The spectrum of the Neumann-Poincaré operator of a bowtie

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3. Elliptic corner singularity functions in metamaterials
4. The resonant spectrum of the bowtie
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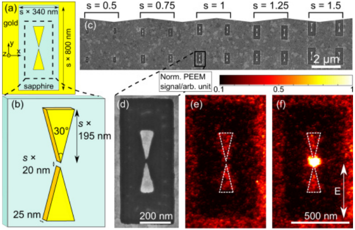
1. Introduction :

Bowtie nano-antennas are extensively studied in the physics literature, as they can produce a remarkably large enhancement of the electrical field near their corners, and particularly in their central neck



(E. Lorek et al, Optics Express Vol. 23, Issue 24, pp. 31460-31471 (2015))

Such plasmon resonances may occur in metallic particles if

- the electric permittivity $\varepsilon(\omega)$ inside the particle depends on the frequency of the excitation, and should have a negative real part and a small imaginary part

  This is the case for metals such as Au, Ag, Al, for frequencies in the visible light range

- the wavelength of the incident excitation $\lambda = 2\pi/\omega$ is much larger than the particle diameter δ

  $$\delta/\lambda \quad = \quad \delta\omega/2\pi \ \prec\prec \ 1$$

  In real life δ is between 10 and 100 nm and $\lambda \sim 650$ nm

The desired resonant frequencies as well as the local fields enhancement may be achieved by tuning the geometry of the nanostructure

[Mayergoyz-Fredkin-Z Zhang Phys. Rev. B 2005, Grieser Rev. Math. Phys. 14, Ammari-Ruiz-Yu-Zhang, Ammari-Millien]

We consider the simplest setting : 2D quasistatic resonances in the TE polarization, which correspond to finding non-trivial solutions to

$$\left\{ \begin{array}{lcll} \operatorname{div}(\dfrac{1}{\varepsilon(\omega,x)}\nabla u(x)) & = & 0 & \text{in } \Omega \\ + \text{ homogeneous BC's on } \partial\Omega & & & \end{array} \right. \tag{1}$$

- Ω is a smooth bounded domain in $\mathbf{R}^2$, that contains a metallic inclusion D homogeneous Dirichlet BC's are applied on $\partial\Omega$

  One can also consider $\Omega = \mathbf{R}^2$ with the radiation condition $u \to 0$ as $|x| \to \infty$

- The frequency ω is fixed and the conductivity $a(x) = \dfrac{1}{\varepsilon(\omega,x)}$ is defined by

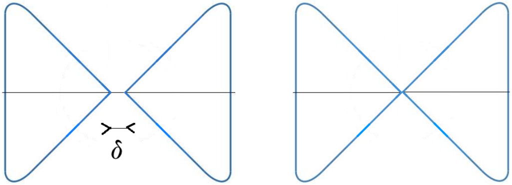
$$a(x) \quad = \quad \left\{ \begin{array}{ll} k, & \text{if } x \in D \\ 1 & \text{otherwise} \end{array} \right.$$

Resonances = values of k for which there exist non trivial solutions to (1)

Objectives

- Understand how the fields concentrate and get enhanced according to the shape of the particles

- In the case of the bowtie, understand the qualitative difference between the perfect and the approximate bowtie



2. Integral representation

2.1. The Neumann-Poincaré operator

We consider the Green function of Ω

$$\begin{cases} -\Delta G(x,y) = \delta_y(x), & \text{in } \Omega \\ G(x,y) = 0 & \text{on } \partial\Omega \end{cases}$$

and seek a solution to $\mathrm{div}(a\nabla u) = 0$ in the form

$$u(x) = S_D\varphi(x) = \int_{\partial D} G(x,y)\varphi(y)\,ds(y) \quad x \in D \cup (\Omega \setminus \overline{D})$$

