

LOCALIZATION AND LANDSCAPE FUNCTIONS ON QUANTUM GRAPHS

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ABSTRACT. We discuss explicit landscape functions for quantum graphs. By a “landscape function” $\Upsilon(x)$ we mean a function that controls the localization properties of normalized eigenfunctions $\psi(x)$ through a pointwise inequality of the form

$$|\psi(x)| \leq \Upsilon(x).$$

The ideal Υ is a function that

- a) responds to the potential energy $V(x)$ and to the structure of the graph in some formulaic way;
- b) is small in examples where eigenfunctions are suppressed by the tunneling effect; and
- c) relatively large in regions where eigenfunctions may - or may not - be concentrated, as observed in specific examples.

It turns out that the connectedness of a graph can present a barrier to the existence of universal landscape functions in the high-energy régime, as we show with simple examples. We therefore apply different methods in different régimes determined by the values of the potential energy $V(x)$ and the eigenvalue parameter E .

1. INTRODUCTION

The overarching question that we investigate in this paper is how the graph structure impacts the behavior of eigenfunctions. A quantum graph is locally one-dimensional and within the realm of Sturm-Liouville theory, but multidimensional features arise from the connectedness. It can be thought of as an intermediate case between one-dimensional and multidimensional models.

This article is an exploration of the degree to which explicit, “landscape functions” can be constructed for the eigenfunctions of quantum graphs. By a “landscape function” $\Upsilon(x)$ we mean a function that controls the localization properties of normalized eigenfunctions $\psi(x)$ through a pointwise inequality of the form

$$|\psi(x)| \leq \Upsilon(x).$$

The ideal Υ will be an explicit function simply expressed in terms of the eigenvalue E , the metric graph Γ , and the potential energy $V(x)$ in the Schrödinger equation living on it. $\Upsilon(x)$ should vary over the graph and usefully distinguish the regions where an eigenfunction may be large from those where it must have small amplitude due to the tunneling effect. The literature abounds with techniques to obtain uniform L^p estimates of eigenfunctions of quantum Hamiltonians for $2 < p \leq \infty$, notably Nelson’s notion of hypercontractivity, as further developed by many later researchers, cf. [28, §X.9], [12, §2], §2. See also [11, 3, 30] for other approaches to pointwise

bounds on eigenfunctions. In [13] Davies showed that hypercontractive estimates can be adapted to the case of quantum graphs, as we shall recall in Theorem 2.1, below.

For differential operators, several techniques have successfully been used to construct landscape functions that vary in useful ways over Euclidean domains or manifolds, and related approaches will be explored here for quantum graphs. The circumstances that determine which method is the most effective depend heavily on the relationship between $V(x)$ and E , and to a lesser extent on the graph structure. The strongest control is obtained in the *tunneling régime*, where $V(x) > E$, which is the subject of §3, using an Agmon metric. An explicit upper bound with tunneling decrease into a barrier is stated in Theorem 3.1. This section follows our previous work [18], but improves it by extending its validity and by making the constants explicit. It is even possible to adapt the Agmon method to obtain landscape bounds when $E > V(x)$, modestly, as we show later in Eq. (28).

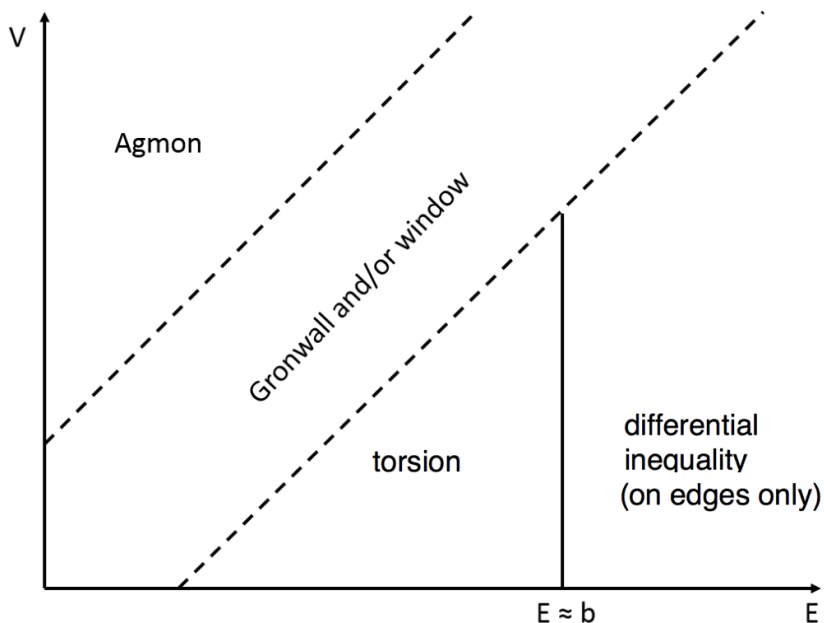
The second established method uses the maximum principle to prove inequalities in terms of functions satisfying other differential equations, especially variants of the torsion function. We innovate in §4 by replacing the torsion function by something more explicit, consisting of functions of the form constant + Gaussian on a covering set of intervals and star graphs. The covering can even in principle be made global for the graph, although the upper bound will become trivial (*i.e.*, worse than the uniform bound) on regions where $E \gg V$. Examples show that the method based on maximum principles can work well where $E > V(x)$ but only modestly.

