Twisting *versus* bending in quantum waveguides

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Based on :

[Chenaud, Duclos, Freitas, D.K.] Differential Geom. Appl. *23* (2005)

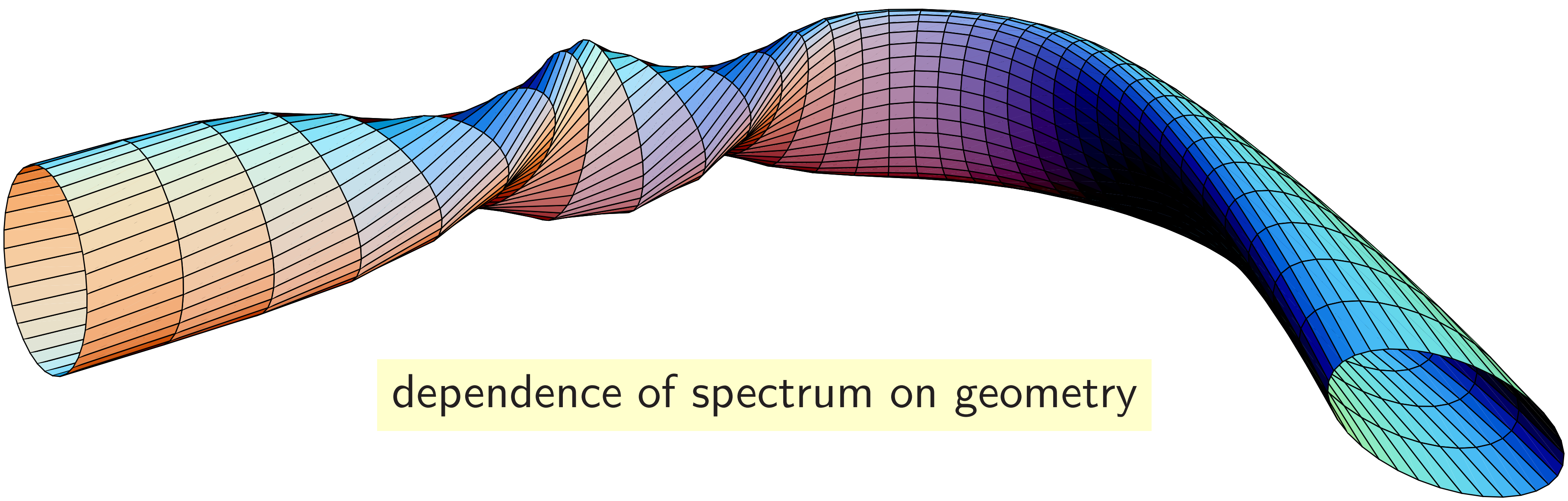
[Ekholm, Kovařík, D.K.] Arch. Ration. Mech. Anal., *to appear*

Graph Models of Mesoscopic Systems, Wave-Guides and Nano-Structures

Cambridge, 10–13 April 2007

The Problem

Hamiltonian $\approx -\dfrac{\hbar^2}{2\,m^*}\,\Delta_D^\Omega$ where Ω = twisted and bent tube



dependence of spectrum on geometry

mathematical model for *quantum waveguides* due to [Exner, Šeba 1989]

Characteristics of the (present) model:
- *unbounded* geometry
- *local* deformation
- *uniform* cross-section

Outline

1. Geometry of a twisted and bent tube
2. Strategy
3. Stability of the essential spectrum
4. Effect of bending
5. Effect of twisting
6. Conclusions

The Geometry

$\Gamma : \mathbb{R} \to \mathbb{R}^3$

unit-speed curve with curvature κ and torsion τ

- possessing an *appropriate* smooth Frenet frame $\{e_1, e_2, e_3\}$

$\Rightarrow$ Serret-Frenet formulae:
$$\begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix}' = \begin{pmatrix} 0 & \kappa & 0 \\ -\kappa & 0 & \tau \\ 0 & -\tau & 0 \end{pmatrix} \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix}$$

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open connected bounded set, $a := \sup_{t \in \omega} |t|$

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tube of cross-section ω

$$\mathcal{L}(s,t) := \Gamma(s) + \sum_{\mu=2}^{3} t_\mu \, e_\mu^\theta(s)$$

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Assumptions: $\|\kappa_1\|_\infty \, a < 1$ and Ω does not overlap itself

