Localization of eigenfunctions on quantum graphs

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Abstract

I'll discuss ways to construct realistic "landscape functions" for eigenfunctions ψ of quantum graphs. This term refers to functions that are easier to calculate than exact eigenfunctions, but which dominate |ψ| in a non-uniform pointwise fashion constraining how ψ can be localized. Our techniques include Sturm-Liouville analysis, a maximum principle, and Agmon's method.

This is joint work with Anna Maltsev of the University of Bristol, *CMP* 2018, and a preprint on the arxiv, recently submitted.

Why do eigenfunctions localize?

- The tunneling effect.
- Randomness (Anderson localization).

  However, here we consider only deterministic Hamiltonians.

- Different mathematical tools needed in different energy régimes.

Why do eigenfunctions localize?

- And how do these mechanisms work on quantum graphs?
  - (to be defined…)

Landscape functions

1. The game is to find an ***easily computed*** $\Upsilon(x, E)$ such that for any normalized eigenfunction $\psi(x)$:

$$H\,\psi(x) = E\,\psi(x),$$

$$|\psi(x)| \le \Upsilon(x, E).$$

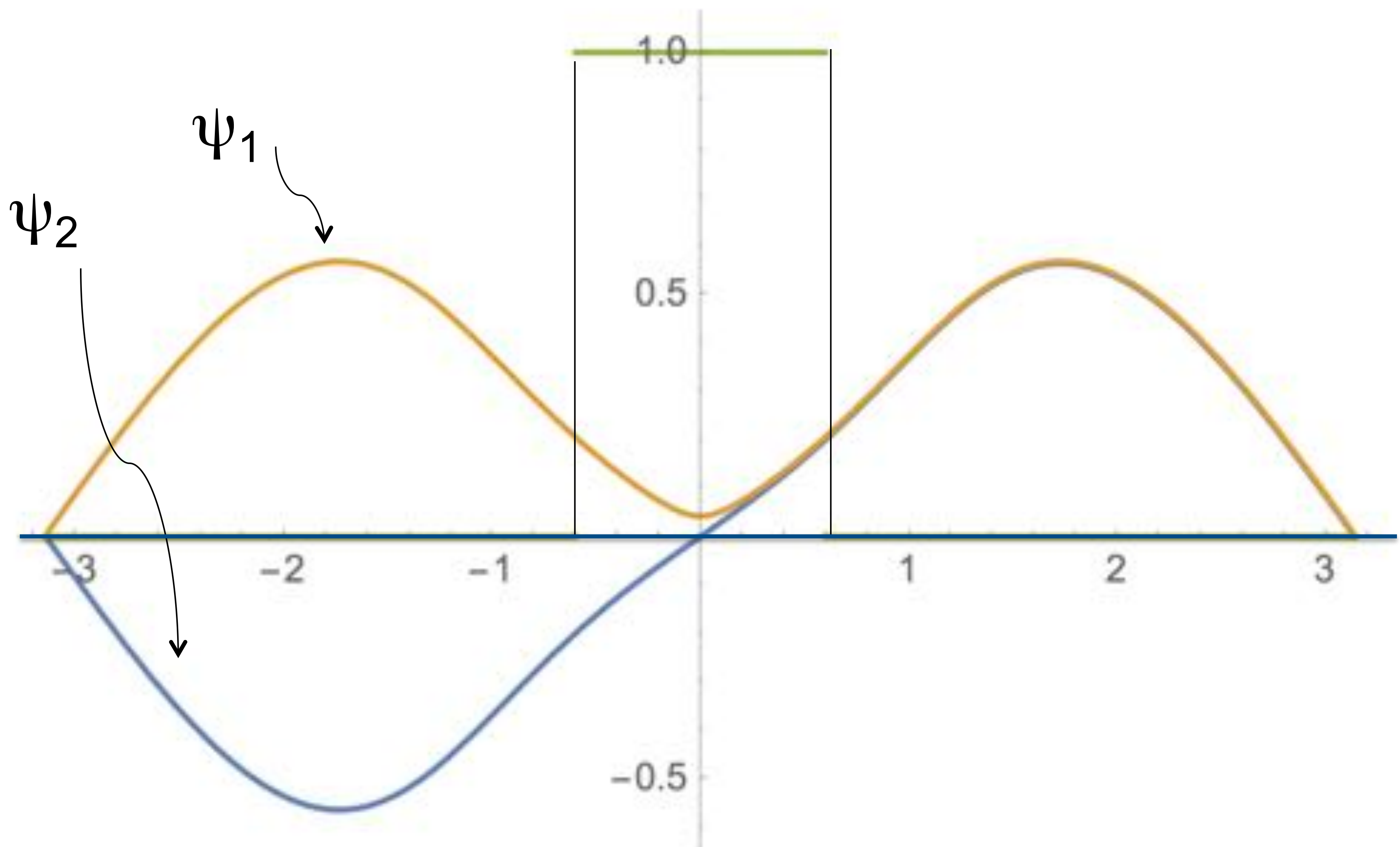
2. cf. Filoche, Mayboroda, Steinerberger

Landscape functions

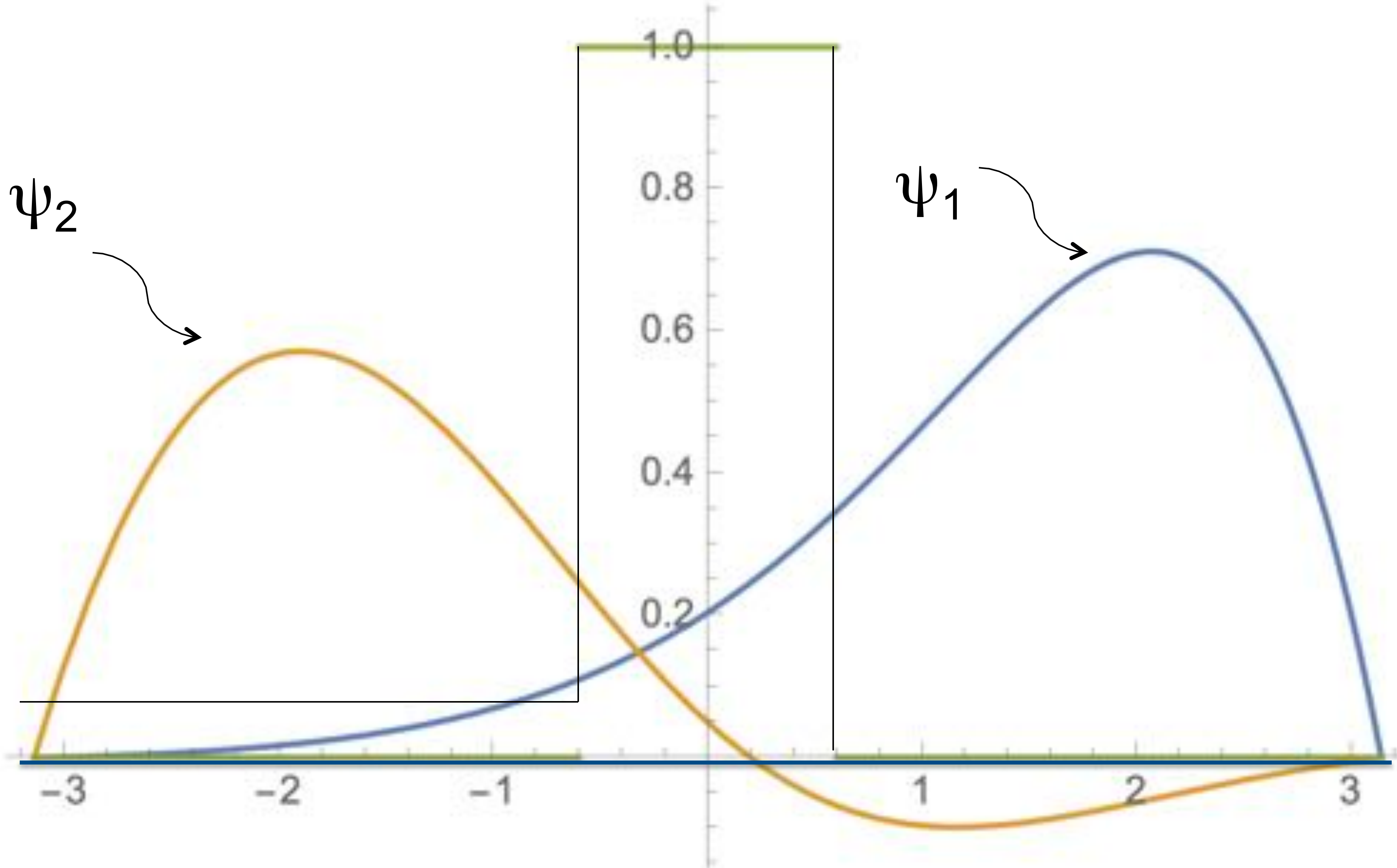
We have to accept that a given eigenfunction may be far smaller than $\Upsilon(x, E)$ in some regions. Consider a non-symmetric double-well problem

$$|\psi(x)| \leq \Upsilon(x, E),$$

and the “flea on the elephant” phenomenon.