Its normal derivatives satisfy the Plemelj jump conditions : for $x \in \partial D$

$$\frac{\partial S_D \varphi}{\partial \nu}\Big|^{\pm}(x) = \lim_{t\to 0^+} \nabla S_D\varphi(x \pm t\nu(x)) \cdot \nu(x) = (\pm\frac{1}{2}I + \mathcal{K}_D^*)\varphi(x)$$

$$\mathrm{NPO}: \quad \mathcal{K}_D^*\varphi(x) = \int_{\partial D} \frac{\partial G}{\partial \nu_x}(x,y)\varphi(y)\,ds(y)$$

so that $u = S_D\varphi$ is a resonance iff $\quad (\lambda I - K_D^*)\varphi \;=\; 0 \qquad \lambda \;=\; \dfrac{k+1}{2(k-1)}$

Prop: [Khavinson-Putinar-Shapiro, 2007]

- $\mathcal{K}_D^*$ extends as an operator $H_0^{-1/2}(\partial D) \to H_0^{1/2}(\partial D)$
- As a consequence of the Calderón identity

$$\mathcal{K}_D S \quad = \quad S\mathcal{K}_D^*$$

  $\mathcal{K}_D^*$ is self adjoint for the scalar product

$$< \varphi, \psi >_S \quad = \quad - < \varphi, S_D\psi >_{H^{-1/2}, H^{1/2}}$$

- the spectrum of $\mathcal{K}_D^*$ is real and contained in $(-1/2, 1/2]$
- If D is smooth, $\mathcal{K}_D^*$ is compact, so its spectrum consists in a set of eigenvalues that accumulate to 0

2.2. The Poincaré variational operator

We define $T_D \ : H^1_0(\Omega) \to H^1_0(\Omega)$ by

$$\forall\, v \in H^1_0(\Omega), \quad \int_\Omega \nabla T_D u \cdot \nabla v \quad = \quad \int_D \nabla u \cdot \nabla v$$

Prop:

- The operator T_D is non-negative, self adjoint, $||T_D|| \leq 1$,
- $Ker(T_D) = \{u \in H^1_0(\Omega),\ u_{|D} = const\}$
- $Ker(I - T_D) = \{u \in H^1_0(\Omega),\ u_{|\Omega \setminus \overline{D}} = 0\}$
- $H^1_0(\Omega) = Ker(T_D) \oplus Ker(I - T_D) \oplus \mathcal{H}$

  where $\mathcal{H}$ is the space of single layer potentials

$$\mathcal{H} \quad = \quad \{u \in H^1_0(\Omega),\ \Delta u = 0 \text{ in } D \cup (\Omega \setminus \overline{D}), \int_{\partial D} \partial_\nu u = 0\}$$

As a consequence, the eigenvalues of the restriction of T_D to $\mathcal{H}$ are given by the min-max principle

$$\beta_n^- = \max_{\substack{F_n \subset \mathcal{H} \\ \dim(F_n) = n}} \min_{u \in F_n \setminus \{0\}} \frac{\int_D |\nabla u|^2}{\int_{\mathbf{R}^2} |\nabla u|^2}$$

$$\beta_n^+ = \min_{\substack{F_n \subset \mathcal{H} \\ \dim(F_n) = n}} \max_{u \in F_n \setminus \{0\}} \frac{\int_D |\nabla u|^2}{\int_{\mathbf{R}^2} |\nabla u|^2}$$

so that, the eigenvalues of T satisfy

$$0 \le \beta_1^+ \le \beta_2^+ \le \cdots \le 1/2 \le \cdots \le \beta_2^- \le \beta_1^{-1} \le 1$$

2.3. Relationship between resonances, the NPO, and the Poincaré variational operator

If β is an eigenvalue of T_D with eigenvector u

$$\int_\Omega \beta \nabla u \cdot \nabla v \quad = \quad \int_\Omega \nabla T_D u \cdot \nabla v \; = \; \int_D \nabla u \cdot \nabla v$$

$$\text{i.e.} \int_{\Omega \setminus D} \beta \nabla u \cdot \nabla v \; + \; \int_D (\beta - 1) \nabla u \cdot \nabla v \quad = \quad 0$$