The motion of the general moving frame

$$\begin{pmatrix} e_1^\theta \\ e_2^\theta \\ e_3^\theta \end{pmatrix}' = \begin{pmatrix} 0 & \kappa\cos\theta & \kappa\sin\theta \\ -\kappa\cos\theta & 0 & \tau - \theta' \\ -\kappa\sin\theta & -(\tau - \theta') & 0 \end{pmatrix} \begin{pmatrix} e_1^\theta \\ e_2^\theta \\ e_3^\theta \end{pmatrix}$$

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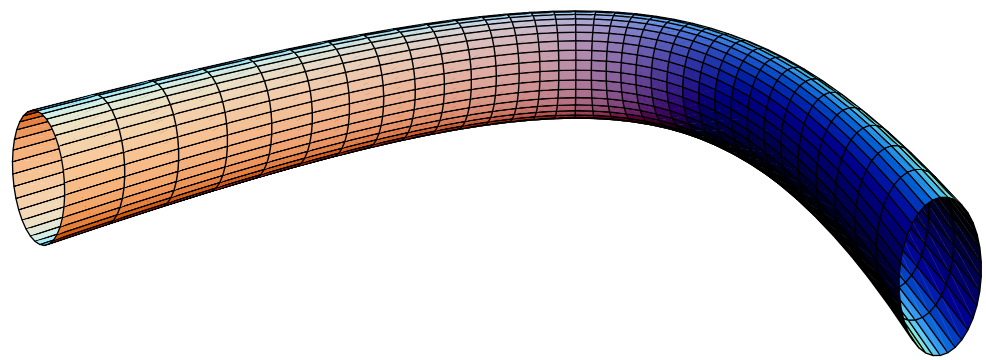

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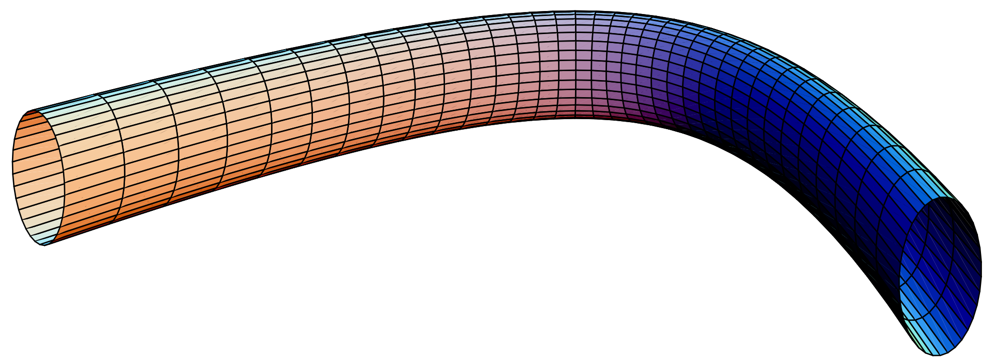
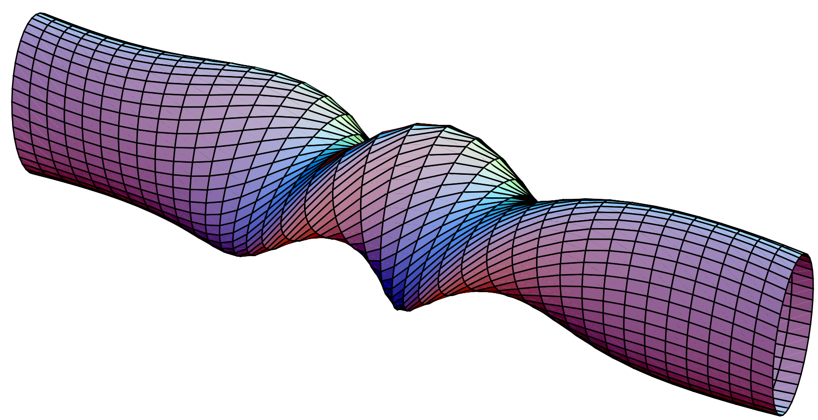


twisting $:\Longleftrightarrow \quad \begin{cases} \tau - \theta' \neq 0 \\ \omega \text{ is not circular} \end{cases}$