(not computationally accurate)



(not computationally accurate)

Landscape functions

The best realistic hope for a landscape function is that it is small and of the right order in the classically forbidden region $V > E$, but it will be much cruder where $V < E$.

Landscape functions

"Case studies" show that even more things can go wrong when we try to landscape quantum graphs. First, we recall what quantum graphs are:

Graphs and quantum graphs

- Combinatorial graphs are abstract networks of vertices (or nodes) and connections (or edges). Graphs originated with Euler's solution of the puzzle of the 7 bridges of Königsberg.
- Graphs are in 1-1 correspondence with a class of matrices, their adjacency matrices.

One way to explain graphs

Graphs and quantum graphs

- *Quantum* graphs are *metric graphs* (so the edges are intervals) coupled with differential operators on the edges.
- My edge operators are going to be 1D linear Schrödinger operators (Sturm-Liouville operators in Liouville normal form), but there are other possibilities

Graphs and quantum graphs

- *Quantum* graphs have been rediscovered many times, of course with uncorrelated terminology and notation.
  - Pauling, 1936, benzene rings; Ruedenberg and Scherr, 1953
  - Quantum wires became popular in 90's
    - Duclos-Exner
  - Smilansky and associates, late 90's, chaotic features.

Quantum graphs

- Vertices are connected by edges, on which $-\psi'' + V(x)\psi = E\psi$.
- The solutions are continuous and connected at the vertices by conditions such as

$$\sum_{e\sim v} f_e'(v^+) = 0.$$

"Kirchhoff conditions"

Quantum graphs

- Kirchhoff conditions correspond to the energy form

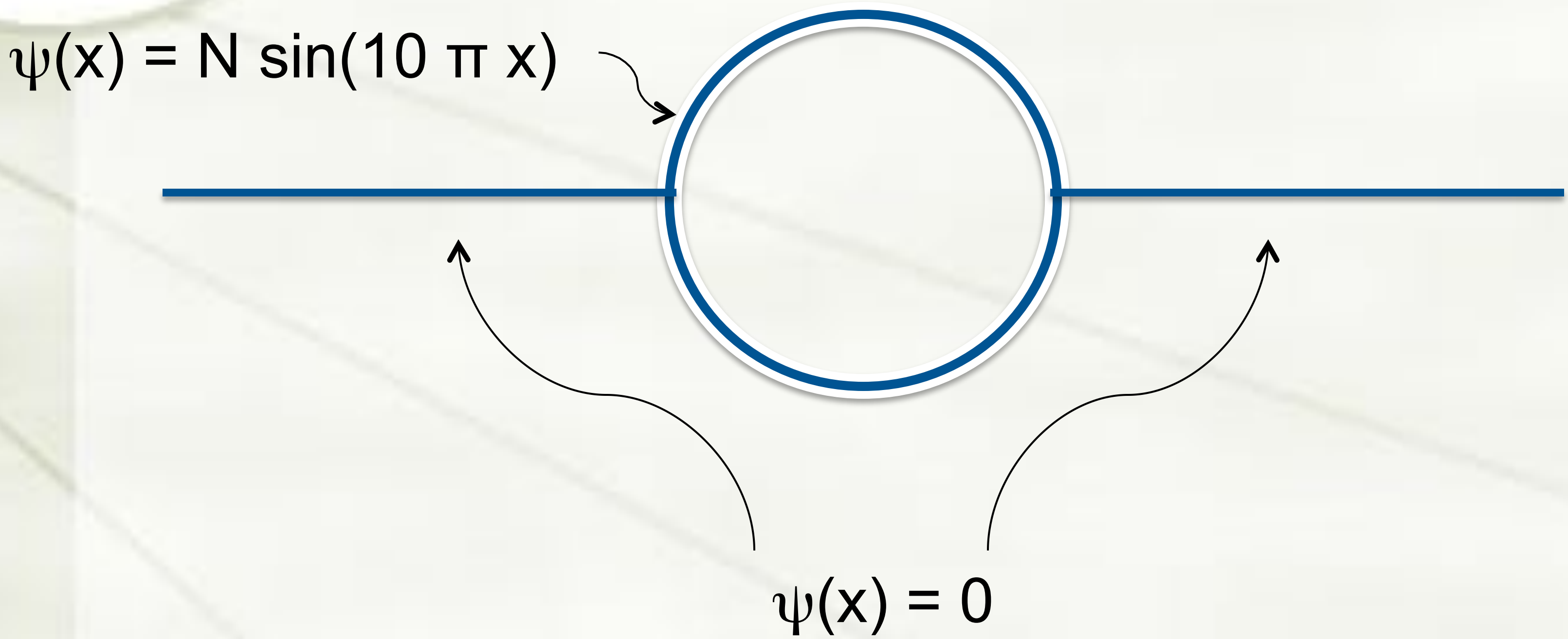
$$\phi \to \sum_e \int_e \left(|\phi'|^2 + V(x)|\phi|^2\right) dx$$

on $H^1(\Gamma)$. (Like Neumann BC)

Quantum graphs

- QGs have some one-dimensional features and some multi-dimensional features.
- But they have one feature that is disturbingly different from ODEs or (elliptic) PDEs⋯

There's no unique continuation principle through vertices!