For completeness, in later sections we work out bounds in the situations not covered in §§3–4, that is, when $E \gg V$ and when $E \approx V(x)$. Classical ODE methods are available to produce good pointwise control of solutions, as we review, and for the transitional régime where $E \approx V(x)$ we are also able to use a variant of the Agmon method, to give pointwise control of an eigenfunction by integrating over an enclosing “window.” In the high-energy régime, there is a key difference from the previous methods, however: Whereas the Agmon method and the maximum principle allow one to control an eigensolution on an appropriate subset by its values on the boundary of the subset, the only methods available in the high-energy régime are shooting methods. That is, they take the value of a solution and its derivative at a point and use them to control the solution as it moves along an edge. Unfortunately, as evidenced by Case Studies 1 and 2, when an edge passes a vertex, the eigensolution on a succeeding vertex can set out with an uncontrolled change in its derivative. As a consequence, the bounds obtained from classical ODE methods do not adapt as well to quantum graphs as do those using the Agmon and maximum-principle methods.

A phase diagram delineating the different régimes for constructing landscape functions is depicted in Figure 1.

2. ASSUMPTIONS ON QUANTUM GRAPHS AND SOME USEFUL FACTS

In this section we lay out some assumptions and review some facts about quantum graphs. We recall that a quantum-graph eigenfunction $\psi(x; E)$ is

FIGURE 1. Phase diagram of upper bounds on $|\psi|$.

an L^2 -normalized function that satisfies

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi(x; E) = E\psi(x; E) \quad (1)$$

on the edges of a metric graph Γ , and certain conditions at the vertices. For simplicity, in this article we confine ourselves to Kirchhoff (a.k.a. Neumann-Kirchhoff [8]) vertex conditions, according to which the sum of the outgoing derivatives at each vertex is 0. We refer to [7, 8, 26] for background and precise definitions of these operators.

We may assume without loss of generality that the graph has no leaves. The Kirchhoff vertex condition at the end of a leaf reduces to the standard Neumann boundary condition. Any quantum-graph eigenvalue problem on a graph Γ with leaves can be restated on a larger graph $\hat{\Gamma}$ with no leaves, where $\hat{\Gamma}$ consists of two copies of Γ after identification of the corresponding end vertices of the leaves. The eigenfunctions on Γ simply correspond to eigenfunctions on $\hat{\Gamma}$ which happen to be even under the symmetry of swapping the two copies Γ that compose $\hat{\Gamma}$.

As shown in Figure 1, we will distinguish different parts of the graph based on the corresponding relationship between V and E . This is captured in the following set of definitions:

Definition 2.1. For any finite $E \geq 0$ we refer to

$$\mathcal{T}_E := V^{-1}((E, \infty))$$

as the *tunneling region* (with respect to E), and to its complement

$$\mathcal{C}_E := V^{-1}([0, E])$$

as the *classically allowed region*. Since eigenfunctions are expected to be more highly oscillatory where $E \gg V(x)$, we will sometimes single out *regions of low potential energy*, $\mathcal{C}_{E'} := V^{-1}([0, E'])$, where $E' < E$ (In physical parlance, these are the “bottoms of the wells.”)

Throughout the manuscript we make the following assumptions on the graph G and potential V :

- (1) The degrees of the vertices are uniformly bounded above by some $d_{\max} < \infty$.
- (2) Every edge is at least as long as some fixed $L_{\min} > 0$.
- (3) $V \geq 0$ and locally integrable
- (4) For the eigenvalues E we consider, the classically allowed region is compact.

