Mode matching methods in spectral and scattering problems

by Denis Grebenkov

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Outline of the talk

- Two major research directions
- Mode matching method
- Conclusions and perspectives

https://pmc.polytechnique.fr/pagesperso/dg/publi/publi_e.htm

I. Spectral theory of diffusion MRI

$\vec{G}$

$$\partial_t m = D_0 \Delta m - i\gamma(\vec{G}\cdot\vec{r})m$$

diffusion precession

$$m(\vec{r}, t=0) = 1$$

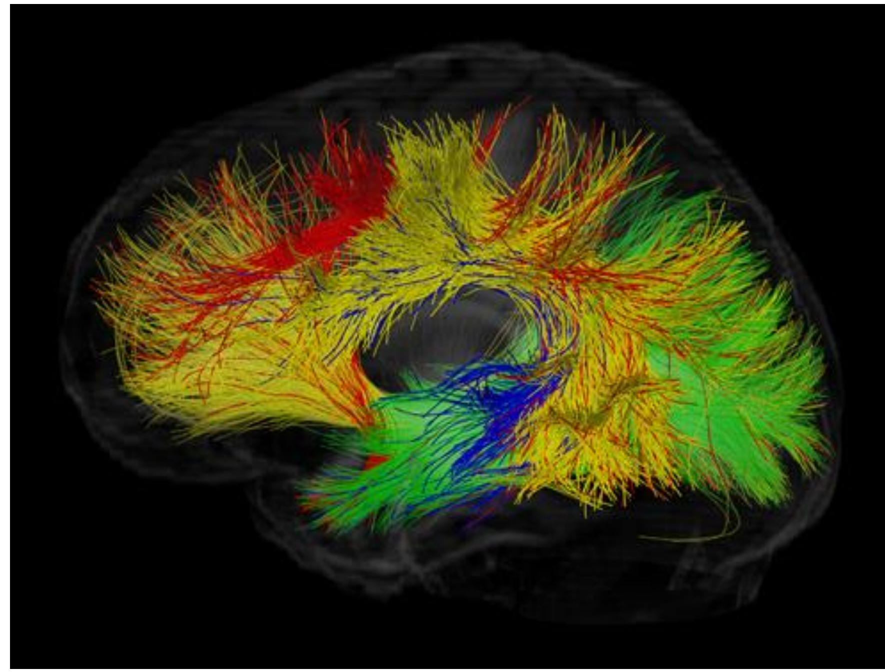
$$\partial_n m = 0$$

Ω

$$m = \exp\left(-D_0 B_g t\right) 1$$

$$B_g = -\Delta + igx$$

Non-self-adjoint Schrödinger operator with purely imaginary linearly growing potential

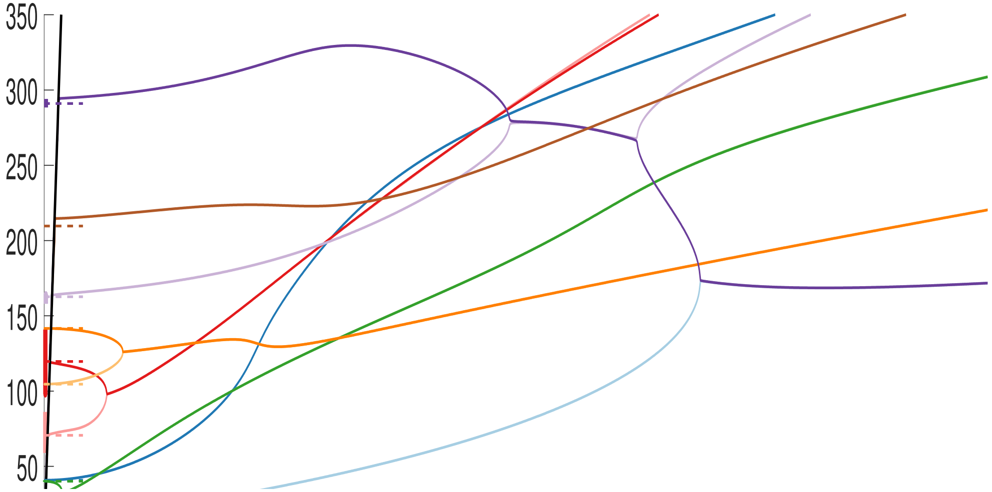


Wedeen et al., Science (2012)

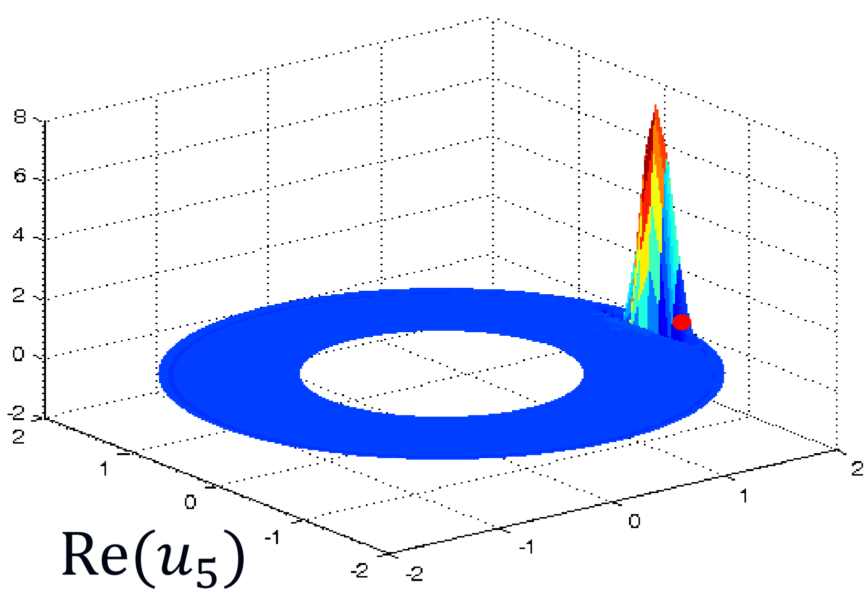
1D domains
bounded domains
unbounded domains
periodic domains