Thus, u is a non-trivial solution to

$$\begin{cases} \operatorname{div}(a(x) \nabla u(x)) = 0 & \text{in } \Omega \\ \qquad u(x) = 0 & \text{on } \partial\Omega \end{cases} \qquad \text{with } a(x) = \begin{cases} 1 & x \in \Omega \setminus \overline{D} \\ k = 1 - 1/\beta & x \in D \end{cases}$$

so that the associated layer potential $\varphi = \partial_\nu u|^+ - \partial_\nu u|^-$ satisfies

$$(\lambda I - \mathcal{K}_D^*)\varphi \quad = \quad 0 \qquad \text{with } \lambda = \frac{k+1}{2(k-1)} = 1/2 - \beta$$

In other words, $\quad \sigma(T_D) = 1/2 - \sigma(\mathcal{K}_D^*)$

When D is merely Lipschitz, $\mathcal{K}_D^*$ is no longer compact in general

Thm : [Perfekt-Putinar 2016]

If D is a planar domain with corners, $\sigma(\mathcal{K}_D^*)$ contains essential spectrum and

$$\begin{aligned} \sigma_{ess}(\mathcal{K}_D^*) &= [\lambda_-, \lambda_+] \subset\subset [-1/2, 1/2] \\ \lambda_\pm &= \pm\frac{1}{2}(1 - \frac{\alpha}{\pi}) \end{aligned}$$

where α is the most acute angle in D

In other words

$$\sigma_{ess}(T_D) = [\beta_-, \beta_+] \subset\subset [0, 1]$$

Singular Weyl sequences

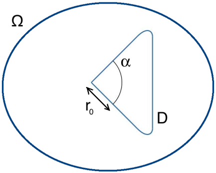
Characterization of the essential spectrum

$\beta \in \sigma_{ess}(T)$ if and only if there exists a sequence $(u_\varepsilon)_{\varepsilon\to 0} \subset H_0^1(\Omega)$ such that

$$\begin{cases} (\beta I - T)u_\varepsilon & \to & 0 & \text{strongly in } H_0^1(\Omega) \\ ||u_\varepsilon||_{H_0^1(\Omega)} & = & 1 & \\ u_\varepsilon & \rightharpoonup & 0 & \text{weakly in } H_0^1(\Omega) \end{cases}$$

3. Corner singularity functions

Assume that D is as in the figure



Consider the transmission problem

$$\begin{cases} -\mathrm{div}(a(x)\nabla u(x)) = 0 & \text{in } \Omega \\ u(x) = f & \text{on } \partial\Omega \end{cases} \quad \text{with } a(x) = \begin{cases} 1 & x \in \Omega \setminus \overline{D} \\ k > 0 & x \in D \end{cases}$$

Prop: [Kondratiev, Grisvard, Dauge-Costabel,...]

$u(x) = u_{reg} + u_{sing}$ with

$$\begin{cases} u_{reg} \in H^2(\Omega) \\ u_{sing}(x) = C r^\eta \varphi(\theta), \quad 0 < r < r_0, \quad 0 \le \theta < 2\pi \end{cases}$$

where θ is a smooth function in each sector

$\eta \in (0,1]$ is determined by α and k (the geometry and the contrast)

How does one find η ?