Equivalent definitions of twisting

a tube of non-circular cross-section is not twisted

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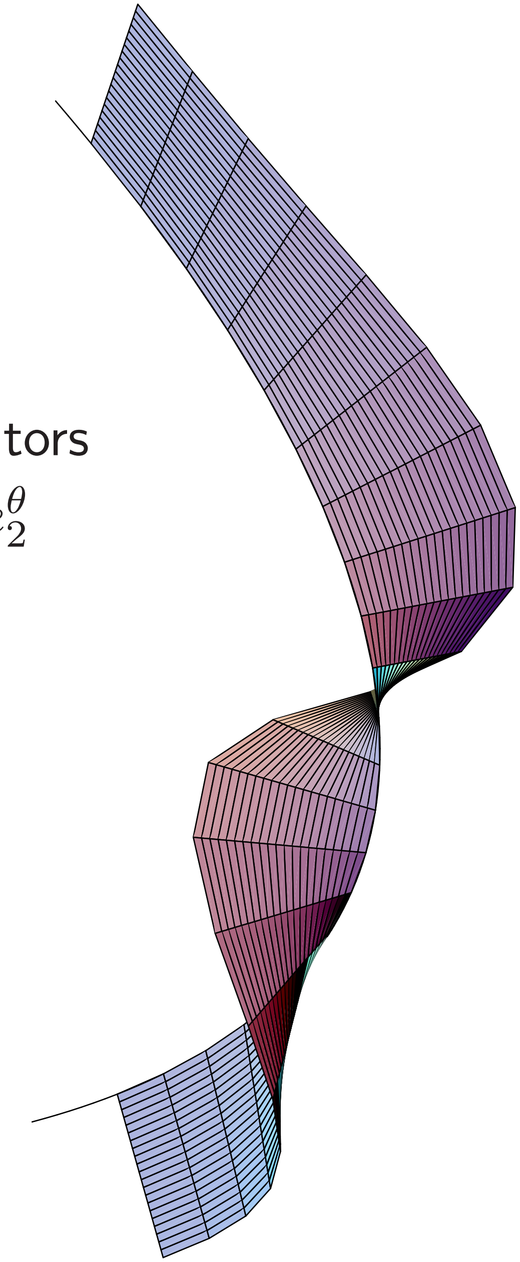

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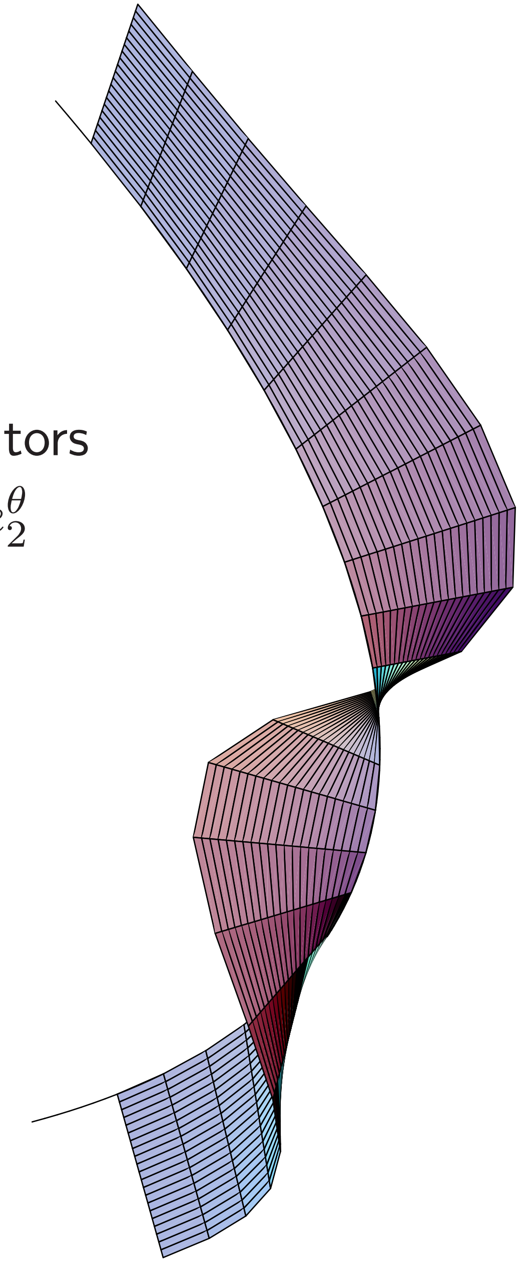