DG, Rev. Mod. Phys. 79, 1077-1137 (2007)
DG & Helffer, SIAM J. Math. Anal. 50, 622 (2018)
Almog, DG, & Helffer, J. Math. Phys. 59, 041501 (2018)
Moutal, Moutal, and DG, J. Phys. A 53, 325201 (2020)

I. Spectral theory of diffusion MRI



- Asymptotic behavior of eigenvalues as $g \to \infty$
- Branching points in the spectrum
- Localization of eigenfunctions



jer operator with
jrowing potential

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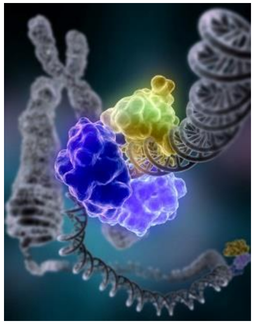
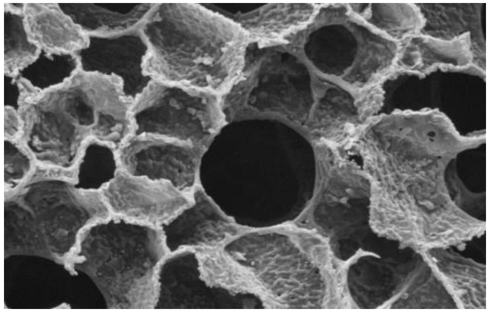
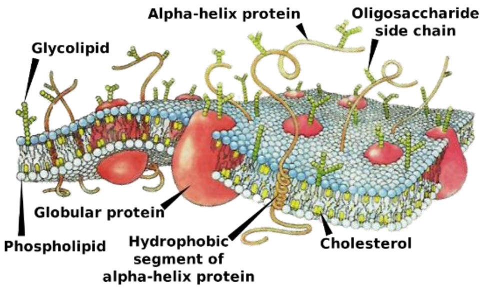
Moutal, Moutal, and DG, J. Phys. A 53, 325201 (2020)

II. Diffusion-influenced reactions







Let τ be the (random) first-passage time to the target

$$S(x,t) = \boldsymbol{P}_x\{\tau > t\}$$

survival probability

Mixed boundary value problem

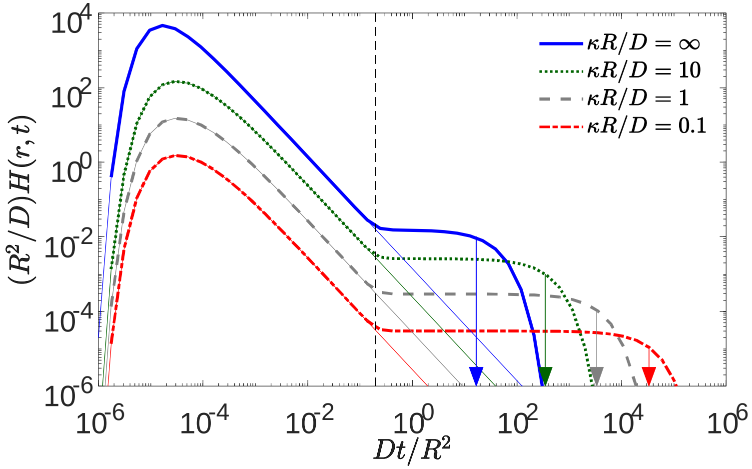
$$\partial_t S = L_{FP}^* S \qquad \text{in the bulk}$$

$$-D\partial_n S = \kappa\, S \qquad \text{on the target}$$

$$-D\partial_n S = 0 \qquad \text{on the rest}$$

S. Redner, *A guide to first-passage processes* (2001)
R. Metzler, et al., *First-passage phenomena and their applications* (2014)
D. Holcman, Z. Schuss, *SIAM Rev. 56, 213-257* (2014)

II. Diffusion-influenced reactions



- **Whole distribution of the FPT**

  DG, et al. Commun. Chem. 1, 96 (2018)

- **Anomalous diffusions**

  Lanoiselée et al., Nat. Commun. 9, 4398 (2018)

- **Effect of multiple particles**

  DG et al., New J. Phys. 22, 103004 (2020)

- **Encounter-based approach**

  Understanding and generalization of Robin BC

  DG, Phys. Rev. Lett. 125, 078102 (2020)

$$S_\kappa(x,t) = \int_0^\infty d\ell \, e^{-\ell\kappa/D} \, P(\ell, t|x)$$

II. Diffusion-influenced reactions

- Whole distribution of the FPT

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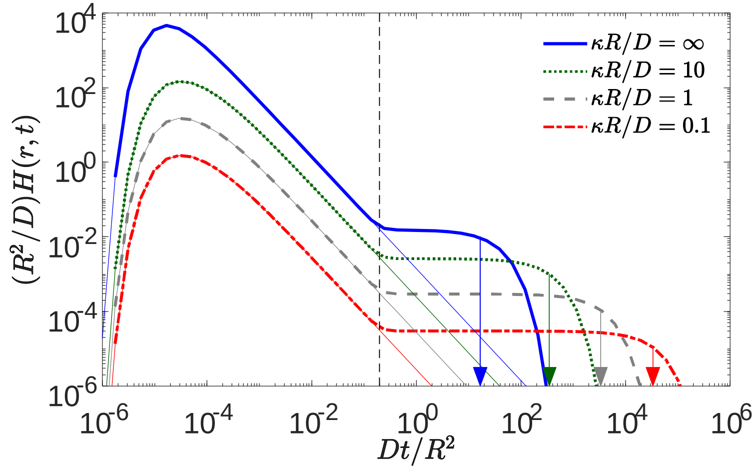

- Anomalous diffusions

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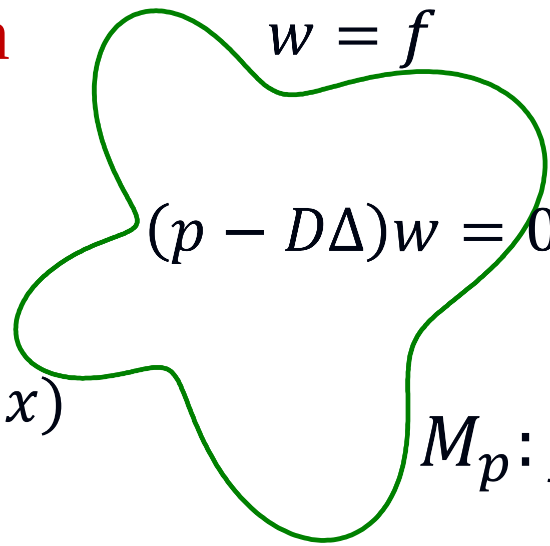
$$S_\kappa(x,t) = \int_0^\infty d\ell \, e^{-\ell\kappa/D} \, P(\ell,t|x)$$