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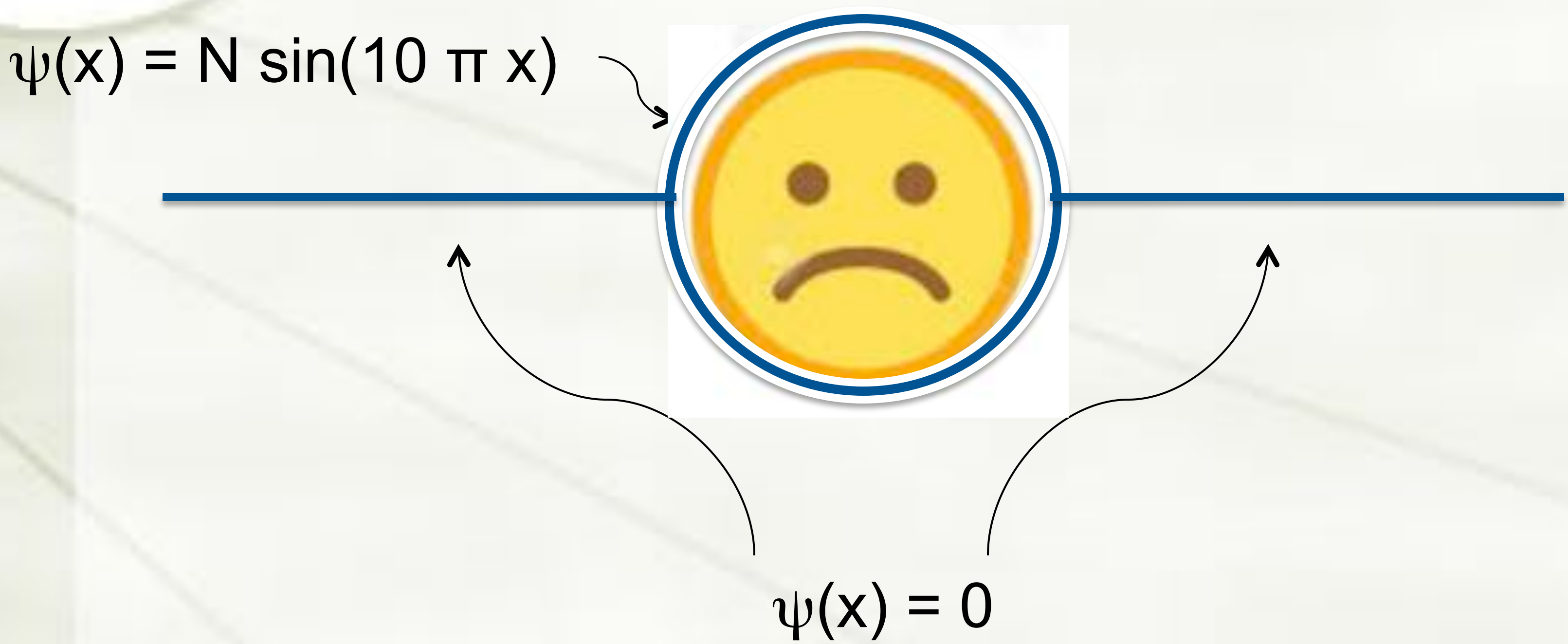
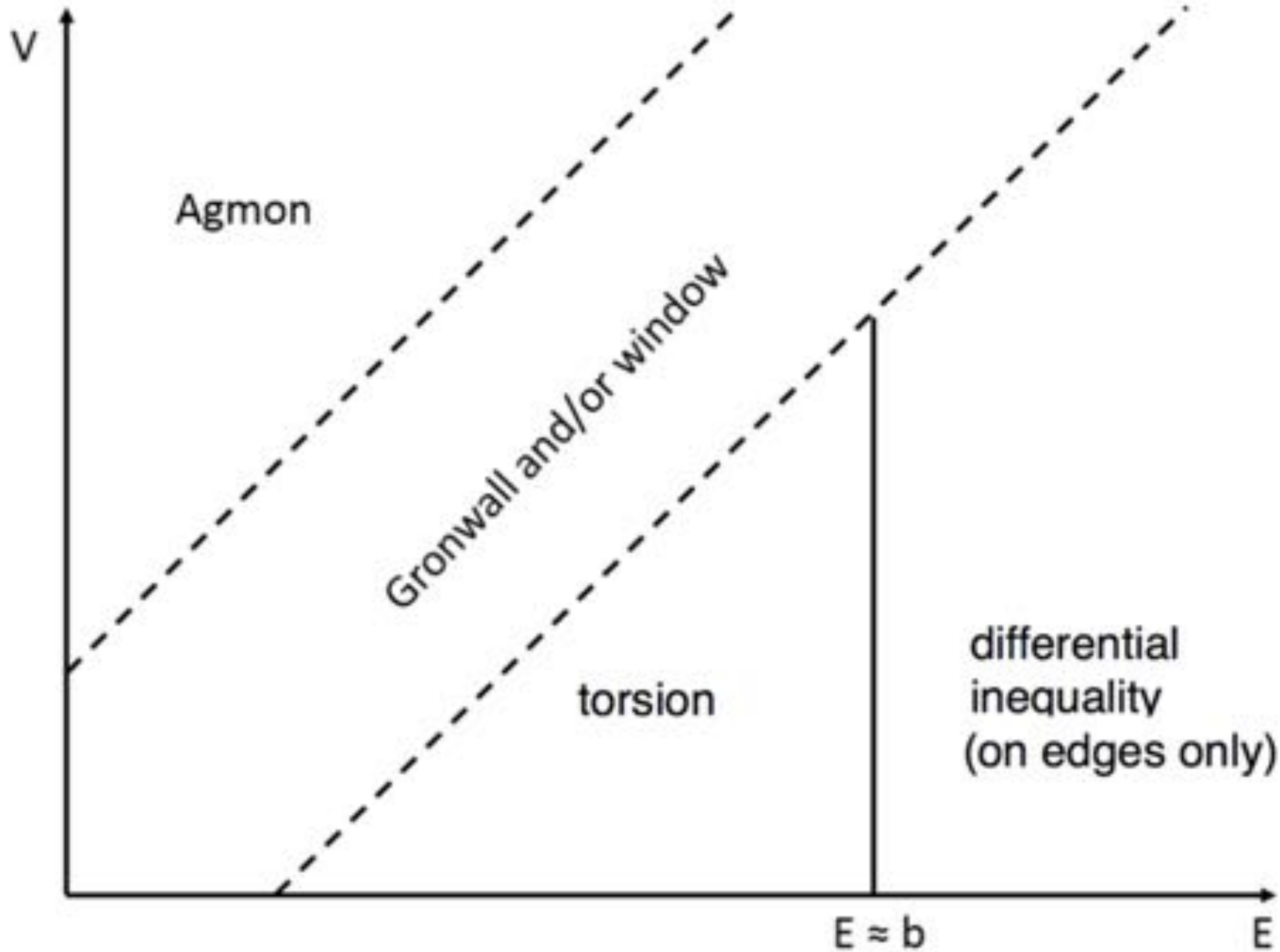


GAME OVER?

Different methods in different régimes

- The tunneling régime – $V(x) > E$
  - Use Agmon's method.
- When $E > V$ but not too much
  - Build on the torsion function.
- Any relationship between E and V but no vertices.
  - Some ODE methods.


V
Agmon
Gronwall and/or window
torsion
differential
inequality
(on edges only)
E ≈ b
E

Step 1. Uniform control

- We provide a standard kind of hypercontractive (heat-kernel) estimate, sharpening a non-explicit formula of Davies. Assuming inf(V)=0, for L^2- normalized eigenfunctions,

$$\sum_{E_j \le E} \|\psi_j\|^2_{L^\infty(\mathbf{e})} \le \sqrt{\frac{2eE}{\pi}} + \frac{\sqrt{e}}{|\mathbf{e}|}$$

Step 1. Uniform control

- The heat kernel is pt-wise bounded above by the heat kernel where the vertex conditions are replaced with Neumann BC – disconnecting the graph into independent intervals.

$$
\begin{aligned}
K_{\mathbf{e}}(t,x,y) &= \frac{1}{|\mathbf{e}|}\left(1+2\sum_{n=1}^{\infty}\exp\left(-\left(\frac{n\pi}{|\mathbf{e}|}\right)^2 t\right)\cos\left(\frac{n\pi}{|\mathbf{e}|}x\right)\cos\left(\frac{n\pi}{|\mathbf{e}|}y\right)\right)\\
&\le \frac{1}{|\mathbf{e}|}\left(1+2\sum_{n=1}^{\infty}\exp\left(-\left(\frac{n\pi}{|\mathbf{e}|}\right)^2 t\right)\right)\\
&= \frac{1}{|\mathbf{e}|}\vartheta_3\left(0,\exp\left(-\left(\frac{\pi}{|\mathbf{e}|}\right)^2 t\right)\right) \qquad (5)
\end{aligned}
$$