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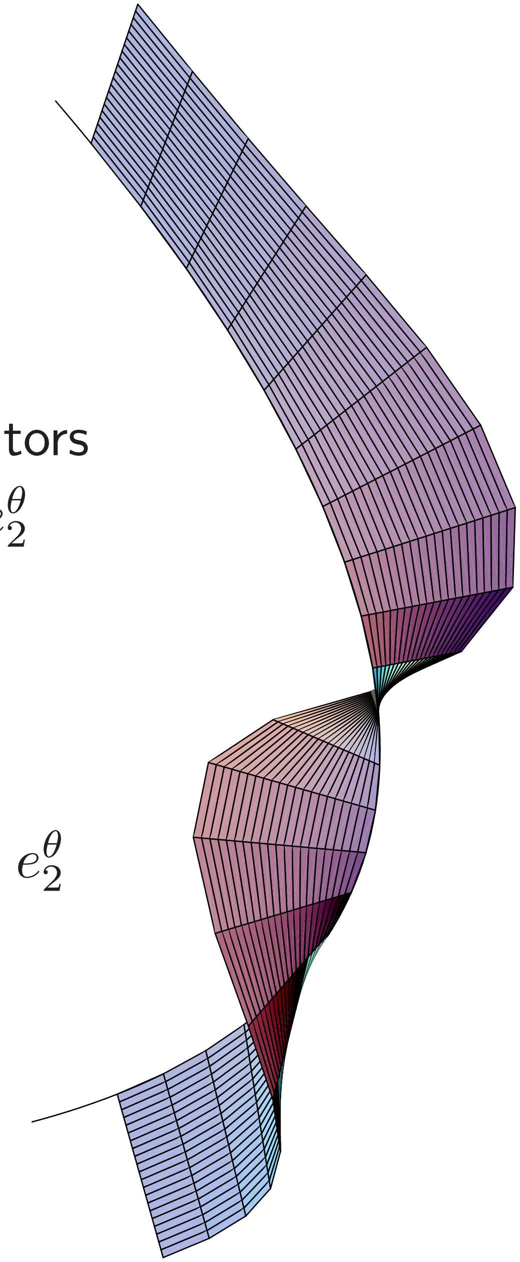
$:\Longleftrightarrow$ $\{e_1^\theta, e_2^\theta, e_3^\theta\}$ is the **Tang frame** *i.e.* $\theta' = \tau$

$\Longleftrightarrow$ **parallel transport** of the surface normal along generators of the ruled surface generated by e_2^θ

$\Longleftrightarrow$ **zero curvature** of the ruled surface

$\Longleftrightarrow$ **no Coriolis acceleration** of the (non-inertial) traveller e_2^θ



The Hamiltonian

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Strategy: $\mathcal{L} : \mathbb{R} \times \omega \to \Omega$ is a diffeomorphism $\Longrightarrow$ $\Omega \simeq (\mathbb{R} \times \omega, G)$

$$G = \begin{pmatrix} h^2 + h_2^2 + h_3^2 & h_2 & h_3 \\ h_2 & 1 & 0 \\ h_3 & 0 & 1 \end{pmatrix}$$

$$h(s,t) := 1 - [t_2 \cos\theta(s) + t_3 \sin\theta(s)]\,\kappa(s)$$

$$h_2(s,t) := -t_3\,[\tau(s) - \theta'(s)]$$

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$$-\Delta_D^\Omega \simeq \quad H \overset{\mathrm{w}}{:=} -|G|^{-1/2}\,\partial_i\,|G|^{1/2}\,G^{ij}\,\partial_j \quad \text{on} \quad L^2(\mathbb{R} \times \omega, d\mathrm{vol})$$

$$|G| := \det(G) = h^2, \qquad (G^{ij}) := G^{-1}, \qquad d\mathrm{vol} := h(s,t)\,ds\,dt$$