Dirichlet-to-Neumann operator M_p

$w = f$



$(p - D\Delta)w = 0$

$\partial_n w = g$

$M_p : f \to g = \partial_n w$

Mode matching methods

in collaboration with A. Delitsyn
(Kharkevich Institute for Information Transmission Problems of RAN, Moscow, Russia)

A. Delitsyn, B.-T. Nguyen, & DG, *Trapped modes in finite quantum waveguides*, Eur. Phys. J. B. 85, 176 (2012)

A. Delitsyn, B.-T. Nguyen, & DG, *Exponential decay of Laplacian eigenfunctions in domains with branches of variable cross-sectional profiles*, Eur. Phys. J. B 85, 371 (2012)

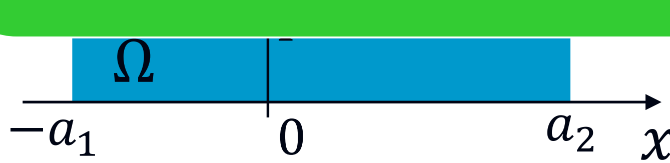
A. Delitsyn & DG, *Mode matching methods in spectral and scattering problems*, Quart. J. Mech. Appl. Math. 71, 537–580 (2018)

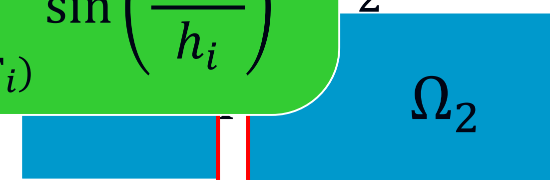
A. Delitsyn & DG, *Resonance scattering in a waveguide with identical thick perforated barriers*, Appl. Math. Comput. 412, 126592 (2022)

Basic idea

$$\frac{\partial u_i}{\partial x}\Big|_\Gamma = T_i(\lambda)\, u_i\Big|_\Gamma$$

$$T_i(\lambda)f = \sum_n \frac{2\gamma_{n,i}}{h_i \tanh(\gamma_{n,i} a_i)} \left(f, \sin\left(\frac{\pi n y}{h_i}\right)\right)_{L_2(\Gamma_i)} \sin\left(\frac{\pi n y}{h_i}\right)$$





$$u_1\Big|_\Gamma = u_2\Big|_\Gamma = u\Big|_\Gamma$$

$$-\Delta u = \lambda u$$

$$\gamma_{n,1} = \sqrt{\frac{\pi^2 n^2}{h_1^2} - \lambda}$$

$$u_1(x,y) = \sum_n c_{n,1} \sin\left(\frac{\pi n y}{h_1}\right) \sinh(\gamma_{n,1}(a_1 + x))$$

$$u_1(x,y) = \sum_n \frac{2\left(u_1|_\Gamma, \sin\left(\frac{\pi n y}{h_1}\right)\right)_{L_2(\Gamma)}}{h_1 \sinh(\gamma_{n,1} a_1)} \sin\left(\frac{\pi n y}{h_1}\right) \sinh(\gamma_{n,1}(a_1 + x))$$

$$u_2(x,y) = \sum_n \frac{2\left(u_2|_\Gamma, \sin\left(\frac{\pi n y}{h_2}\right)\right)_{L_2(\Gamma)}}{h_2 \sinh(\gamma_{n,2} a_2)} \sin\left(\frac{\pi n y}{h_2}\right) \sinh(\gamma_{n,2}(a_2 - x))$$

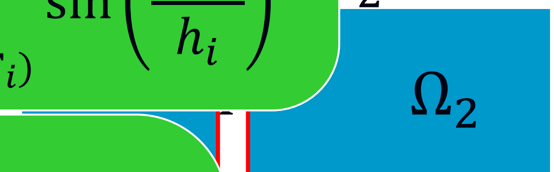
A. Delitsyn & DG, Quart. J. Mech. Appl. Math. 71, 537–580 (2018)

Basic idea

$$\frac{\partial u_i}{\partial x}\bigg|_\Gamma = T_i(\lambda)\, u_i\bigg|_\Gamma$$

$$T_i(\lambda)f = \sum_n \frac{2\gamma_{n,i}}{h_i \tanh(\gamma_{n,i} a_i)} \left(f, \sin\left(\frac{\pi n y}{h_i}\right)\right)_{L_2(\Gamma_i)} \sin\left(\frac{\pi n y}{h_i}\right)$$

$u_2 = 0$



$$\frac{\partial u_1}{\partial x}\bigg|_\Gamma = \frac{\partial u_2}{\partial x}\bigg|_\Gamma \quad \forall y \in \Gamma$$

$= u_2\big|_\Gamma = u\big|_\Gamma$

$$\left(T_1(\lambda)u\big|_\Gamma - T_2(\lambda)u\big|_\Gamma, v\right)_{L_2(\Gamma)} = 0 \quad \forall v \in \mathrm{H}^{\frac{1}{2}}(\Gamma)$$