We shall have occasion below to invoke the maximum principle, which is easy to extend to the setting of quantum graphs (cf e.g. [25, 2]). We provide a version here that applies to quantum graphs in a form that is convenient for our purposes.

Lemma 2.1. *Let H be a quantum-graph Hamiltonian with $V(x) \geq 0$ on an open subset \mathcal{S} of G . Suppose that $w \in C^2$ and that $Hw := -w'' + V(x)w$ on edges, with “super-Kirchhoff” conditions at the vertices v , that*

$$\sum_{\mathbf{e} \sim v} w'_{\mathbf{e}}(x_0^+) \geq 0, \quad (2)$$

i.e., the sum of the outgoing derivatives of w at a vertex is nonnegative. If $Hw \leq 0$ on the edges contained in \mathcal{S} , then $w_+ := \max(w, 0)$ does not have a strict local maximum on \mathcal{S} .

Proof. (See also [17]) We follow a standard proof of the maximum principle for elliptic partial differential equations, taking special care at the vertices.

For this purpose we may assume that $w > 0$ at the putative maximum, as the value 0 cannot logically be a strict local maximum value of w_+ . We next argue that it suffices to prove the maximum principle under the assumption that $Hw \leq -\epsilon^2$ on \mathcal{S} for some $\epsilon \neq 0$, since if w has a strict local maximum on \mathcal{S} , then so does $w_{\delta}(x) := \exp(\delta x)w(x)$ for sufficiently small $|\delta(x)|$, at a point $x_1 \in \mathcal{S}$. But $Hw_{\delta}(x) = \exp(\delta x)(-\delta^2 w - \delta w' + Hw)$, and therefore for δ of sufficiently small magnitude and with the same sign as $w'(x_1)$ (supposing that $w'(x_1) \neq 0$), this will be strictly negative in a neighborhood of x_1 .

Thus we posit without loss of generality that $Hw \leq -\epsilon^2$ for some $\epsilon > 0$. If we suppose that w is maximized at some x_0 interior to an edge, then $w'(x_0) = 0$ and $w''(x_0) \leq 0$, but this contradicts the assumption that $Hw \leq -\epsilon^2$. If on the other hand the maximizing x_0 is a vertex, then for each edge \mathbf{e} emanating from x_0 , $w'_{\mathbf{e}}(x_0^+) \leq 0$. Because of the super-Kirchhoff conditions, if for any edge, $w'_{\mathbf{e}}(x_0^+) < 0$, there must be at least one other edge \mathbf{e}' on which $w'_{\mathbf{e}'}(x_0^+) > 0$, which would contradict maximality. Therefore $w'_{\mathbf{e}}(x_0^+) = 0$ for all edges \mathbf{e} , and a necessary condition for maximality is again that $w''_{\mathbf{e}}(x_0^+) \leq 0$. This, as before, would contradict $Hw \leq -\epsilon^2$. \square

As mentioned above, eigenfunctions of quantum graphs are bounded above in the L^∞ sense, using hypercontractive (heat-kernel) estimates. The next result provides a specific bound of this type, using an argument of [13].

The following theorem refers to the edges of the metric graph Γ . Any point of an edge can be regarded as a degree-two vertex, however, since the Kirchhoff condition reduces at a degree-two vertex to the condition that the solutions are C^1 there. Hence in these estimates edges can be subdivided into smaller edges, if convenient.

Theorem 2.1. *Let $\psi_\ell(x) := \psi(x; E_\ell)$ for a particular eigenvalue E_ℓ . On each edge \mathbf{e} of a quantum graph, the L^2 normalized eigenfunctions $\psi_j(x)$ satisfy*

$$\sum_{E_j \leq E} \|\psi_j\|_{L^\infty(\mathbf{e})}^2 \leq \sqrt{\frac{2e(E - \inf_\Gamma(V))}{\pi}} + \frac{\sqrt{e}}{|\mathbf{e}|}. \quad (3)$$

For an individual eigenfunction ψ_j , therefore, if $E_j \leq E$, then

$$|\psi_j(x)| \leq \sqrt{\sqrt{\frac{2e(E - \inf_\Gamma(V))}{\pi}} + \frac{\sqrt{e}}{|\mathbf{e}(\mathbf{x})|}}, \quad (4)$$

where $\mathbf{e}(\mathbf{x})$ denotes the edge containing x . If $\mathbf{e}(\mathbf{x})$ has infinite length, the terms containing $|\mathbf{e}(\mathbf{x})|$ in the denominator are interpreted as 0.