Stability of essential spectrum

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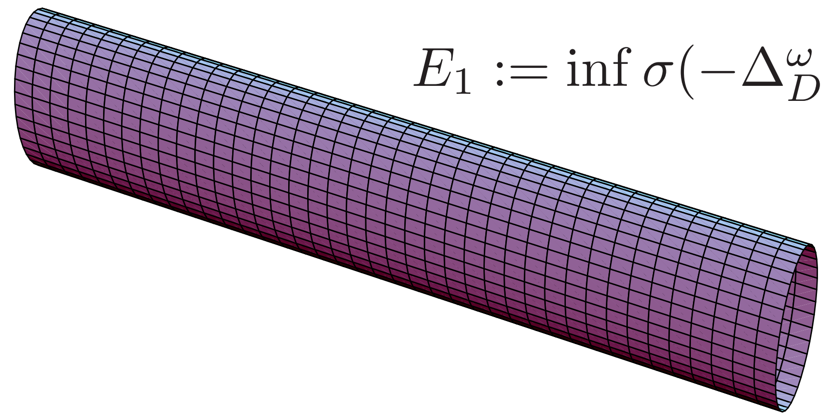
Remark. Straight tube $(\kappa = 0 = \tau - \theta')$:

$$E_1 := \inf \sigma(-\Delta_D^{\omega})$$

$$\sigma(-\Delta_D^{\mathbb{R}\times\omega}) = \sigma_{\text{ess}}(-\Delta_D^{\mathbb{R}\times\omega}) = [E_1, \infty)$$



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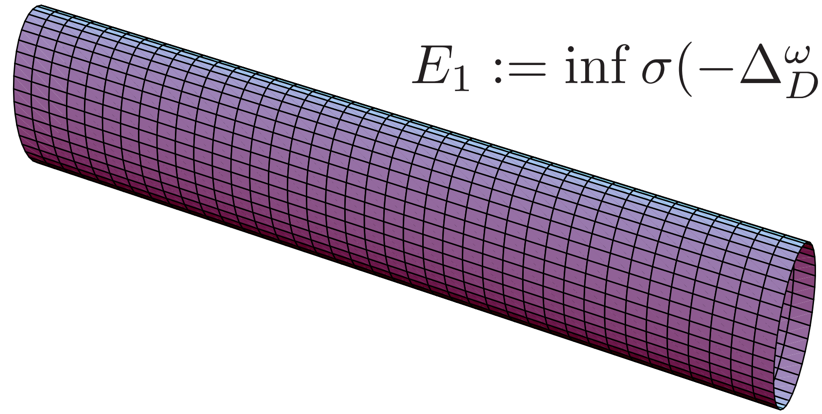

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Theorem. $$\lim_{|s|\to\infty}\big(|\kappa(s)| + |\tau(s) - \theta'(s)|\big) = 0 \quad \Longrightarrow \quad \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) = [E_1, \infty)$$

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Classical Weyl's criterion requires to impose additional conditions on derivatives!

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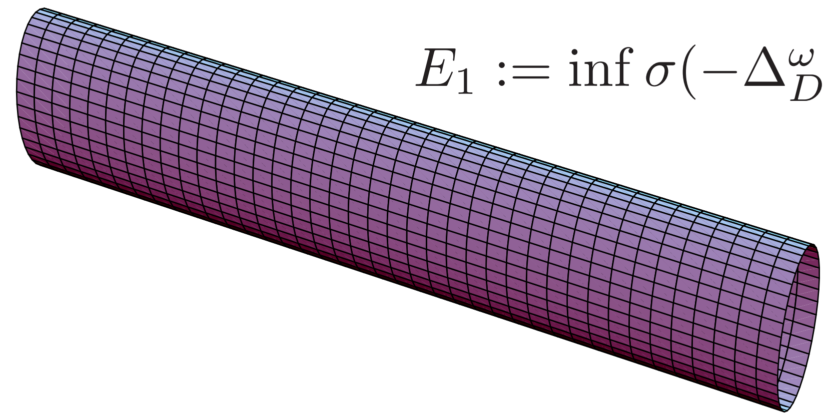

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History :

[Goldstone, Jaffe 1992] ... κ of compact support & $\omega =$disc

[Duclos, Exner 1995] ... additional vanishing of κ' and κ'' & $\omega =$disc

[Dermenjian, Durand, Iftimie 1998] ... σ_{ess} of multistratified cylinders

[Chenaud, Duclos, Freitas, D.K. 2005] ... $\theta' = \tau$ (ω arbitrary)

The effect of bending

Theorem. $\kappa \neq 0 \quad \& \quad \theta' = \tau \quad \Longrightarrow \quad \inf \sigma(-\Delta_D^\Omega) < E_1$

Proof. Trial function based on $\mathcal{J}_1$ ($\leftrightarrow$ E_1). q.e.d.

