $\psi \in \mathrm{Dom}(q)$ the following inequality takes place, $(H\psi,\psi) \geq (H_{int} \oplus H_{ext}\psi,\psi)$ which implies

$$\inf\sigma_{ess}\,(H) \geq \inf\sigma_{ess}\,(H_{int} \oplus H_{ext})\,.$$

But the domain Ω_R^{int} is bounded so by standard arguments $\sigma_{ess}(H_{int}) = \emptyset$, [9]. Then

$$\inf\sigma_{ess}\,(H_{int} \oplus H_{ext}) = \sigma_{ess}(H_{ext}).$$

On the other hand $\forall\varphi \in \mathrm{Dom}(q_{ext})$, $\|\varphi\|_{L^2(\Omega_{ext})} = 1$ we have

$$(H_{ext}\varphi,\varphi) \geq (\partial_x^2 \otimes \mathbb{1}_y\varphi,\varphi).$$

For $y \in \mathbb{R}, |y| > R$, let $(u,v) \in \mathbb{R}^2$ be the solution of $f(u)+d = f(v) = y$, $|u|, |v| \to \infty$ as $y \to \infty$. By usual arguments then there exists $\xi \in (u,v)$ s.t. $d = |f(v)-f(u)| = |v-u||f'(\xi)|$ so $b(y) = \dfrac{d}{|f'(\xi)|} \to 0$ as $y \to \infty$.

This implies that

$$(\partial_x^2 \otimes \mathbb{1}_y\varphi,\varphi) = \int\limits_{|y|>R} dy \int\limits_u^v \partial_x^2\varphi\varphi \geq \left(\frac{\pi}{\sup_{|y|>R} b(y)}\right)^2 := i(R).$$

So $\inf\sigma_{ess}(H^{ext}) \geq i(R)$ for any $R > 0$ and large. But $i(R) \to \infty$ as $R \to \infty$, the theorem is proved. $\square$

3. Hardy inequalities

Theorem 3.1 (repulsive shearing)**.** *Suppose $\beta \in \mathbb{R}$, $f' \in L^\infty_{loc}(\mathbb{R})$, $\varepsilon \neq 0$ and $\beta\varepsilon \geq 0$. Then there exists $c > 0$ s.t.*

$$-\Delta_D - E_1(\beta) \geq \frac{c}{1+s^2}, \tag{3}$$

holds in the quadratic form sense in $L^2(\Omega)$.

Remark 3.1.
- *The theorem implies the non-existence of bound states for the system.*
- *Because of the presence of positive term in the r.h.s, the result is stable by adding a small perturbation.*
- *If $\varepsilon = 0$, simple arguments show that the theorem cannot be true, [4].*

Sketch of proof. The proof of the Theorem follows the same lines as in [1]. The key point is given by the following identity. Let $\psi \in C_0^\infty(\Omega_0)$, χ denoting the first transverse mode, then

$$q[\psi] - E_1(\beta)\|\psi\|^2 = \|\partial_s\psi - \varepsilon\partial_t\psi - \beta\chi\partial_t(\chi^{-1}\psi)\|^2 + \|\chi\partial_t(\chi^{-1}\psi)\|^2 + \int\limits_{\Omega_0} \beta\varepsilon\left(E_1(\beta) + (\frac{\chi'}{\chi})^2\right)|\psi|^2. \tag{4}$$

This comes from the ground state decomposition i.e. by choosing $\psi(s,t) = \chi(t)\phi(s,t)$, $\phi \in C_0^\infty(\Omega_0)$ (see [9]) in the formula (1). Notice that by (4), since the r.h.s. is positive if $\beta\varepsilon \geq 0$ then the associated operator $H_{f'}$ has no spectrum below $E_1(\beta)$.

Let I be an real interval s.t. $\mathrm{essinf}\{|\varepsilon|\} > 0$ on I and $\Omega_0^I = I \times (0,d)$. Denoting by:

$$\tilde{q_I}[\psi] := \|\partial_s\psi - \varepsilon\partial_t\psi - \beta\chi\partial_t(\chi^{-1}\psi)\|^2_{L^2(\Omega_0^I)} + \|\chi\partial_t(\chi^{-1}\psi)\|^2_{L^2(\Omega_0^I)}$$

$\mathrm{Dom}(\tilde{q_I}) = \{\psi\lfloor_{\Omega_0^I}, \psi \in H_0^1(\Omega_0)\}$. It is shown in [1] that $\tilde{q_I}$ is a closed quadratic form and:

$$\lambda_I = \inf_{\psi \in \mathrm{Dom}(q_I), \psi \neq 0_{\mathcal{H}_I}} \frac{\tilde{q}_I[\psi]}{\|\psi\|^2_{\mathcal{H}_I}} > 0.$$

Hence this gives a a local Hardy inequality i.e.:

$$q[\psi] - E_1\|\psi\|^2 \geq \int_{\Omega_0} \beta\varepsilon \left(E_1(\beta) + (\frac{\chi'}{\chi})^2\right)|\psi|^2 + \lambda_I \|\mathbb{I}_I \psi\|^2. \tag{5}$$