We remark that the proof implies a slightly stronger bound than that stated in the theorem, at the price of minimizing a less intuitive expression involving theta functions.

Proof. In this proof, if an edge has infinite length, we regard it as the union of an edge of arbitrarily large finite length and countably many other edges of, say, length 1, by inserting degree-two vertices as necessary. We can afterwards take the limit as the length of the large edge tends to ∞ .

Following the proof of Lemma 4.1 in [13], we note that the heat kernel on a metric graph is pointwise bounded above on each edge by the heat kernel on that edge with Neumann boundary conditions at its ends,

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

If a potential energy $V(x) \geq V_{\min}$ is included, the kernel of $\exp(-tH)$ is bounded above by $\exp(-V_{\min}t)K_{\mathbf{e}}(t, x, y)$ according to a standard result (an exercise using the Lie-Trotter product formula, cf. Lemma 1.1 of [10]). By expanding $\exp(-tH)$ in eigenfunctions, we obtain

$$\sum_{E_j \leq E} |\psi_j(x)|^2 \leq e^{(E - \inf_\Gamma(V))t} K_{\mathbf{e}(\mathbf{x})}(t, x, x), \quad (6)$$

For the sake of simplicity, after inserting (5) we replace the theta function by a larger but more elementary quantity, getting

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

Finally we choose $t = \frac{1}{2(E - \inf_{\Gamma}(V))}$ (which is the minimizing value if we ignore “1+” on the right side), and obtain the claim. \square

Another inequality that we can adapt to quantum graphs with a simple proof is the Harnack inequality.

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

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

Proof. We may assume $\psi > 0$. Abbreviating $Hf := -f'' + Vf$ as usual,

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

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 $r = \ln\left(\frac{\psi(x_2)}{\psi(x_1)}\right)$ 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 $\tilde{P} = P \cup J$ where $J = \cup I_i$, and I_i are short intervals of two kinds adjacent to P (i.e. they are short enough that they do not reach the next vertex):

- (1) Short extensions beyond $x_{1,2}$
- (2) Some neighborhoods of the vertices, i.e. including little bits of edges whose vertices lie in P

Now let η be a piecewise C^1 function such that $\eta := 1$ on P and $\eta := 0$ on \tilde{P}^c . (Specifically, \tilde{P} could be chosen as $\{x \in U : \operatorname{dist}(x, P) < L_{\min}/2\}$, and η as a linear ramp going from 1 to 0 as x goes from P to $\partial\tilde{P}$.) Then

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

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

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

Choosing $\alpha = 1/2$ we obtain

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

which is independent of ψ as claimed. \square

A final tool we adapt to quantum graphs is a lower-bound inequality of Boggio (more often attributed to Barta; see [16] for some discussion of the contribution of Boggio [9]), *viz.*, i.e. if Δ is the Dirichlet Laplacian on a domain and $v(x) > 0$ is a suitably regular function, then, in the weak sense,

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

Since the graph Laplacian is more analogous to a domain's Neumann Laplacian than to its Dirichlet Laplacian, it may be surprising that Boggio's inequality extends without complications:

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. For notational simplicity, the proof is carried out in the case where f is real valued. According to Picone's inequality,

$$\begin{aligned} (f'(x))^2 &\geq \Phi'(x) \frac{d}{dx} \left(\frac{(f(x))^2}{\Phi(x)} \right) \\ &= \frac{d}{dx} \left(\Phi(x) \frac{d}{dx} \left(\frac{(f(x))^2}{\Phi(x)} \right) \right) + (f(x))^2 \left(\frac{-\Phi''(x)}{\Phi(x)} \right). \end{aligned}$$

When the first term in the last line is integrated on an edge \mathbf{e} , it contributes

$$-2f(0+)f'(0+) + (f(0+))^2 \frac{\Phi'(0+)}{\Phi(0+)}$$

in the outgoing sense at both of the vertices bounding \mathbf{e} . When all such contributions are summed at a given vertex, the result is nonnegative according to the assumptions on f and Φ . \square

3. LANDSCAPE UPPER BOUNDS ON TUNNELING REGIONS,
USING AGMON'S METHOD

It is in the tunneling régime \mathcal{T}_E that the estimation of eigenfunctions in terms of a landscape function is at the same time the most explicit and the tightest when compared with examples. We thus start by recalling and sharpening some bounds derived with Agmon's method, which were first established for quantum graphs in [18].