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Theorem ([Ekholm, Kovařík, D.K. 2005]).
Let $\kappa = 0$. Let θ be such that $\theta' \neq 0$, $\theta' \in C_0(\mathbb{R})$ and $\theta'' \in L^\infty(\mathbb{R})$.
Assume that ω is not circular. Then

$$-\Delta_D^\Omega - E_1 \ \geq \ \frac{c}{1 + |\Gamma(\cdot) - \Gamma(s_0)|^2}$$

Hardy inequality !

where $s_0 \in \mathbb{R}$ is such that $\theta'(s_0) \neq 0$ and $c = c(s_0, \theta', \omega) > 0$.

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Proof. Writing $\psi(s,t) = \mathcal{J}_1(t)\,\phi(s,t)$, $\psi \in C_0^\infty(\mathbb{R} \times \omega)$, $\qquad \partial_\sigma := t_3\,\partial_2 - t_2\,\partial_3$,

$$\big(\psi, [H - E_1]\,\psi\big) = \|\mathcal{J}_1 \partial_1 \phi\|^2 + \|\mathcal{J}_1 \partial_2 \phi\|^2 + \|\mathcal{J}_1 \partial_3 \phi\|^2$$

$$+ \|\theta'\,(\mathcal{J}_1 \partial_\sigma \phi + \phi\,\partial_\sigma \mathcal{J}_1)\|^2 + \text{ mixed terms} \qquad \ldots \qquad \text{q.e.d.}$$

Twisting *vs* bending

Theorem ([Ekholm, Kovařík, D.K. 2005]).

Let θ be such that $\tau - \theta' \neq 0$, $\theta' \in C_0(\mathbb{R})$ and $\theta'' \in L^\infty(\mathbb{R})$.
Assume that ω is not circular. Assume also that $\kappa \in C_0^1(\mathbb{R})$.
Then there exists $\varepsilon > 0$ such that

$$\|\kappa\|_\infty + \|\kappa'\|_\infty \leq \varepsilon \quad \Longrightarrow \quad \sigma\big(-\Delta_D^\Omega\big) = [E_1, \infty)$$

where $\varepsilon = \varepsilon(\tau, \theta', \omega)$.

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Theorem ([Bouchitté, Mascarenhas, Trabucho 2006]). $\longleftarrow$ graph model

Let $\Omega_\varepsilon = \mathcal{L}(I \times \varepsilon\omega)$, I bounded. Then

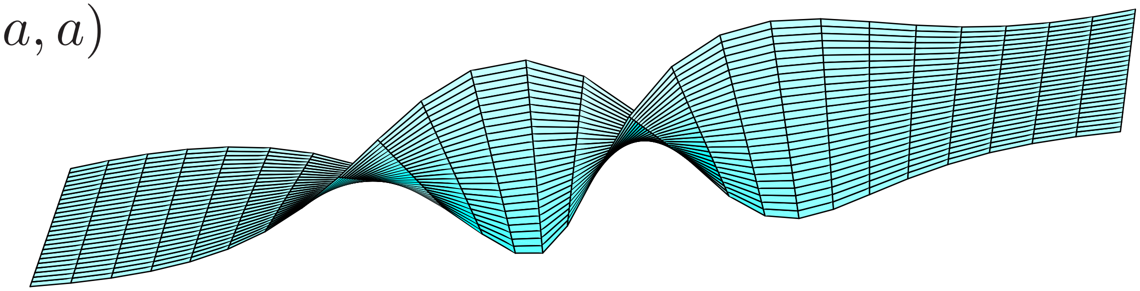
$$-\Delta_D^{\Omega_\varepsilon} - \varepsilon^{-2} E_1(\omega) \underset{\varepsilon \to 0}{\simeq} -\Delta_D^I - \frac{\kappa^2}{4} + C(\omega)(\tau - \theta')^2 + \mathcal{O}(\varepsilon)$$

where $C(\omega) > 0$ *iff* ω is not circular.