$u_1($ … $_{,1} = \sqrt{\frac{\pi^2 n^2}{h_1^2} - \lambda}$

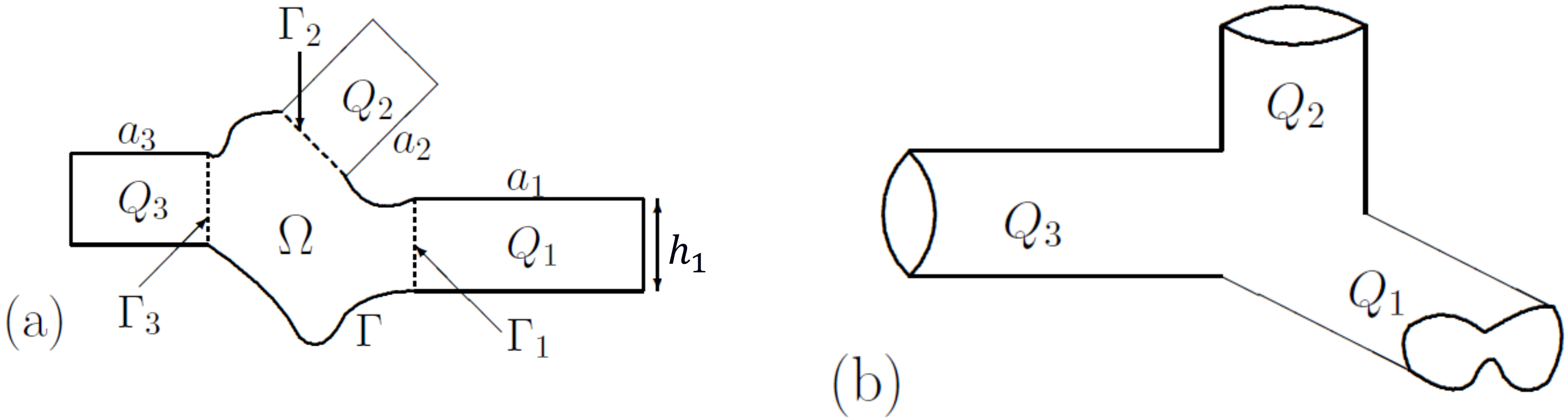
$$a_\lambda(u\big|_\Gamma, v) = 0 \quad \forall v \in \mathrm{H}^{\frac{1}{2}}(\Gamma)$$

$u_1($ … $+ x))$

$$a_\lambda(f,g) = \sum_n \frac{2\gamma_{n,1}}{h_1 \tanh(\gamma_{n,1} a_1)} \left(f, \sin\left(\frac{\pi n y}{h_1}\right)\right)_{L_2(\Gamma)} \left(g, \sin\left(\frac{\pi n y}{h_1}\right)\right)_{L_2(\Gamma)}$$
$$+ \sum_n \frac{2\gamma_{n,2}}{h_2 \tanh(\gamma_{n,2} a_2)} \left(f, \sin\left(\frac{\pi n y}{h_2}\right)\right)_{L_2(\Gamma)} \left(g, \sin\left(\frac{\pi n y}{h_2}\right)\right)_{L_2(\Gamma)}$$

$u_2($

Finite quantum waveguides



$-\Delta u = \lambda u$ in $D = \Omega \cup Q_1 \cup \cdots \cup Q_n$ $\qquad u = 0$ on ∂D

$$\boldsymbol{T_i(\lambda)f} = \sum_{\boldsymbol{n}} \frac{\gamma_{n,i}}{\tanh(\gamma_{n,i} a_i)} \left(f, \psi_{n,i}\right)_{L_2(\Gamma_i)} \psi_{n,i}(y) \qquad \gamma_{n,i} = \sqrt{\nu_{n,i} - \lambda}$$

$$\frac{2}{h_i}\left(f, \sin\left(\frac{\pi n y}{h_i}\right)\right)_{L_2(\Gamma_i)} \sin\left(\frac{\pi n y}{h_i}\right)$$

$-\Delta u = \lambda u$ in Ω $\qquad u = 0$ on Γ $\qquad \left.\frac{\partial u}{\partial n}\right|_{\Gamma_i} = -T_i(\lambda)u\Big|_{\Gamma_i}$

$-\Delta u = \mu(\lambda)u$ in Ω $\qquad u = 0$ on Γ $\qquad \left.\frac{\partial u}{\partial n}\right|_{\Gamma_i} = -T_i(\lambda)u\Big|_{\Gamma_i}$

A. Delitsyn, B.-T. Nguyen, & DG, Eur. Phys. J. B. 85, 176 (2012)

Finite quantum waveguides

Sufficient condition for trapping

$$\exists v \in H(\Omega) \quad \text{s.t.} \qquad \sum_i \left(\frac{\sigma_i}{a_i} + \frac{\kappa_i}{\tanh(a_i \sqrt{\nu_2 - \nu_1})} \right) < \beta$$

$$\beta = \nu_1 (v, v)_{L_2(\Omega)} - (\nabla v, \nabla v)_{L_2(\Omega)}$$

$$\sigma_i = (v, \psi_1)^2_{L_2(\Gamma_i)} \qquad \kappa_i = \sum_n \sqrt{\nu_n - \nu_1}\, (v, \psi_n)^2_{L_2(\Gamma_i)}$$