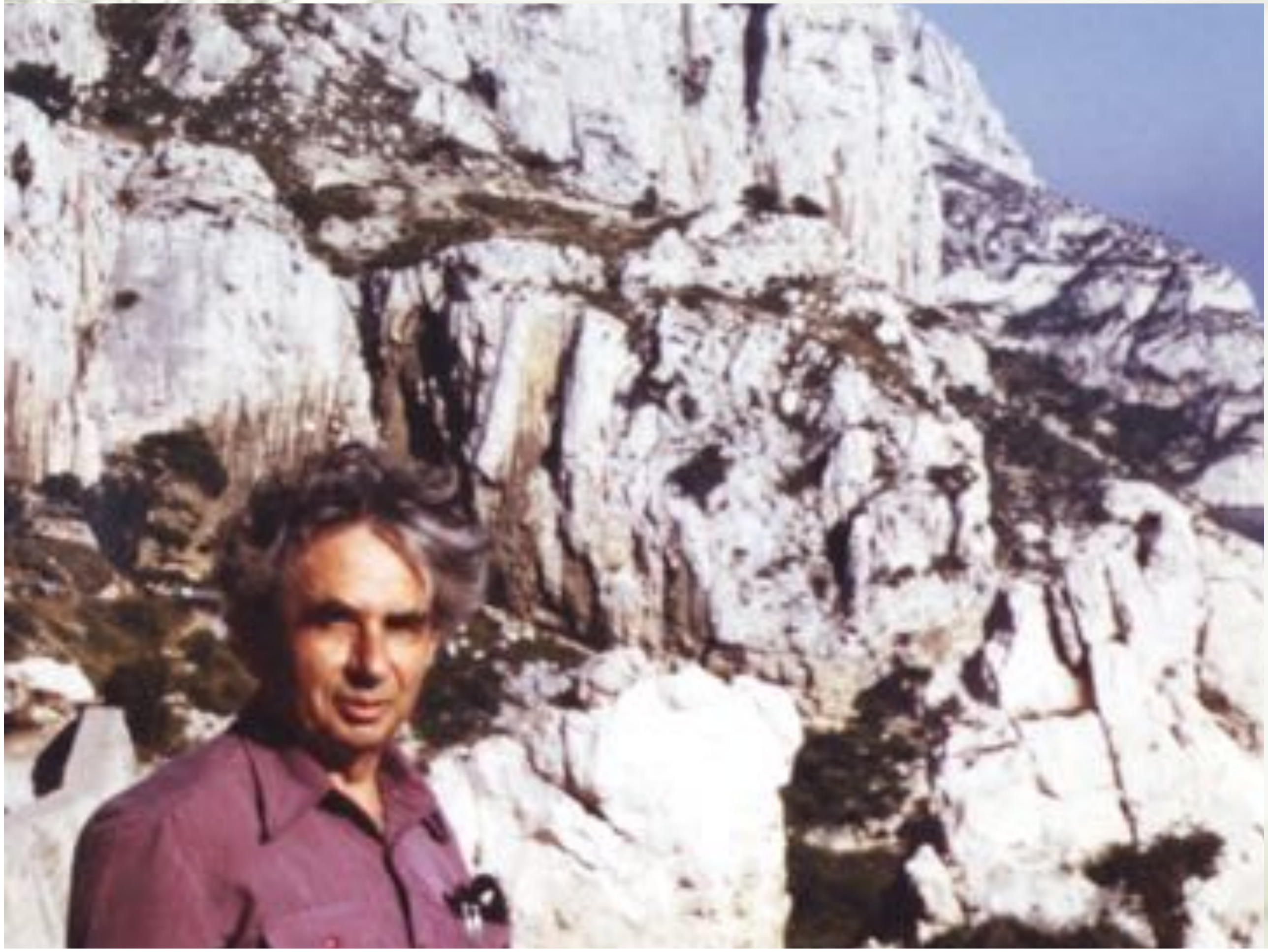
Step 1. Uniform control

- With the Lie-Trotter product formula and a bound on the theta fn., we get:

$$\sum_{E_j \le E} |\psi_j(x)|^2 \le \frac{e^{(E-\inf_\Gamma(V))t}}{|\mathbf{e}|}\left(1 + \frac{|\mathbf{e}|}{\sqrt{\pi t}}\right)$$

- This is true for all t, so we pick a somewhat optimal value, $t = 1/2(E-V_m)$

Step 2. nonuniform control in the tunneling régime following Agmon



Luminy,1993

Agmon estimates

- The decrease of eigenfunctions is a geometric concept.
- In the 80’s, Agmon produced many-dimensional estimates that resemble Liouville-Green in 1D.
- The book of Hislop-Sigal has a good treatment.

Agmon estimates

- In the "tunneling régime" for a given E, $\mathcal{T}_E := V^{-1}([E,\infty))$ define the Agmon (or Liouville-Green) metric by

$$\rho_A(x,y;E) := \min_{P\text{: paths } y \text{ to } x} \int_P \sqrt{V-E}.$$

Agmon for quantum graphs

Theorem 3.1. *For* $x \in \tau_E$ *with* $\operatorname{dist}(x, \partial\tau_E) \geq \ell$,

$$|\psi(x)| \leq \frac{\sqrt{\operatorname{dist}(x, \partial\tau_E)}\,\|\psi\|_{L^2(\cup_{j=1}^m [b_j, b_j+\ell])}}{\ell} \exp(-\rho_A(x, \partial\tau_E; E)).$$

- The Agmon method works regardless of vertices!

What's the effect of connectness?

- Do connections at vertices enhance or diminish localization?

Agmon for infinite *q- graphs*

- If the graph tends to ∞, and $E < \liminf V$, how well localized are the eigenfunctions?

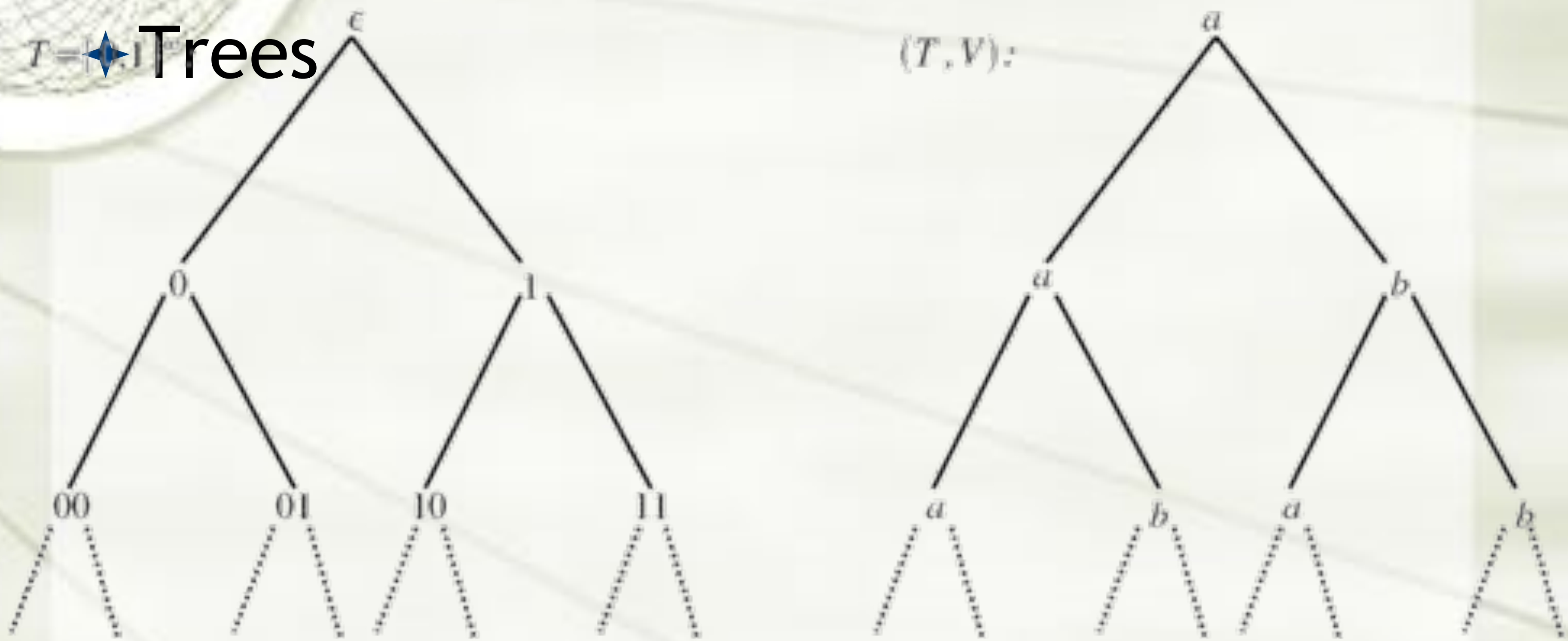
Case studies

- Infinite ladders

- Let V=0, E=-1 (outside a finite region). There is a symmetric solution that looks like e^{-x} on the sides and constant on the rungs, and an antisymmetric one of the form $ge^{-|\ln \lambda_-|x}$ where g is periodic and $|\ln \lambda_-| > 1.$

Case studies

- Trees



Examples

- Trees
  - With branching number b and length L, the transfer matrix for the regular tree has smaller eigenvalue