Twisted strips

$$\omega = (-a, a) \times (-b, b) \xrightarrow[b \to 0]{} (-a, a)$$

$$E_1 = \left(\frac{\pi}{2a}\right)^2$$



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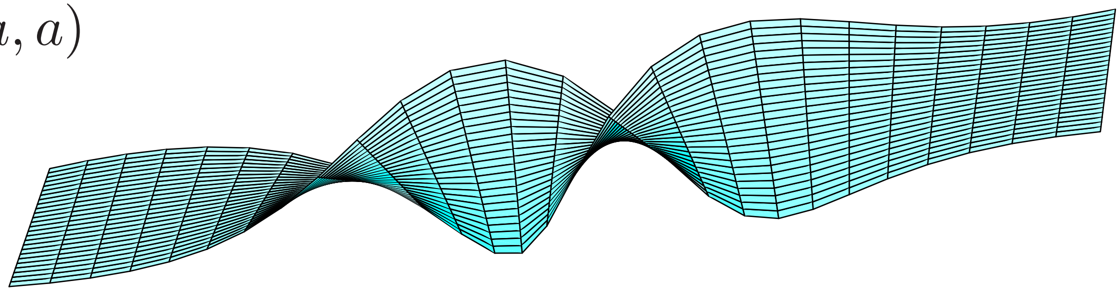

Theorem ([D.K. 2006]).
Assume that $\kappa \cos\theta = 0$ and $0 < \|\tau - \theta'\|_\infty \, a \leq \sqrt{2}$. Then

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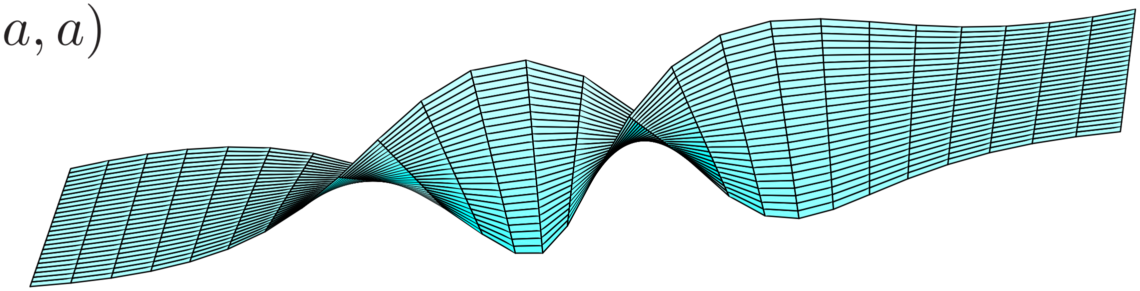

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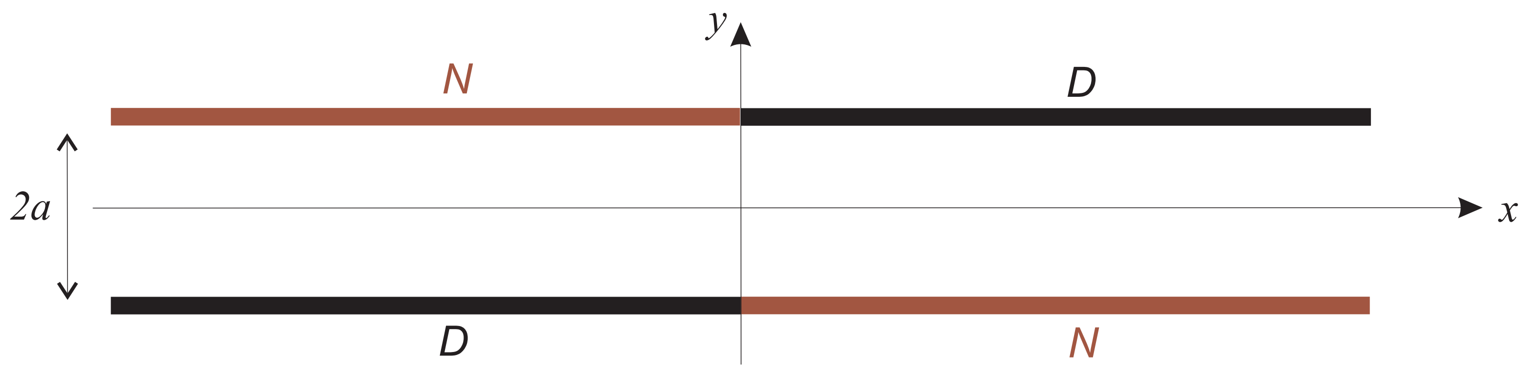
negative curvature of the ambient space acts as a *repulsive* interaction