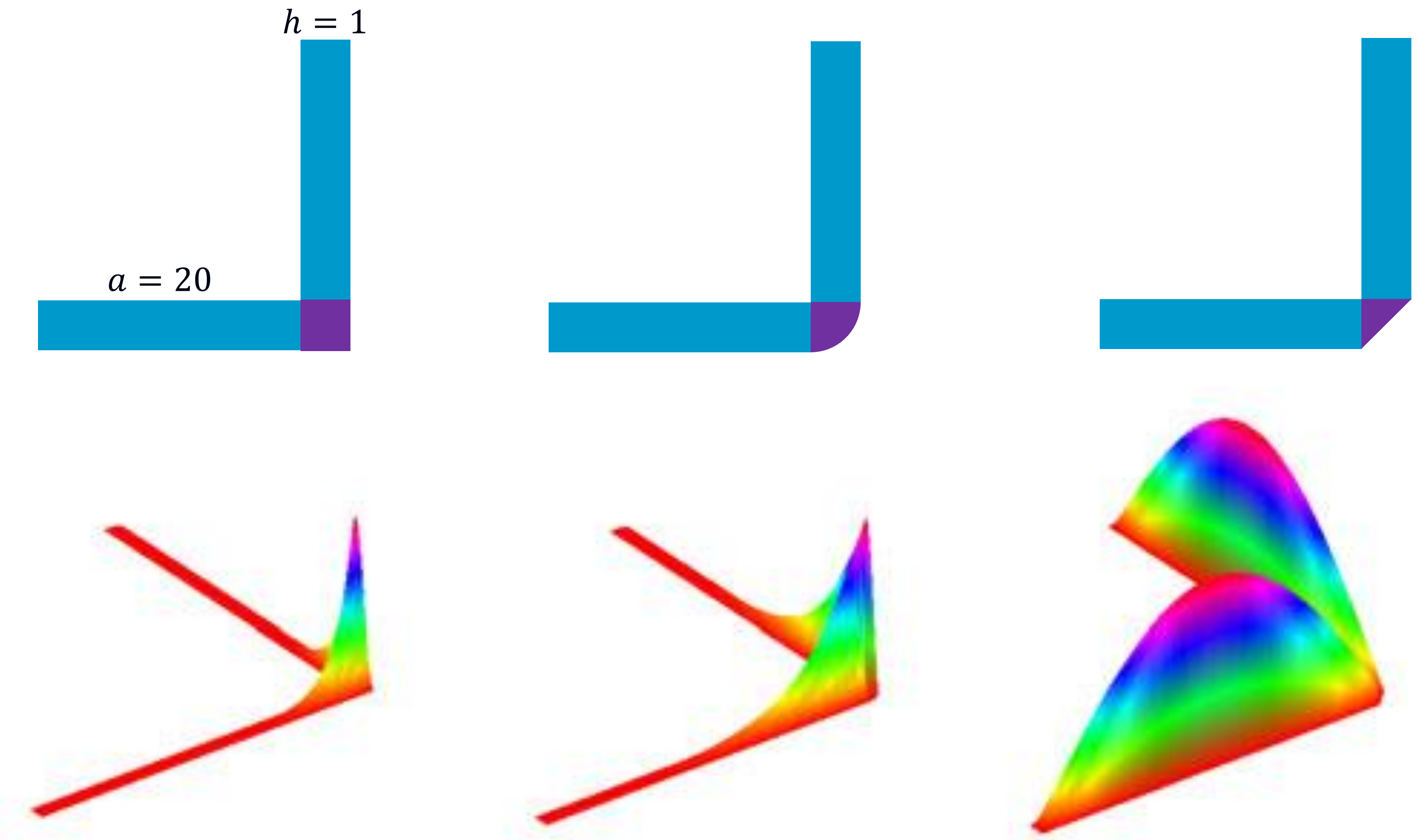
For long enough branches of the same profile:

$$\sum_i \frac{1}{a_i} < \eta = \frac{\beta}{\sigma_1} - \frac{1}{\sigma_1} \sum_i \kappa_i$$

$$-\Delta u = \mu(\lambda) u \ \text{ in } \Omega \qquad u = 0 \ \text{ on } \Gamma \qquad \left. \frac{\partial u}{\partial n} \right|_{\Gamma_i} = -T_i(\lambda) u \Big|_{\Gamma_i}$$

A. Delitsyn, B.-T. Nguyen, & DG, Eur. Phys. J. B. 85, 176 (2012)

Finite quantum waveguides

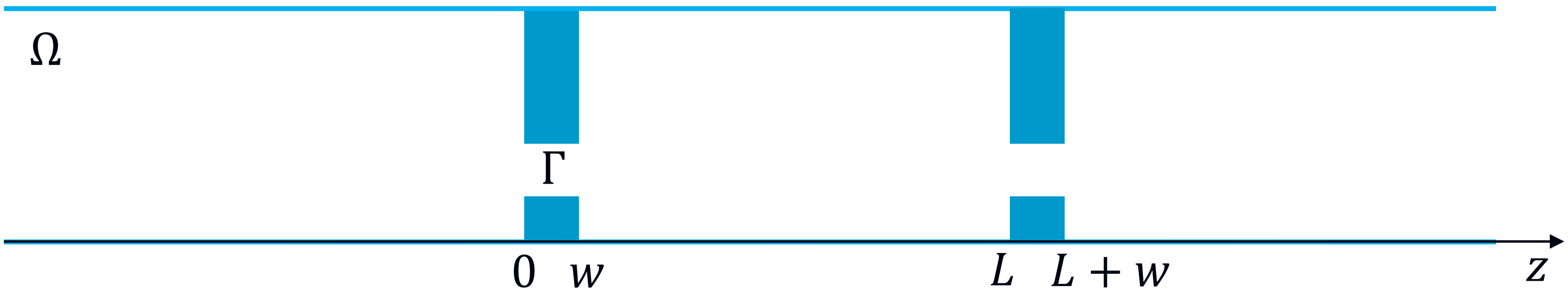


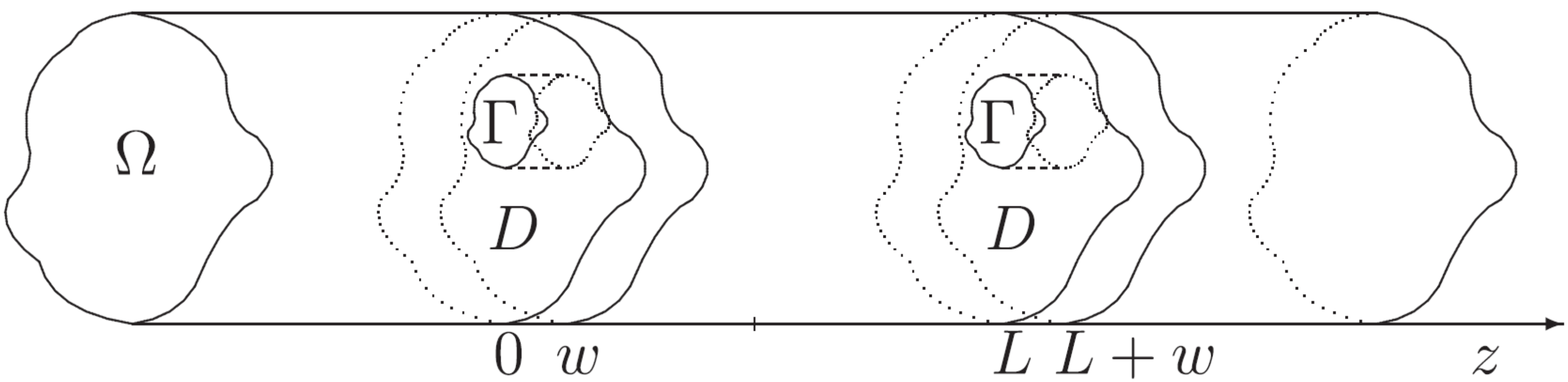
$\lambda_1 \approx 0.9302\,\pi^2$ $\lambda_1 \approx 0.9879\,\pi^2$ $\lambda_1 \approx 1.0032\,\pi^2$