Seek u_{sing} as a solution to $\mathrm{div}(a\nabla u) = 0$ in the whole plane, with

$$a(x) = a(\theta) = \begin{cases} k < 0 & |\theta| < \alpha/2 \\ 1 & \text{otherwise} \end{cases}$$

which has the form $u_{sing} = r^\eta \varphi(\theta)$ with $0 < \eta < 1$

$$\varphi(\theta) = \begin{cases} a_1 \cos(\eta\theta) + b_1 \sin(\eta\theta) & |\theta| < \alpha/2 \\ a_2 \cos(\eta\theta) + b_2 \sin(\eta\theta) & \text{otherwise} \end{cases}$$

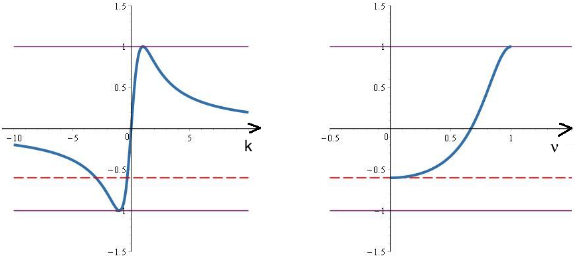
Expressing the transmission conditions $[u] = [a\partial_\theta u] = 0$ on the interfaces $\theta = \pm\alpha/2$ yields a homogeneous linear system for the a_i, b_i's

Condition for the existence of non-trivial solutions

$$\frac{2k}{k^2+1} = \frac{\sin(\alpha\eta)\sin((2\pi-\alpha)\eta)}{1-\cos(\alpha\eta)\cos((2\pi-\alpha)\eta)}$$

$$\frac{2k}{k^2+1} = \frac{\sin(\alpha\eta)\sin((2\pi-\alpha)\eta)}{1-\cos(\alpha\eta)\cos((2\pi-\alpha)\eta)}$$

Picture when $\alpha = \Pi/3$:



$$\frac{(k_\pm+1)}{2(k_\pm-1)} = \pm(1-\alpha/\pi)/2 = \lambda_\pm$$

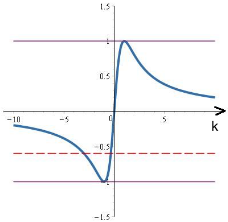
When $k_+ < k < k_- < 0$, one may seek more singular functions in the form

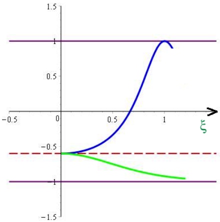
$$u_{sing} \quad = \quad r^{i\xi}\varphi(\theta) \quad \text{with } \xi \in \mathbf{R}$$

for which $\varphi(\theta) \ = \ a_i \cosh(\xi\theta) + b_i \sinh(\xi\theta)$ in each sector

Condition for the existence of non-trivial solutions:

$$\frac{2k}{k^2+1} \quad = \quad \frac{\sinh(\alpha\xi)\sinh((2\pi-\alpha)\xi)}{1-\cosh(\alpha\xi)\cosh((2\pi-\alpha)\xi)}$$

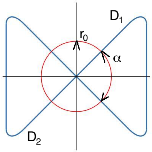




see also [Daugé-Teixier, Bonnet-Chesnel,Bonnet-Chesnel-Clayes]

4. The resonant spectrum of the bowtie

Let D be a bowtie antenna, contained in a set $\Omega \subset \mathbf{R}^2$



Strictly speaking, the bowtie is not a Lipschitz domain : the definition of the Neumann-Poincaré operator may require caution

However, defining a Poincaré variational operator is straightforward

$$\begin{aligned} T_D \;:\; H^1_0(\Omega) \quad &\longrightarrow \quad H^1_0(\Omega) \\ \forall\, v \in H^1_0(\Omega), \quad \int_\Omega \nabla T_D u \cdot \nabla v \quad &= \quad \int_D \nabla u \cdot \nabla v \end{aligned}$$

The resonant frequencies are related to $\sigma(T_D)$ as (generalized) eigenfunctions of T_D satisfy (in $\mathcal{D}'$)

$$T_D(u) \;=\; \beta u \qquad \Leftrightarrow \qquad \mathrm{div}(a \nabla u) \;=\; 0$$

where

$$a \;=\; \begin{cases} 1 & \text{in } \Omega \setminus D \\ 1 - 1/\beta & \text{in } D \end{cases}$$