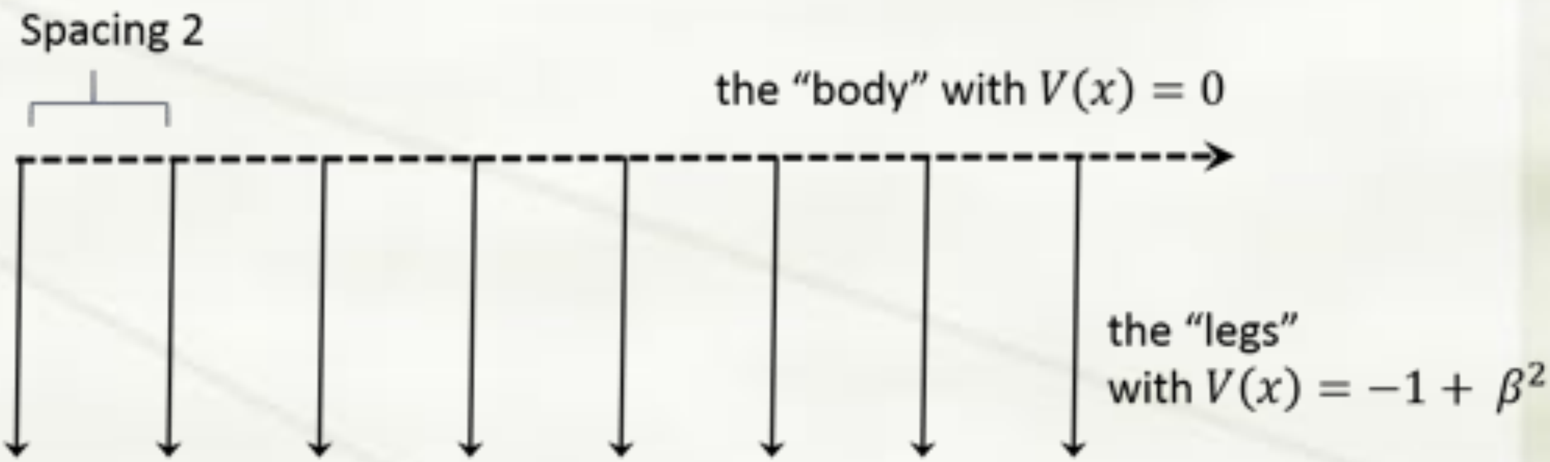
$$= \frac{1}{\left(\frac{b}{2}+\frac{1}{2}\right)\cosh kL + \sqrt{\left(\left(\frac{b}{2}+\frac{1}{2}\right)\cosh kL\right)^2 - b}}$$

$$< \frac{1}{b\cosh kL}$$

(Here, $E = k^2$.)

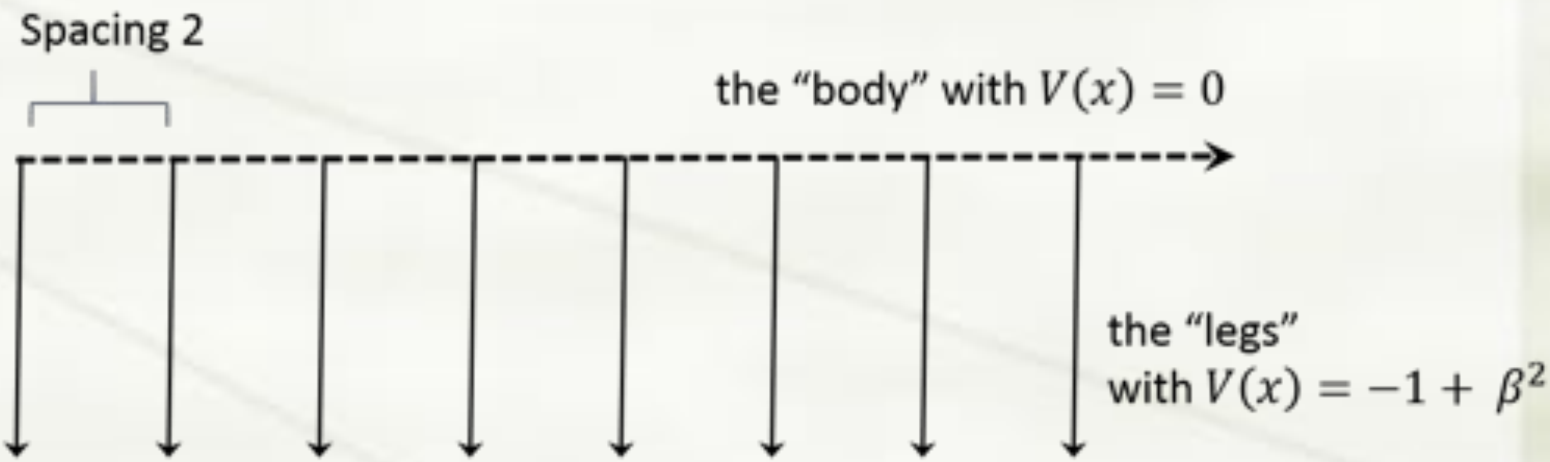
Case studies

- Millipedes



Case studies

- Millipedes

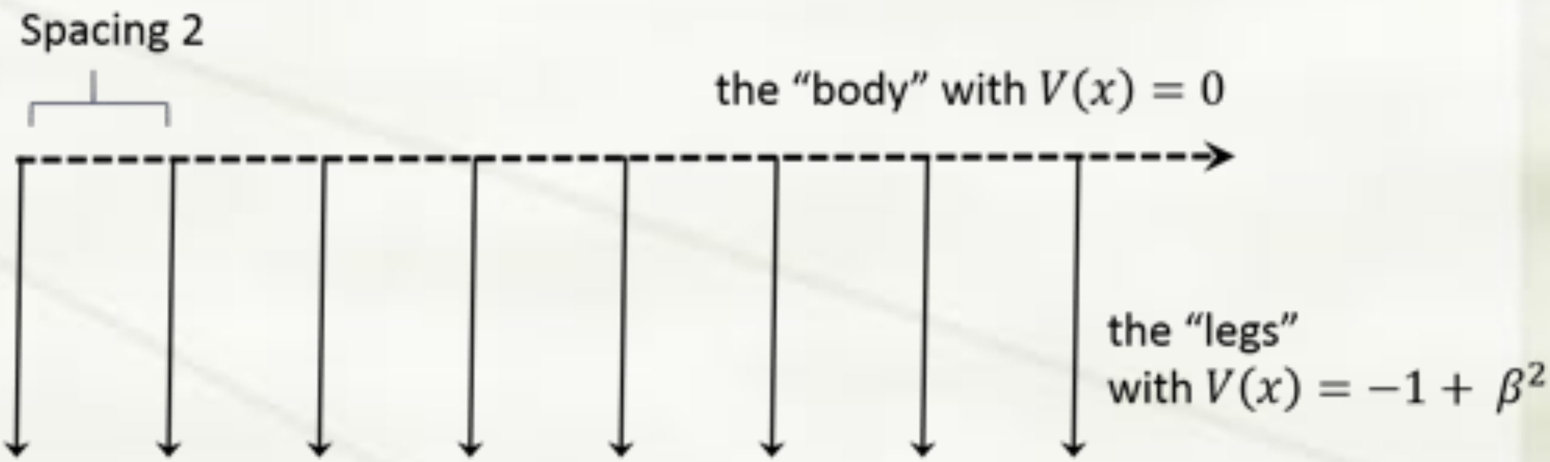


$$\lambda_- = e^{-2}\left(1 - \frac{\beta}{2}\right) + 0(\beta^2)$$

$$= e^{-2-\frac{\beta}{2}+0(\beta^2)}.$$

Case studies

- Millipedes



The spectral problem is equivalent to a problem on a half line, with delta potentials at regular intervals.

Results in the CMP paper for infinite graphs

1. The “classical action” estimate for eigensolutions on the line is valid for graphs. *Vertices are not a barrier for Agmon!* 

Results in the CMP paper for infinite graphs

Theorem 1.1. *Suppose that* $\Gamma_0 \subset \Gamma$ *is a connected, infinite subgraph on which* $\liminf(V(x) - E) > 0$. *If* $\psi \in L^2(\Gamma) \cap \mathcal{K}(\Gamma_0)$ *satisfies*

$$-\psi'' + V(x)\psi = E\psi$$

on the edges of Γ_0, *then for any* $\delta < \liminf(V - E)$,

$$e^{\rho_a(x;E-\delta)}\psi \in H^1(\Gamma_0) \cap L^\infty(\Gamma_0). \tag{9}$$

$$\rho_a(y, x; E) := \min_{\text{paths } P\, y \text{ to } x} \int_P (V(t) - E)_+^{1/2} dt.$$

Results in the CMP paper for infinite graphs

1. The "classical action" estimate for eigensolutions on the line is valid for graphs.
2. Along a path, a refined estimate is possible in terms of the "fractions of the derivative" p_k. (Here we need assumptions that imply that eigenfunctions decay without changing sign.)