A. Delitsyn, B.-T. Nguyen, & DG, Eur. Phys. J. B. 85, 176 (2012)

Scattering problem

Infinite cylinder Q_0 of a bounded cross-section Ω with a “hole” Γ





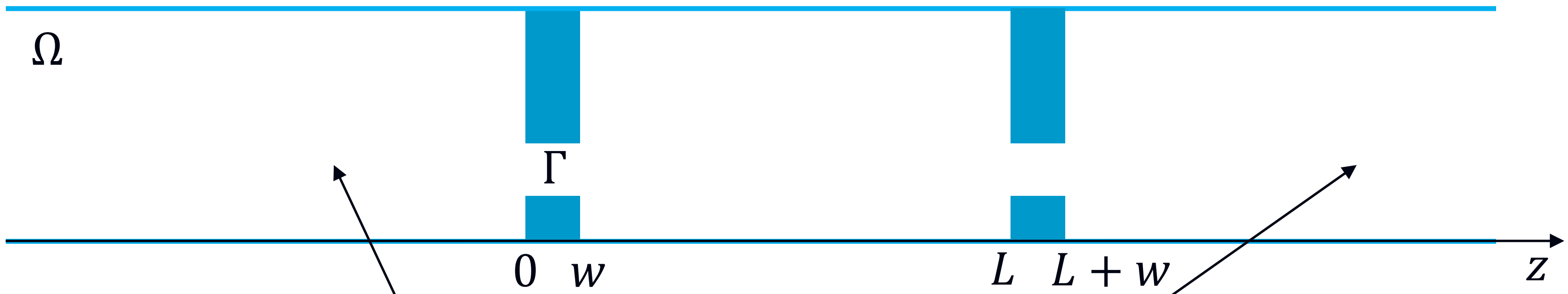
A. Delitsyn & DG, Quart. J. Mech. Appl. Math. 71, 537–580 (2018) $w = 0$

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022) $w > 0$

L. Chesnel, S.A. Nazarov, *Abnormal acoustic transmission in a waveguide with perforated screens*, C. R. Mécanique, 349, 1:9-19 (2021)

Scattering problem

Infinite cylinder Q_0 of a bounded cross-section Ω with a “hole” Γ



$$\Delta u + k^2 u = 0 \quad \text{in } Q_0 \qquad u = 0 \quad \text{on } \partial Q_0$$

$$u(x,z) = e^{i\gamma_1 z}\psi_1(x) + r_1 e^{-i\gamma_1 z}\psi_1(x) + \sum_{n\geq 2} r_n e^{\gamma_n z}\psi_n(x) \qquad z < 0$$

$$u(x,z) = t_1 e^{i\gamma_1 z}\psi_1(x) + \sum_{n\geq 2} t_n e^{-\gamma_n z}\psi_n(x) \qquad z > L + w$$

$$-\Delta\psi_n = \lambda_n\psi_n \quad \text{in } \Omega \qquad \psi_n = 0 \quad \text{on } \partial\Omega$$

$$\gamma_1 = \sqrt{k^2 - \lambda_1}$$

$$\gamma_n = \sqrt{\lambda_n - k^2}$$

$$\boxed{\lambda_1 < k^2 < \lambda_2}$$

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Scattering problem

Infinite cylinder Q_0 of a bounded cross-section Ω with a “hole” Γ

Theorem (main result)

Let Γ be an open subset of Ω, and $\delta = \mathrm{diam}\{\Gamma\}$

1) $\forall\, k \in \left(\sqrt{\lambda_1}, \sqrt{\lambda_2}\right)$ fixed, $\lim\limits_{\delta \to 0} r_1 = -1$

i.e., the wave is fully reflecting in the limit of closing barriers

2) $\forall \epsilon > 0 \;\; \exists \delta' > 0 \;\; \forall \Gamma \text{ with } \delta < \delta' \;\; \exists k_D \text{ s.t. } |r_1| < \epsilon$

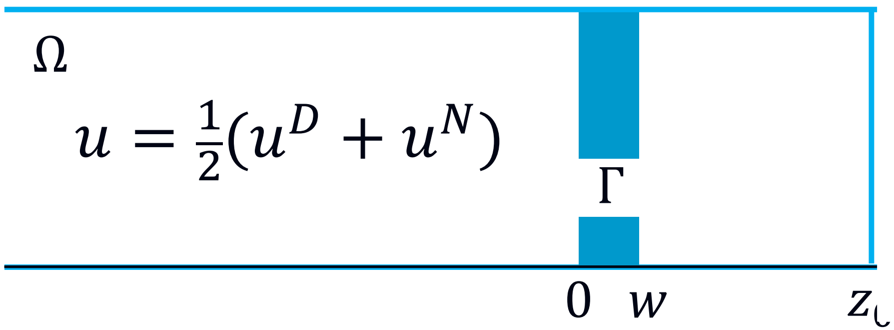
i.e., the wave is almost fully propagating across two almost closed barriers at the resonance wavenumber k_{D}

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Main steps of derivation

1

Infinite cylinder Q_0 of a bounded cross-section Ω with a “hole” Γ



$$\Delta u^D + k^2 u^D = 0 \text{ in } Q$$

$$u^D = 0 \text{ on } \partial Q_0$$

$$u^D(x,z) = -u^D(x, 2z_0 - z)$$

$$u^D(x,z) = e^{i\gamma_1 z}\psi_1(x) + r_1^D e^{-i\gamma_1 z}\psi_1(x) + \sum_{n\ge 2} r_n^D e^{\gamma_n z}\psi_n(x)$$

$$u^D = 0 \text{ at } z = z_0$$

$$\Delta u^N + k^2 u^N = 0 \text{ in } Q$$

$$u^N = 0 \text{ on } \partial Q_0$$

$$u^N(x,z) = +u^N(x, 2z_0 - z)$$

$$u^N(x,z) = e^{i\gamma_1 z}\psi_1(x) + r_1^N e^{-i\gamma_1 z}\psi_1(x) + \sum_{n\ge 2} r_n^N e^{\gamma_n z}\psi_n(x)$$