The two central lemmas in [18] can be distilled into the following pointwise identities for an Agmon function F , a smooth cutoff η , and a real-valued function ψ satisfying $(H - E)\psi = 0$ on $\text{supp}(\eta)$. First:

$$F^2(x)\eta(x)\psi(x)(H - E)\eta(x)\psi(x) = F^2(x)(-\eta''(x)\psi^2(x) - \eta\psi(x)\eta'(x)\psi'(x)), \quad (10)$$

where the quantity on the right is supported within $\text{supp}(\eta') =: \mathcal{S}$, and can therefore be estimated in terms of $\|\eta''\|_\infty$, $\|\eta'\|_\infty$, $\sup(F)\chi_{\mathcal{S}}$, and $\|\psi\|_{H^1(\mathcal{S})}$. With a little algebraic juggling, we can rewrite (10) so that the derivatives ψ' and η'' do not appear:

$$F^2(x)\eta(x)\psi(x)(H - E)\eta(x)\psi(x) = \psi^2(x)\left(\eta'(x)(\eta(x)F^2(x))'\right) - G'(x), \quad (11)$$

except inside $G(x) = \eta(x)\eta'(x)F^2(x)\psi^2(x)$, which will be arranged to integrate to 0 on any edge by requiring the support of η' to lie within the edge. In (11) the quantity on the right can therefore be estimated in terms of $\|\eta'\|_\infty$, $\sup(F)\chi_{\mathcal{S}}$, $\sup(F')\chi_{\mathcal{S}}$, and $\|\psi\|_{L^2(\mathcal{S})}$. In particular, this will allow us to relax the assumption that $\eta \in C^2$ and choose it to be a ramp function below.

By a second direct calculation,

$$F^2(x)\eta(x)\psi(x)(H - E)\eta(x)\psi(x) = ((F\eta\psi)')^2 + \left(V - E - \left(\frac{F'}{F}\right)^2\right)(F\eta\psi)^2 - H'(x), \quad (12)$$

where $H = F^2\eta\psi(\eta\psi)'$ will produce boundary contributions when integrated, but if F is continuous and ψ satisfies Kirchhoff conditions, they will sum to 0.

Suppose initially that for some $\ell > 0$ the finite, closed interval $[a - \ell, b + \ell]$ is contained within an edge belonging to \mathcal{T}_E . In order to obtain estimates on $I = [a, b]$, let

$$\begin{aligned} F_E(x) &= 1, & x \notin (a, b) \\ F_E(x) &= e^{\min \int_a^x \sqrt{V-E}, \int_x^b \sqrt{V-E}}, & x \in [a, b] \end{aligned} \quad (13)$$

We let η be a linear ramp on $[a - \ell, a]$ and $[b, b + \ell]$, with $\eta = 0$ on $\mathbb{R} \setminus [a - \ell, b + \ell]$ and $\eta = 1$ on I . Then equations (11) and (12) yield that

$$\int_{\Gamma} \psi^2(x)\left(\eta'(x)(\eta(x)F_E^2(x))'\right) \geq \int_{\Gamma} ((F_E\eta\psi)')^2. \quad (14)$$

Now fixing $x \in I$ we apply Cauchy-Schwarz to the right side:

$$\begin{aligned}
\int_{\Gamma} ((F_E \eta \psi)')^2 &= \int_{a-\ell}^x ((F_E \eta \psi)')^2 + \int_x^{b+\ell} ((F_E \eta \psi)')^2 \\
&\geq \frac{(\int_{a-\ell}^x (F_E \eta \psi)')^2}{x-a+\ell} + \frac{(\int_x^{b+\ell} (F_E \eta \psi)')^2}{b+\ell-x} \\
&= \frac{(F_E(x)\psi(x))^2}{x-a+\ell} + \frac{(F_E(x)\psi(x))^2}{b+\ell-x} \\
&= \psi(x)^2 \left(\frac{F_E(x)^2(b-a+2\ell)}{(x-a+\ell)(b+\ell-x)} \right).
\end{aligned} \tag{15}$$