Results in the CMP paper for infinite graphs

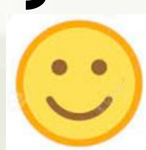
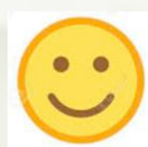
Theorem 1.2. *Suppose that $\Gamma_0 \subset \Gamma$ is a connected, infinite subgraph on which $\liminf(V(x) - E) > 0$ and that $\psi \in L^2(\Gamma) \cap \mathcal{K}(\Gamma_0)$ satisfies*

$$-\psi'' + V(x)\psi = E\psi$$

on the edges of Γ_0 and $\psi' < 0$ outside of a set of compact support. Consider any infinite path $P \subset \Gamma_0$, on which the fraction of the derivative exiting from a vertex v is designated p_v. Then for any $\delta < \liminf(V - E)$, $e^{\rho_P(x,E-\delta)}\psi \in L^2(P)$. That is,

$$\sqrt{\prod_{v \in P} \frac{1}{p_v}} e^{\rho_a(x,E-\delta)}\psi \in L^2(P) \cap L^\infty(P).$$

Results in the CMP paper for infinite graphs

1. The "classical action" estimate for eigensolutions on the line is valid for graphs.
2. Along a path, a refined estimate is possible.
3. On sufficiently regular graphs, an averaged wave function **must decay more rapidly** than the classical-action estimate.  

Results in the CMP paper for infinite graphs

Theorem 1.3. *Suppose that* Ψ *is the averaged eigenfunction on a quantum graph with regular topology corresponding to a solution* ψ *of* (1), *for which* $\psi \in L^2(\Gamma) \cap \mathcal{K}$, *and that for all* x *such that* $\operatorname{dist}(0,x) = y$, $V(x) \geq V_m(y)$, *where* $\liminf(V_m(y) - E) > 0$. *Define*

$$F_{\mathrm{ave}}(y,E) := \left(\prod_{j; v_j < y} \sqrt{\frac{b_j}{a_j}} \right) e^{\int_0^y \sqrt{V_m(t) - E}\, dt}. \tag{12}$$

Then for each $0 < \delta < \liminf(V_m - E)$,

$$F_{\mathrm{ave}}(y, E - \delta)\Psi \in H^1(\mathbb{R}^+) \cap L^\infty(\mathbb{R}^+).$$

Step 2. Agmon's method

- In our interpretation, in part inspired by Hislop-Sigal, we play off three quantities

  (i) An eigenfunction ψ, or more generally a function such that $\psi(x)H\,\psi(x) \leq E\,(\psi(x))^2$.

  (ii) A smooth cut-off function $\eta(x)$.

  (iii) A weight $F(x)$, which is usually exp(?).

Step 2. Agmon estimates

- There is a marvelous local Sobolev-energy bound,

$$|\nabla\eta(x)F(x)\psi(x)|^2 + \left(V(x) - E - \left|\frac{\nabla F(x)}{F(x)}\right|^2\right)(\eta(x)F(x)\psi(x))^2$$

$$\leq$$

$$(\psi(x))^2\nabla\eta(x)\cdot(\text{some stuff}) + \nabla\cdot(\text{some other stuff})\,.$$

- F is chosen (in various ways) so (⋯)≥0 on supp η, while $\nabla\eta$ is supported where its coefficient, which involves F, is small.

Step 3, E > V but not too much.

- $-\Delta\ T(x) = 1$ defines the "torsion function," which has been studied by van den Berg and others. It can be used to cook up landscape functions that are global on graphs (but only good where $E - V$ is not too big).

"Landscape functions" and E > V.

- The landscape functions of Filoche et al. are solutions of H *L*(x) = 1, H = -Δ + V(x), V(x) ≥ 0, for then if

$$W(x) := \pm\psi(x) - E\|\psi\|_\infty L(x),$$

$$HW(x) = E\left(\pm\psi(x) - \|\psi\|_\infty\right) \leq 0,$$

so by the maximum principle, if W(x) ≤ 0 on the boundary of some set, it is ≤ 0 on the interior of the set. (There is a max principle for quantum graphs.)

“Landscape functions” and E > V.

- W(x) ≤ 0 means that

$$|\psi(x)| \leq E\|\psi\|_\infty L(x).$$

Step 3, E > V but not too much.

- The first simplification is to realize that it suffices to have $-\Delta\ L(x) \geq 1$, because then we can offer *explicit* functions L, for instance Gaussians:
- If $V \geq b\,x^2$, $b > 0$, and

$$\Upsilon_0(x,b) := \frac{1}{b}\left(\frac{1}{2} + e^{-bx^2/2}\right)$$

then

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\Upsilon_0(x,b) \geq 1.$$

Step 3, E > V but not too much.

- The first simplification is to realize that it suffices to have $-\Delta\ L(x) \geq 1$, because then we can offer *explicit* functions L, for instance Gaussians:
- Even if torsion bounds have limited utility, *vertices are not a barrier for them!*

Example: Mathieu with periodic conditions

- $-\psi'' + 2q(1 + \cos(2x))\psi = E\psi$ (the classical normalization)
- The tunneling and classically allowed regimes each have 2 conn. components, so the lsf is obtained by concatenating truncated Gaussians and adding a constant. We set q = 10.

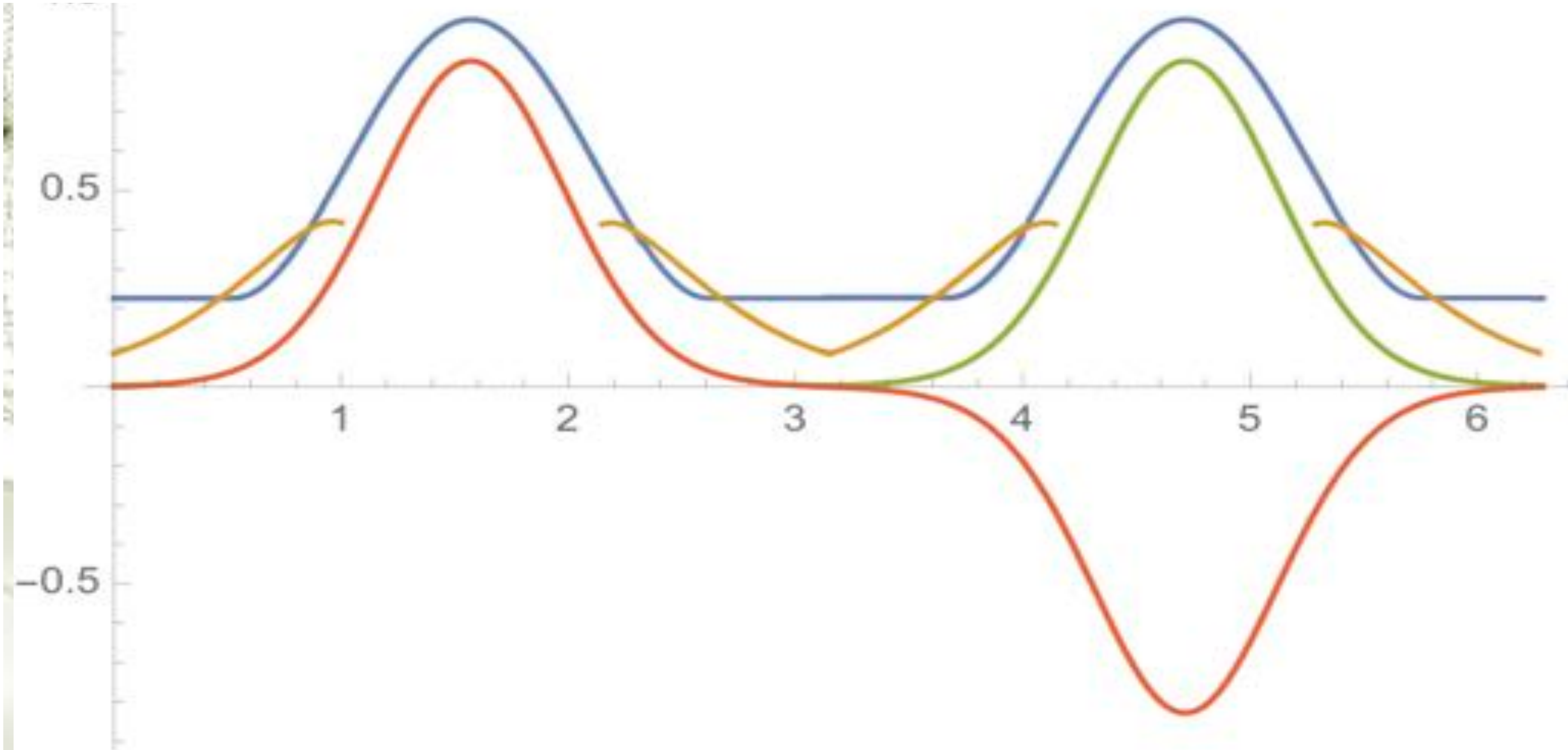


FIGURE 4. The first two Mathieu eigenfunctions for $q = 10$ (green and red), along with landscape bounds using a simplified torsion function (blue) and Agmon's method (gold) (Case Study 7), calculated with *Mathematica*. In the torsion-type bound we have used a numerical calculation of the maximum of the Mathieu functions. The Agmon bound is self-contained, but we have not attempted to optimize details such as the choice of ℓ.