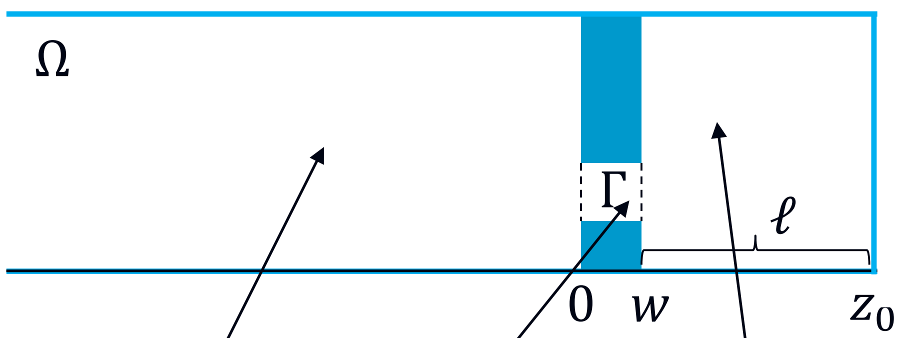
$$\partial u^N / \partial z = 0 \text{ at } z = z_0$$

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Main steps of derivation

2

Infinite cylinder Q_0 of a bounded cross-section Ω with a "hole" Γ



$$u_0 = u^D(x,0)\Big|_\Gamma$$

$$u_1 = u^D(x,w)\Big|_\Gamma$$

$$1 + r_1^D = (u_0, \psi_1)_{L_2(\Gamma)}$$

$$r_n^D = (u_0, \psi_n)_{L_2(\Gamma)}$$

$$u^D(x,z) = e^{i\gamma_1 z}\psi_1(x) + \left((u_0,\psi_1)_{L_2(\Gamma)} - 1\right) e^{-i\gamma_1 z}\psi_1(x) + \sum_{n\geq 2} (u_0,\psi_n)_{L_2(\Gamma)} e^{\gamma_n z}\psi_n(x)$$

$$u^D(x,z) = -\frac{(u_1,\psi_1)_{L_2(\Gamma)} \sin\left(\gamma_1(z-z_0)\right)}{\sin(\gamma_1 \ell)}\psi_1(x) - \sum_{n\geq 2} \frac{(u_1,\psi_n)_{L_2(\Gamma)} \sinh\left(\gamma_n(z-z_0)\right)}{\sinh(\gamma_n \ell)}\psi_n(x)$$

$$u^D(x,z) = \sum_n \frac{-(u_0,\phi_n)_{L_2(\Gamma)} \sinh\left(\beta_n(z-w)\right) + (u_1,\phi_n)_{L_2(\Gamma)} \sinh(\beta_n z)}{\sinh(\beta_n w)}\phi_n(x)$$

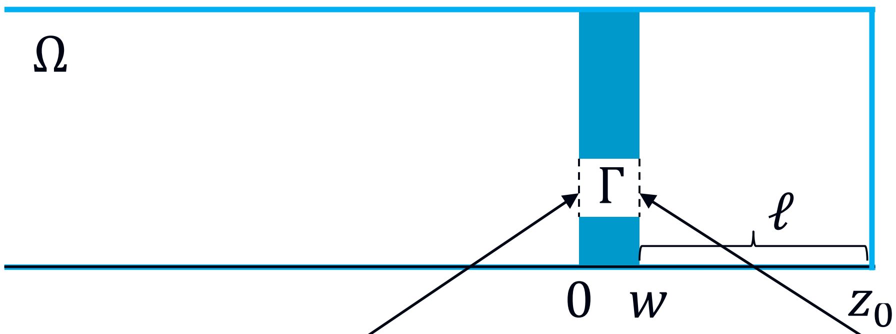
$-\Delta\phi_n = \mu_n \phi_n$ in Γ $\qquad$ $\phi_n = 0$ on $\partial\Gamma$ $\qquad$ $\beta_n = \sqrt{\mu_n - k^2}$

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Main steps of derivation

3

Infinite cylinder Q_0 of a bounded cross-section Ω with a "hole" Γ



$$u_0 = u^D(x,0)\Big|_\Gamma$$

$$u_1 = u^D(x,w)\Big|_\Gamma$$

$$1 + r_1^D = (u_0, \psi_1)_{L_2(\Gamma)}$$

$$r_n^D = (u_0, \psi_n)_{L_2(\Gamma)}$$

$$\frac{\partial u^D}{\partial z}\Big|_{z=0-0} = \frac{\partial u^D}{\partial z}\Big|_{z=0+0} \qquad \frac{\partial u^D}{\partial z}\Big|_{z=w-0} = \frac{\partial u^D}{\partial z}\Big|_{z=w+0}$$

We get two functional equations on u_0 and u_1

$$-i\gamma_1(u_0,\psi_1)\psi_1 + A_0 u_0 + C u_1 = -2i\gamma_1\psi_1$$

$$B u_0 + \gamma_1 \mathrm{ctan}(\gamma_1 \ell)(u_1,\psi_1)\psi_1 + A_1 u_1 = 0$$

→ Two linear equations (u_0, ψ_1) (u_1, ψ_1)

$$A_0 f = \sum_{n\geq 2} \gamma_n (f,\psi_n)\psi_n(x) + \sum_{n\geq 1} \beta_n \mathrm{ctanh}(\beta_n w)(f,\phi_n)\,\phi_n(x)$$

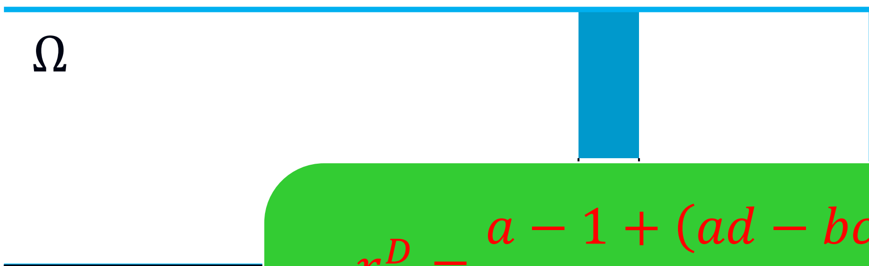
$$A_1 f = \cdots \qquad B f = \cdots \qquad C f = \cdots$$