Twist via boundary conditions

$$E_1 = \left(\frac{\pi}{4a}\right)^2$$



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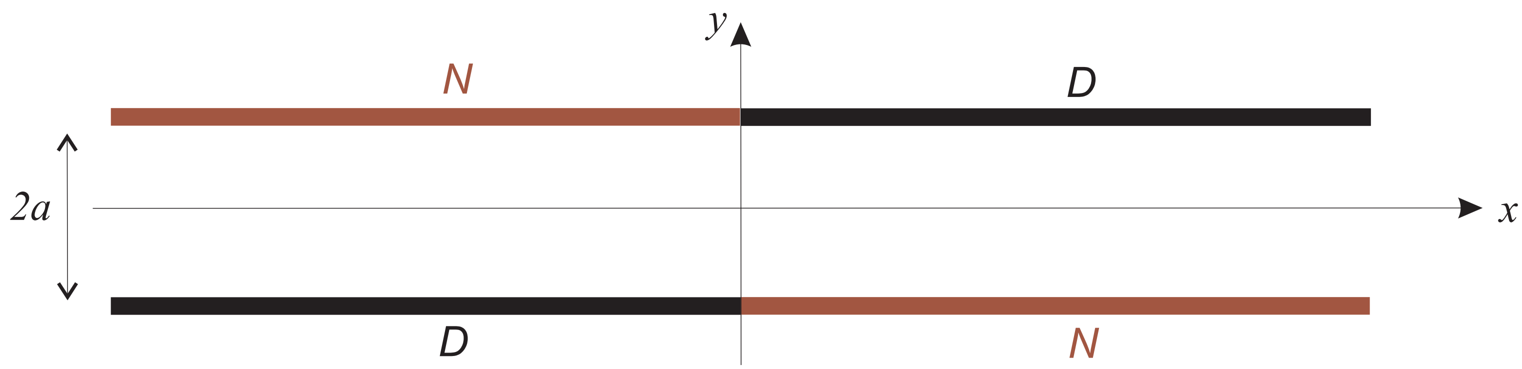

Theorem ([Kovařík, D.K. 2006]).

$$-\Delta_{DN} - E_1 \;\geq\; \frac{c}{1+x^2}$$

where $c = c(a) > 0.$

Conclusions

Moral :

→ bending acts as an *attractive* interaction

→ twisting acts as a *repulsive* interaction

→ Hardy inequalities in twisted tubes

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$\longrightarrow$ Hardy inequalities in twisted tubes

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Open problems :

¿ higher-dimensional generalisations ?

¿ effect of twisting on the essential spectrum ?

¿ other physical motivations ?

Mourre's theory for twisted tubes ?

Theorem ([D.K., Tiedra de Aldecoa 2004]).

Assume that $\theta' = \tau$ (plus some fast decay of κ, τ at infinity).

Then $A := -\frac{i}{2}(s\,\partial_s + \partial_s\, s)$ is strictly conjugate to H on $\mathbb{R} \setminus \{E_n\}_{n=1}^{\infty}$,

i.e. $\mathcal{P}^H i[H, A]\mathcal{P}^H \geq c\,\mathcal{P}^H$ with some $c > 0$.

Corollary. Eigenvalues of H are countable and can accumulate at E_n only.

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i.e. $\mathcal{P}^H i[H,A]\mathcal{P}^H \geq c\,\mathcal{P}^H$ with some $c > 0$.

Corollary. Eigenvalues of H are countable and can accumulate at E_n only.

Commutator for the straight tube: $i[H_0, A] = 2(-\partial_s^2)$

$\Longrightarrow$ $\psi_n := 1 \otimes \mathcal{J}_n$ represent the 'bad' functions.

Mourre's theory for twisted tubes ?

Theorem ([D.K., Tiedra de Aldecoa 2004]).
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However, $\big(\psi_n, i[H,A]\,\psi_n\big) = \|\theta'\partial_\sigma \mathcal{J}_n\|^2 > 0$ for a straight but twisted tube!

Conjecture. The result of Mourre theory can be improved for twisted tubes.