Step 4. Local Sobolev estimates for arbitrary E

- There is a Gronwall-type bound for a local Sobolev norm of eigenfunctions of The Schrödinger equation on an interval: If y > x, and

$$g(x) := (\psi(x))^2 + \frac{(\psi'(x))^2}{E}$$

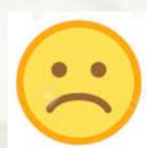
then

$$g(y) \leq g(x) \exp\left(\frac{1}{\sqrt{E}} \int_x^y |V(t)| dt \right)$$

(possibly due to Davies)

Step 4. Local Sobolev estimates for arbitrary E

- The Gronwall-type bound is valid for any E and gives excellent control for large E
- It can be usefully combined with the local Sobolev estimates using the Agmon identities, but ⋯
- *It does not remain valid past a vertex.*



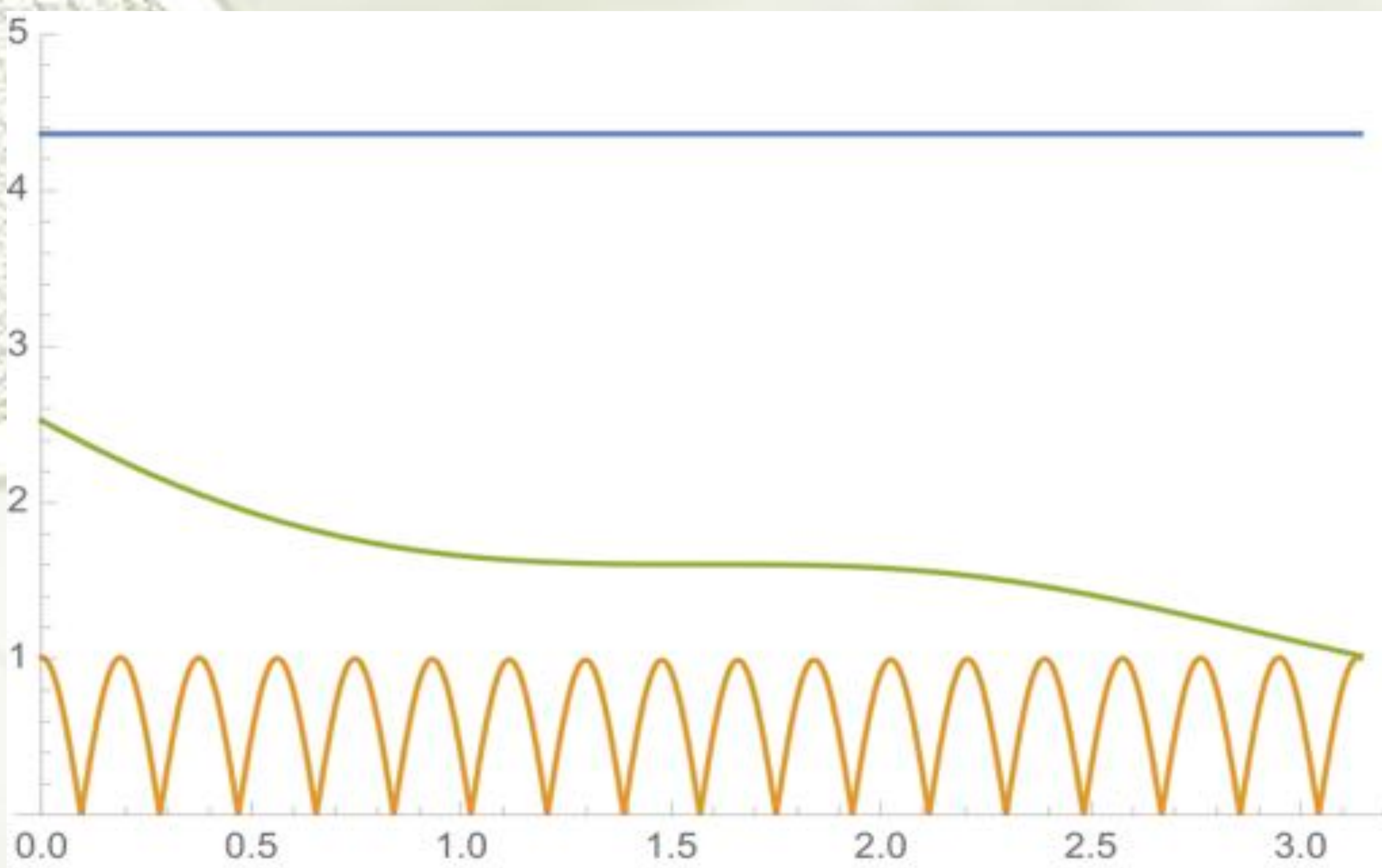


Figure 6. An even Mathieu-type eigenunction on an edge of a tetrahedron, with $q = 5$, $E = 300$ (red), along with the uniform upper bound of Theorem 2.1 and the upper bound from Theorem 5.1 (green). (Case Study 8).

Step 5. Harnack estmates

- On a compact region where $\psi > 0$,

  $\max(\psi) \leq C \min(\psi)$
- *C only depends on the region and V(x).*
- *Harnack remain valid even past vertices!* 