Thm : The essential spectrum of the bowtie antenna saturates the interval of possible values

$$\sigma_{ess}(T_D) \quad = \quad [0,1]$$

1. The corner singularity functions associated to the central neck of D are easily determined :

Assume that $\beta \in (0,1), \beta \neq 1/2$. Set $k = 1 - 1/\beta$ and

$$a(x) \ = \ a(\theta) \quad = \quad \begin{cases} k & \text{if } |\theta| < \alpha/2 \quad \text{and} \quad |\pi - \theta| < \alpha/2 \\ 1 & \text{otherwise} \end{cases}$$

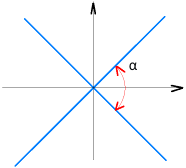
Then there exists a solution u to $\mathrm{div}(a\nabla u) = 0$ in $\mathbf{R}^2$, of the form

$$u(r,\theta) \quad = \quad Re(r^{i\xi})\varphi(\theta), \quad r > 0, \quad 0 \leq \theta < 2\pi$$

for some $\xi > 0$, where

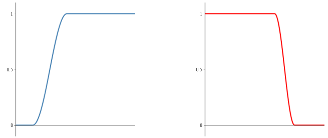
$$\varphi(\theta) \quad = \quad a_i \cosh(\xi\theta) + b_i \sinh(\xi\theta)$$

in each angular sector

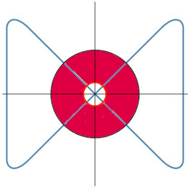


2. The function $u = r^{i\xi}\varphi(\theta)$ is not in H^1_{loc}, as $\nabla u = O(r^{-1})$ near the corner

Let $\varepsilon > 0$ and $\chi_1(r)$, $\chi_2(r)$ be 2 smooth cut-off functions of the form



and define $\qquad u_\varepsilon(x) \;=\; s_\varepsilon\,\chi_1(\frac{r}{\varepsilon})\chi_2(r)u(x) \in H^1_0(\Omega)$



3. We choose s_ε so that $||u_\varepsilon||_{H^1} = ||s_\varepsilon \chi_1(r/\varepsilon)\chi_2 u||_{H^1} = 1$

$$s_\varepsilon^2 \left(\int_{\varepsilon<r<2\varepsilon} |u\nabla\chi_1^\varepsilon + \chi_1^\varepsilon \nabla u|^2 + \int_{2\varepsilon<r<r_0/2} |\nabla u|^2 + \int_{\frac{r_0}{2}<r<r_0} |u\nabla\chi_2 + \chi_2\nabla u|^2 \right) \quad = \quad 1$$

The first and second terms are $O(1)$ while the second tends to ∞

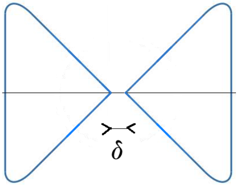
It follows that $\quad s_\varepsilon \to 0 \quad$ and thus that $\quad u_\varepsilon \rightharpoonup 0 \quad$ weakly in H^1

4. We finally show that $\quad (\beta I - T_D)u_\varepsilon \to 0$ in $H_0^1(\Omega)$

Conclusion : u_ε is a singular Weyl sequence for any $\beta \in (0,1)$, and consequently

$$[0,1] \quad \subset \quad \sigma_{ess}(T_D)$$

4. The spectrum of the bowtie with close-to-touching wings



In the case of a bowtie D_δ whose wings are separated by a distance $\delta > 0$, the situation is qualitatively different :

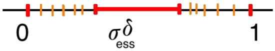
- In that case $\sigma_{ess}(T_{D_\delta}) = [\alpha/\pi, 1-\alpha/\pi] \subsetneq (0,1)$ independently of δ
- When $k > 0$, the regularity of the associated field u_δ also changes qualitatively

$$\begin{cases} u_\delta = r^\eta \varphi(\theta), & \eta \geq 2/3 \quad \forall \alpha, k \\ u_0 = r^\eta \varphi(\theta), & \eta > 0 \quad \text{arbitrary small}(\alpha, k) \end{cases}$$