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Main steps of derivation

3

Infinite cylinder Q_0 of a bounded cross-section Ω with a "hole" Γ



$$u_0 = u^D(x,0)\Big|_\Gamma$$

$$u_1 = u^D(x,w)\Big|_\Gamma$$

$)_{L_2(\Gamma)}$

$)_{L_2(\Gamma)}$

$$\frac{\partial u^D}{\partial z}\Big|_{z=0-0}$$

$$r_1^D = \frac{a-1+(ad-bc-d)\,\mathrm{ctan}(\gamma_1\ell)}{a+1+(ad-bc+d)\,\mathrm{ctan}(\gamma_1\ell)}$$

a,b,c,d being expressed as $\left(E_{a,\ldots}\psi_1,\psi_1\right)_{L_2(\Gamma)}$

with $E_{a,\ldots}$ given explicitly in terms of A_0, A_1, B, C

We get two functional equations on u_0 and u_1

$-i\gamma_1($

$Bu_0 + \gamma_1 \mathrm{ctan}$

$$r_1^N = \frac{\bar a-1+\left(\bar a\bar d-\bar b\bar c-\bar d\right)\tan(\gamma_1\ell)}{\bar a+1+\left(\bar a\bar d-\bar b\bar c+\bar d\right)\tan(\gamma_1\ell)}$$

Two linear equations

(u_0,ψ_1)

(u_1,ψ_1)

$$A_0 f = \sum_{n\ge 2}\gamma_n (f,\psi_n)\psi_n(x) + \sum_{n\ge 1}\beta_n \mathrm{ctanh}(\beta_n w)(f,\phi_n)\,\phi_n(x)$$

$A_1 f = \cdots \qquad Bf = \cdots \qquad Cf = \cdots$

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Main steps of derivation

4

Infinite cylinder Q_0 of a bounded cross-section Ω with a "hole" Γ

$$u_0 = u^D(x,0)\Big|_\Gamma$$

$$u_1 = u^D(x,w)\Big|_\Gamma$$

$$1 + r_1^D = (u_0, \psi_1)_{L_2(\Gamma)}$$

$$r_n^D = (u_0, \psi_n)_{L_2(\Gamma)}$$

$\mathrm{ctan}(\gamma_1 \ell)$ does NOT depend on Γ

$$\gamma_1 = \sqrt{k^2 - \lambda_1}$$

$$r_1^D = \frac{a - 1 + (ad - bc - d)\,\mathrm{ctan}(\gamma_1 \ell)}{a + 1 + (ad - bc + d)\,\mathrm{ctan}(\gamma_1 \ell)}$$

$$r_1^N = \frac{\bar a - 1 + \left(\bar a \bar d - \bar b \bar c - \bar d\right)\tan(\gamma_1 \ell)}{\bar a + 1 + \left(\bar a \bar d - \bar b \bar c + \bar d\right)\tan(\gamma_1 \ell)}$$

As $\delta \to 0$, all a, b, c, d vanish, all $\bar a, \bar b, \bar c, \bar d$ vanish → $r_1^D \to -1$, $r_1^N \to -1$ → $r_1 \to -1$ (full reflection)

For a fixed δ, at the resonance wavenumber k_D satisfying $d\,\mathrm{ctan}(\gamma_1 \ell) = -1$, one has → $r_1^D = 1$

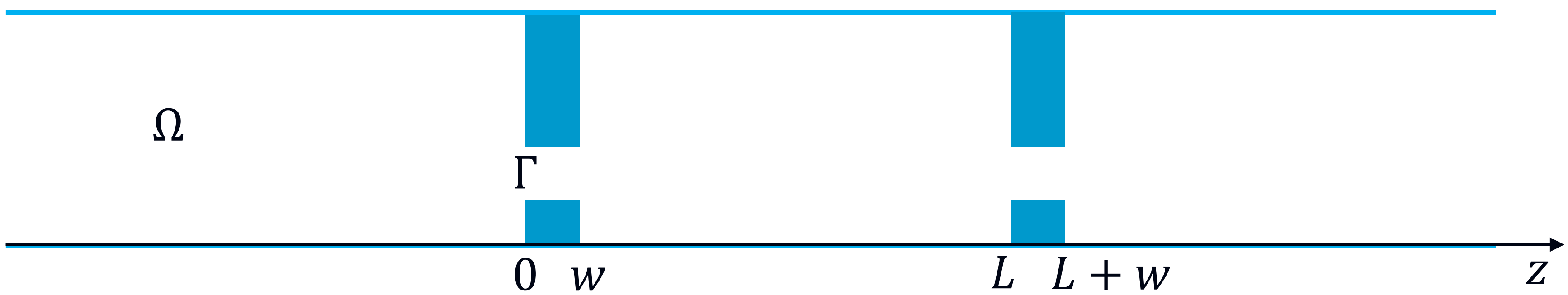
But if δ is small enough, then still → $r_1^N \approx -1$

→ $r_1 \approx 0$ (almost full transmission)

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Another limit: large w

Infinite cylinder Q_0 of a bounded cross-section Ω with a “hole” Γ



There are two main parameters: δ and w

$\delta \to 0$

$w \to \infty$

$\bar{b}, \bar{c} \to 0$
$\bar{a} \to a$ ⇒ $r_1^N \to \dfrac{a-1}{a+1}$

If k is s.t. $r_1^D = -\dfrac{a-1}{a+1}$ ⇒ $r_1 \approx 0$ (almost full transmission)

A. Delitsyn & DG, Appl. Math. Comput. 412, 126592 (2022)

Conclusions

- Mode matching methods are powerful tools for spectral and scattering problems
- Eigenmodes in finite quantum waveguide can be localizated in a junction region
- Waveguide with two identical thick barriers may transmit even for almost closed or very thick barriers

Looking for collaborations!

DG & B.-T. Nguyen, *Geometrical structure of Laplacian eigenfunctions*, SIAM Rev. 55, 601 (2013)