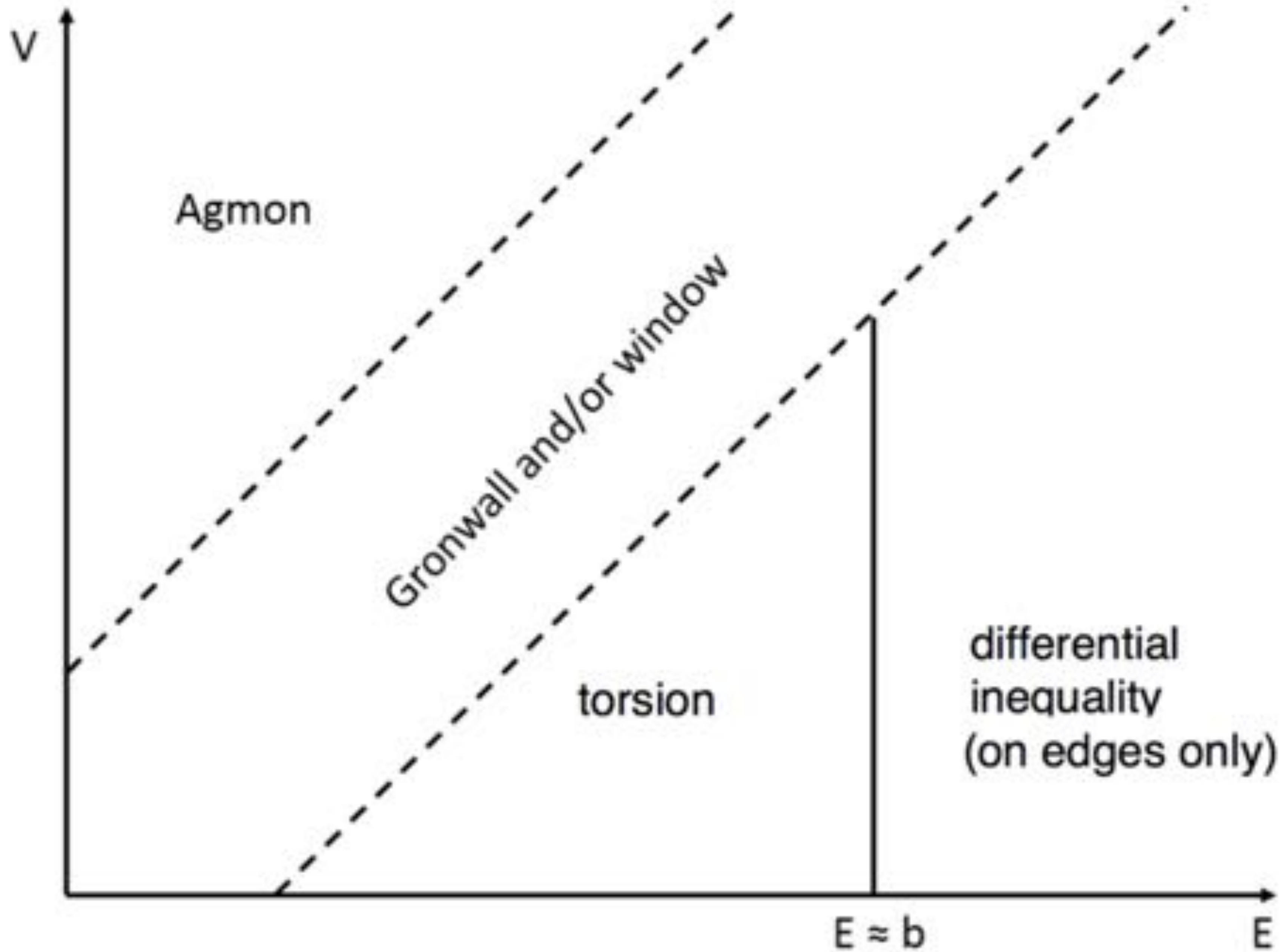
Step 5. Harnack *(careful statement)*

Theorem 2.2 (Harnack inequality for quantum graphs). *Let U be an open subset of Γ and let $W \subset U$ be connected and compact. Then there exists a constant C depending only on U, W, $V(x)$, and E, such that every real-valued $\psi(x)$ defined on U, which never vanishes and satisfies*

$$\operatorname{sgn}(\psi(x))(-\psi''(x) + (V(x) - E)\psi) \geq 0$$

on the edges and Kirchhoff conditions at the vertices, obeys the inequality

$$\frac{\max_W |\psi|}{\min_W |\psi|} \leq C.$$


V
Agmon
Gronwall and/or window
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E ≈ b
E

The End

Selected further details

- Agmon lower bounds and Boggio’s inequality
- Proof of Gronwall-type estimate
- Proof of Harnack

Agmon bounds with Boggio's inequality

- An old bound that has been rediscovered many times:

$$-\Delta \geq \frac{-\Delta v(x)}{v(x)}.$$

Lemma 2.2. *Let Γ_0 be a quantum graph with Kirchhoff or Dirichlet boundary conditions at vertices, possibly independently assigned. Suppose that $\Phi > 0$ is a C^2 function on the edges and satisfies super-Kirchhoff conditions* (2) *at all vertices. Then for every $f \in H^1(\Gamma)$,*

$$\sum_{\mathbf{e}\in\Gamma_0} \int_{\mathbf{e}} |f'(x)|^2 \geq \sum_{\mathbf{e}\in\Gamma_0} \int_{\mathbf{e}} |f(x)|^2 \left(\frac{-\Phi''(x)}{\Phi(x)} \right).$$

Proof of Gronwall-type estimate

$$g(x) := (\psi(x))^2 + \frac{(\psi'(x))^2}{E}$$

$$g(y) \leq g(x) \exp\left(\frac{1}{\sqrt{E}} \int_x^y |V(t)| dt\right)$$

Proof. Using the freedom to redefine $V \to V - E_m$ if simultaneously $E - E_m$, we may set $E_m = 0$ in the proof. We take the derivative of g:

$$g' = 2\psi\psi' + \frac{2\psi'\psi''}{E} = 2\psi\psi'\left(1 + \frac{V - E}{E}\right) = \frac{2V}{E}\psi\psi'. \tag{35}$$

This yields

$$g' \leq \frac{|V|}{\sqrt{E}}(\psi^2 + (\psi')^2/E) = \frac{|V|}{\sqrt{E}}g. \tag{36}$$

Dividing by g and integrating yields the result. $\square$

Proof of Harnack

$$
\begin{aligned}
(H-E)\ln\psi &= -\frac{d}{dx}\left(\frac{\psi'}{\psi}\right) + (V-E)\ln\psi \\
&= \frac{1}{\psi}(H-E)\psi + \left(\frac{\psi'}{\psi}\right)^2 + (V-E)(\ln\psi - 1).
\end{aligned} \tag{7}
$$

By assumption the first term on the right is nonnegative, and so for all x (other than vertices) in U, we get

$$
\left(\frac{\psi'}{\psi}\right)^2 \leq -\frac{d^2}{dx^2}\ln\psi + (V-E). \tag{8}
$$

Let $r = \ln(\frac{\psi(x_2)}{\psi(x_1)})$ for some fixed pair of points $x_{1,2} \in W$ (for example, x_2 maximizing ψ and x_1 minimizing ψ). Then if P is any path from x_1 to x_2,

$$
r^2 = \left(\int_P \frac{\psi'(t)}{\psi(t)}\,dt\right)^2 \leq |P| \int_P \left(\frac{\psi'(t)}{\psi(t)}\right)^2 dt.
$$

Let $r = \ln(\frac{\psi(x_2)}{\psi(x_1)})$ for some fixed pair of points $x_{1,2} \in W$ (for example, x_2 maximizing ψ and x_1 minimizing ψ). Then if P is any path from x_1 to x_2,

$$r^2 = \left(\int_P \frac{\psi'(t)}{\psi(t)} \, dt \right)^2 \leq |P| \int_P \left(\frac{\psi'(t)}{\psi(t)} \right)^2 dt.$$

$$r^2 \leq |P| \int_{\tilde{P}} \eta^2 \left(\frac{\psi'}{\psi} \right)^2 \leq |P| \int_{\tilde{P}} \eta^2 \left(-\frac{d^2}{dx^2} \ln \psi + V - E \right)$$

We now integrate by parts and use the fact that the contributions at the vertices add up to zero by Kirchhoff, leaving

$$\begin{aligned} \int_{\tilde{P}} \eta^2 \left(\frac{\psi'}{\psi} \right)^2 &\leq \int_{\tilde{P}} \eta^2 (V - E) + \int_{\tilde{P}} 2\eta'\eta \, \frac{\psi'}{\psi} \\ &\leq \int_{\tilde{P}} \eta^2 (V - E) + \frac{1}{\alpha} \int_{\tilde{P}} (\eta')^2 + \alpha \int_{\tilde{P}} \left(\eta \frac{\psi'}{\psi} \right)^2 . \end{aligned} \tag{9}$$

Choosing $\alpha = 1/2$ we obtain

$$\int_{\tilde{P}} \eta^2 \left(\frac{\psi'}{\psi} \right)^2 \leq 2 \int_{\tilde{P}} \eta^2 (V - E) + 4 \int_{\tilde{P}} (\eta')^2,$$

L^2 and L^∞ estimates

$$
\begin{aligned}
|\phi(x_0)| = |\chi(x_0)\phi(x_0)| &= \left| \int_{x_0 - \frac{\ell_{\min}}{2}}^{x_0} (\chi(y)\phi(y))' dy \right| \\
&= \left| \int_{x_0 - \frac{\ell_{\min}}{2}}^{x_0} \left(\chi'(y)\phi(y) + \chi(y)\phi'(y)\right) dy \right| \\
&\le \frac{1}{2} \int_{x_0 - \frac{\ell_{\min}}{2}}^{x_0} \left((\chi')^2(y) + (\phi(y))^2 + (\chi(y))^2 + (\phi'(y))^2\right) dy,
\end{aligned}
$$

Comparison with examples

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Comparison with examples

1. The ladder shows that the classical-action bound is sometimes best possible.
2. The millipede has decay faster than the classical-action bound, and our path-dependent estimate captures that.
3. The regular tree shows that the averaged bound is sharp. (Even one with two lengths.)