[E.B., M. Vogelius]

Thm : As $\delta \to 0$, $\sigma(T_{D_\delta})$ must contain eigenvalues outside of its essential spectrum

$$\sigma(T_{D_\delta}) \quad = \quad \sigma_{ess}(T_{D_\delta}) \cup \{\beta_i^{\pm}, 1 \leq i \leq N\}$$



The proof is based on

Lemma [Allaire-Conca]

Let $S_\delta \ : H \longrightarrow H$ be a sequence of self-adjoint operators in a Hilbert space H

Assume that the S_δ's converge pointwise to a limit operator S

$$\forall\, u \in H, \quad ||S_\delta u - Su|| \quad \to \quad 0$$

Then $$\sigma(S) \subset \lim_{\delta \to 0} \sigma(S_\delta)$$

For the Poincaré operators, one easily sees that $\quad T_{D_\delta} \to T_D$ pointwise
Applying the Lemma, it follows that

$$[0,1] \;=\; \sigma(T) \quad = \quad \lim_{\delta \to 0} \sigma(T_\delta)$$

and thus that $\sigma(T_\delta)$ must contain eigenvalues when δ is small enough

A more direct approach
(that hopefully gives insight on what the eigenfunctions may look like)

Let $\beta > 1 - \alpha/\pi$ so that $\beta \notin \sigma_{ess}(T_{D_\delta})$ for any $\delta > 0$, and let

$$u(x) \quad = \quad Re(r^{i\xi})\varphi(\theta)$$

be a generalized eigenfunction for T_D (i.e. when $\delta = 0$)

Set also

$$u_\varepsilon(x) \quad = \quad s_\varepsilon \chi_1(\frac{r}{\varepsilon})\chi_2(r)u(x)$$

The constant s_ε is chosen so that $||u_\varepsilon|| = 1$ (and thus, $s_\varepsilon \to 0$)

The sequence u_ε satisfies

$$\lim_{\varepsilon \to 0} ||(\beta I - T_D)u_\varepsilon||_{H^1} \quad = \quad 0$$

so that in particular

$$\beta \quad = \quad \lim_{\varepsilon \to 0} \frac{\int_D |\nabla u_\varepsilon|^2}{\int_\Omega |\nabla u|^2}$$

Consider now

$$v_{\varepsilon,\delta}(x_1,x_2) = \begin{cases} u_\varepsilon(x_1+\delta/2,x_2) & \text{if } x_1 < -\delta/2 \\ u_\varepsilon(0,x_2) & \text{if } |x_1| < \delta/2 \\ u_\varepsilon(x_1-\delta/2,x_2) & \text{if } x_1 > \delta/2 \end{cases}$$

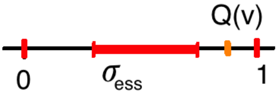
By construction $v_{\varepsilon,\delta} \in H_0^1(\Omega)$ and one can estimate

$$\begin{aligned} \int_\Omega |\nabla v_{\varepsilon,\delta}|^2 &= \int_\Omega |\nabla u_\varepsilon|^2 + s_\varepsilon^2 \int_{|x_1|<\delta/2} |\partial_{x_2}[\chi_1(x_2/\varepsilon)\chi_2(x_2)u(0,x_2)]|^2 \\ &= 1 + s_\varepsilon^2 O(\delta/\varepsilon) \end{aligned}$$

and choosing $\varepsilon = \delta$, and setting $v_\delta = v_{\delta,\delta}$, it follows that

$$\left| \beta - \frac{\int_{D_\delta} |\nabla v_\delta|^2}{\int_\Omega |\nabla v_\delta|^2} \right| \leq \frac{C}{|\ln(\delta)|} \to 0$$

For δ sufficiently small, the function v_δ has a Rayleigh quotient above the essential spectrum of T_{D_δ}