We now finish the proof of the theorem. We can check that if $\varepsilon(s_0) \neq 0$ that

$$Q[\psi] := \|\partial_s\psi - \varepsilon\partial_t\psi - \beta\chi\partial_t(\chi^{-1}\psi -)\alpha\frac{\chi}{s-s_0}\phi\|^2,\ \alpha = \frac{1}{2(1+\beta^2)}; \forall\psi \in C_0^\infty(\Omega_0 \setminus \{s_0\}).$$

satisfies the estimate:

$$0 \leq Q[\psi] \leq \|\partial_s\psi - \varepsilon\partial_t\psi - \beta\chi\partial_t(\chi^{-1}\psi)\|^2 + \|\chi\partial_t(\chi^{-1}\psi)\|^2 - \frac{1}{4(1+\beta^2)}\|\frac{\psi}{s-s_0}\|^2$$

and then:

$$\frac{1}{4(1+\beta^2)}\|\frac{\psi}{s-s_0}\|^2 \leq \|\partial_s\psi - \varepsilon\partial_t\psi - \beta\chi\partial_t(\chi^{-1}\psi)\|^2 + \|\chi\partial_t(\chi^{-1}\psi)\|^2. \tag{6}$$

Let $\psi \in C_0^\infty(\Omega_0, \mathbb{R})$ and η be the following function:

$$\eta(s) = \begin{cases} 1, & |s-s_0| > l; \\ -\frac{1}{l}(s-s_0), & s \in (s_0 - l, s_0)\,; \\ \frac{1}{l}(s-s_0), & s \in (s_0, s_0+l)\,. \end{cases}$$

Set $\Omega_l := (s_0 - l, s_0 + l) \times (0, d)$. By using the decomposition, $\psi = \eta\psi + (1-\eta)\psi$, evidently we have,

$$\int_{\Omega_0} \frac{|\psi|^2}{1+(s-s_0)^2} \leq \quad 2(\int_{\Omega_0} \frac{|\eta\psi|^2}{(s-s_0)^2} + \int_{\Omega_l} |\psi|^2). \tag{7}$$

We use (6) to estimate the first term of the r.h.s. of (7). Then

$$\begin{aligned} \int_{\Omega_0} \frac{|\eta\psi|^2}{(s-s_0)^2} &\leq 8(1+\beta^2)\left(\|\partial_s\eta\psi - \eta\varepsilon\partial_t\psi - \beta\eta\chi\partial_t(\chi^{-1}\psi)\|^2 + \|\eta\chi\partial_t(\chi^{-1}\psi)\|^2\right) \\ &\leq 8(1+\beta^2)\left(\|\partial_s\psi - \varepsilon\partial_t\psi - \beta\chi\partial_t(\chi^{-1}\psi)\|^2 + \|\beta\chi\partial_t(\chi^{-1}\psi)\|^2\right) + \|\eta'\psi\|^2) \\ &\leq 8(1+\beta^2)\left(q[\psi] - E_1(\beta)\|\psi\|^2 + \|\eta'\psi\|^2)\right). \end{aligned}$$

Hence, we get:

$$\int_{\Omega_0} \frac{|\psi|^2}{1+(s-s_0)^2} \leq 16(1+\beta^2)(q[\psi] - E_1(\beta)\|\psi\|^2) + 2(8(1+\beta^2)\frac{1}{l^2} + 1)\int_{\Omega_l} |\psi|^2. \tag{8}$$

Combining this last inequality with (5), we obtain (3) for such a vector ψ. But (3) can be extended for all vector $\psi \in \mathrm{Dom}(q)$ and the theorem is proved.

4. Discrete spectrum

Theorem 4.1 (Attractive shearing)**.** *Suppose that ε satisfies $\varepsilon^2 + 2\beta\varepsilon \in L^1(\mathbb{R})$ and either*

$$\int_{\mathbb{R}} (\varepsilon^2 + 2\beta\varepsilon) < 0 \tag{9}$$

or

$$\varepsilon \in W^1_{loc}(\mathbb{R}), \varepsilon \neq 0, \varepsilon \neq -2\beta \ and \ \int_{\mathbb{R}} (\varepsilon^2 + 2\beta\varepsilon) = 0. \tag{10}$$

Then $\sigma_d(H_f) \neq \emptyset$.

Proof. i) follows from the following : Let $\psi_n(s,t) = \varphi_n(s)\chi(t); n \in \mathbb{N}$ where $(\varphi_n)_{n\in\mathbb{N}}$ is a suitable mollification of the identity on $\mathbb{R}$ then from (4),

$$q[\psi_n] - E_1(\beta)\|\psi_n\|^2 =$$

$$\|\partial_s\psi_n - f'\partial_t\psi_n - \varepsilon\chi'\varphi_n\|^2 + \|\chi\partial_t\phi_n\|^2 + \int\limits_{\Omega_0} \beta\varepsilon \left(E_1(\beta) + (\frac{\chi'}{\chi})^2\right)|\psi_n|^2 =$$

$$\|\varphi_n'\|^2_{L^2(\mathbb{R})} + E_1(\beta)\int\limits_{\mathbb{R}} (\varepsilon^2 + 2\beta\varepsilon)|\varphi_n|^2 ds$$

$$\to E_1(\beta)\int\limits_{\mathbb{R}} (\varepsilon^2 + 2\beta\varepsilon) ds \quad \text{as} \quad n \to \infty.$$

Then the condition (9), implies, for n large enough that $q[\psi_n] - E_1(\beta)\|\psi_n\|^2 < 0$.

ii) follows in a similar way by choosing a slightly different sequence of test functions,

$$\psi_{n,\delta}(s,t) = \chi(t)(\varphi_n(s) + \delta t\xi(s)); n \in \mathbb{N}, \delta > 0$$

where $\xi \in C_0^\infty((-n,n))$ and $\delta > 0$ is chosen in a suitable way.

Remark 4.1. *The assumptions* (9) *and* (10) *of the theorem are clearly not satisfied for repulsive shearing. They require no positive deviation and of course the condition* $\varepsilon < 0$ *is too strong.*

□

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Information about the authors:

Ph. Briet – Aix Marseille Université, Université de Toulon, CNRS, CPT, Marseille France; briet@univ-tln.fr

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