However, to give a relevant bound for an eigenvalue above the essential spectrum, the functions v_δ should be orthogonal to the subspace associated to $\beta = 1$, i.e. to $Ker(T_{D_\delta} - I) \sim H_0^1(D_\delta)$

One can show that

$$\left| \beta - \frac{\int_{D_\delta} |\nabla v_\delta|^2}{\int_\Omega |\nabla v_\delta|^2} \right| \sim \left| \beta - \frac{\int_{D_\delta} |\nabla Z_\delta|^2}{\int_\Omega |\nabla Z_\delta|^2} \right| \to 0$$

$Z_\delta =$ projection of v_δ on $Ker(T_{D_\delta} - I)^\perp$

Remarks :

- One can also show that there are eigenvalues $\beta \in (0, \alpha/\pi)$
- In fact the spectrum contains more and more eigenvalues in the range $[0, \alpha/\pi) \cup (1 - \alpha/\pi, 1]$ as $\delta \to 0$
- [Helsing-Kang-Lim, 2016] contains very nice numerical illustrations of similar phenomena
- The situation is reminiscent of the case of close-to-touching disks [EB-Triki]

5. Conclusion

- We established a link between the spectral properties of the Neumann-Poincaré operator (or the Poincaré variatonal op.) and the corner singularity functions

- Extension to 3D possible

- The behavior of the associated eigenmodes is interesting, in view of their properties of localization, concentration of energy

- Are shapes with singularities
  more interesting for applications ?

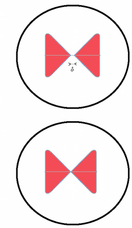
  Can that be quantified ?

Save the date !

Let W_δ denote the orthogonal projection of $v_{\delta,\delta}$ on $H_0^1(D_\delta)$

$$v_\delta = W_\delta + Z_\delta \qquad \text{with} \int_\Omega \nabla W_\delta \cdot \nabla Z_\delta = 0$$

Construct U_δ as



$$U_\delta(x) = \begin{cases} W_\delta(x_1 - \delta/2, x_2) & \text{if } x_1 < 0 \\ W_\delta(x_1 + \delta/2, x_2) & \text{if } x_1 > 0 \end{cases}$$

Then $U_\delta \in H_0^1(D) = Ker(T_D - I)$

We can estimate

$$
\begin{aligned}
(1-\beta)||W_\delta||^2_{H^1} &= (1-\beta)\int_\Omega |\nabla W_\delta|^2 \; = \; (1-\beta)\int_\Omega \nabla W_\delta \cdot \nabla v_\delta \\
&= \int_\Omega \nabla (T_{D_\delta} - \beta I) W_\delta \cdot \nabla v_\delta \; = \; \int_\Omega \nabla (T_{D_\delta} - \beta I) v_\delta \cdot \nabla W_\delta \\
&= \int_\Omega \nabla (T_D - \beta I) u_\delta \cdot \nabla U_\delta \\
&\leq ||(T_D - \beta I) u_\delta||_{H^1} \, ||W_\delta||_{H^1}
\end{aligned}
$$

It follows that $\lim_{\delta \to 0} ||W_\delta||_{H^1} = 0$

It follows from the decomposition

$$v_\delta = W_\delta + Z_\delta, \qquad Z_\delta \perp Ker(T_{D_\delta} - I)$$

that

$$\left| \beta - \frac{\displaystyle\int_{D_\delta} |\nabla v_\delta|^2}{\displaystyle\int_\Omega |\nabla v_\delta|^2} \right| \quad \sim \quad \left| \beta - \frac{\displaystyle\int_{D_\delta} |\nabla Z_\delta|^2}{\displaystyle\int_\Omega |\nabla Z_\delta|^2} \right| \to 0$$

where $Z_\delta \in Ker(T_{D_\delta} - I)^\perp$

and therefore, T_{D_δ} has at least one eigenvalue above its essential spectrum