This yields the estimate

$$\begin{aligned}
|\psi(x)| &\leq \sqrt{\frac{(x-a+\ell)(b+\ell-x)}{b-a+2\ell}} \\
&\times \frac{1}{F_E(x)} \left(\int_{\text{supp } \eta'} \psi^2(y) (\eta'(y) (\eta(y) F_E^2(y))') dy \right)^{\frac{1}{2}} \\
&= \sqrt{\frac{(x-a+\ell)(b+\ell-x)}{b-a+2\ell}} \frac{1}{F_E(x)} \left(\int_{\text{supp } \eta'} \psi^2(y) (\eta'(y))^2 dy \right)^{\frac{1}{2}} \\
&\leq \sqrt{\frac{(x-a+\ell)(b+\ell-x)}{b-a+2\ell}} \frac{\|\psi\|_{L^2([a-\ell, a] \cup [b, b+\ell])}}{\ell F_E(x)}.
\end{aligned} \tag{16}$$

We now extend this argument in two ways. The first is to potentially allow the interval to be infinite, as was the case in [18]. We may parametrize I as $[a, \infty)$, in which case F_E can be simply defined on I as

$$F_E(x) := e^{\int_a^x \sqrt{V-E}}.$$

In this case we can drop one of the contributions to the first line of (15), obtaining

$$\int_{\Gamma} ((F_E \eta \psi)')^2 \geq \frac{(F_E(x)\psi(x))^2}{x-a+\ell}$$

and thus for $x > a$,

$$|\psi(x)| \leq \sqrt{x-a+\ell} F_E^{-1}(x) \frac{\|\psi\|_{L^2([a-\ell, a])}}{\ell}.$$

Secondly, we extend the analysis to connected regions of the graph on which $V - E > 0$ as follows. Since we assume V to be continuous, we know that the set \mathcal{T}_E is open. It may consist of disconnected components, in which case we may restrict ourselves to working on one component at a time, so without loss of generality we may assume that \mathcal{T}_E is connected. Let the boundary of \mathcal{T}_E (henceforth denoted $\partial\mathcal{T}_E$) be $\{b_1, \dots, b_m\}$. Note that $\partial\mathcal{T}_E$ is a finite collection of points, because we assume that $\gamma \setminus \mathcal{T}_E$ is compact, all degrees are finite, and all edges have a minimum length. We define

$$F_E(x) = \exp \left(\min_{1 \leq j \leq m} \min_{P: \text{paths } b_j \text{ to } x} \int_P \sqrt{V-E} \right) \quad \text{for } x \in \mathcal{T}_E \tag{17}$$

$$F_E(x) = 1 \quad \text{for } x \notin \mathcal{T}_E \tag{18}$$

By construction, F_E is again continuous. For $x \in \mathcal{T}_E$ we can think of $F_E(x)$ as defining an *Agmon metric* on \mathcal{T}_E ,

$$\rho_A(x, y; E) := \min_{P: \text{paths } y \text{ to } x} \int_P \sqrt{V - E}. \quad (19)$$

If S is a set, $\rho_A(x, S, E)$ will denote the infimum of $\rho_A(x, y; E)$ for $y \in S$.

To define η , for each j we parametrize the part of the edge containing b_j and lying outside of \mathcal{T}_E with b_j mapped to 0. Then η is taken as a ramp on each of m segments $[0, \ell]$ associated to each point in $\partial\mathcal{T}_E$ (denote them $[0, \ell]_{b_j}$) so that $\eta = 1$ on \mathcal{T}_E and $\eta = 0$ on $\mathcal{T}_E^c \setminus \cup_j [0, \ell]_{b_j}$. This construction yields $\eta'(x) = -1/\ell$ on each of $[0, \ell]_{b_j}$. With η and F_E in place, we carry out a similar calculation. Let P be any path from any of the points $b_j \in \partial\mathcal{T}_E$ to the point $x \in \mathcal{T}_E$.

$$\int_{\Gamma} ((F_E \eta \psi)')^2 \geq \int_P ((F_E \eta \psi)')^2 \geq \frac{(\int_P (F_E \eta \psi)')^2}{|P|} = \frac{(F_E(x) \psi(x))^2}{|P|}. \quad (20)$$

We can then minimize over paths P to obtain an upper bound, which decreases exponentially into the tunneling region. This proves:

Theorem 3.1. *For $x \in \mathcal{T}_E$ with $\text{dist}(x, \partial\mathcal{T}_E) \geq \ell$,*

$$|\psi(x)| \leq \frac{\sqrt{\text{dist}(x, \partial\mathcal{T}_E)} \|\psi\|_{L^2(\cup_{j=1}^m [b_j, b_j + \ell])}}{\ell} \exp(-\rho_A(x, \partial\mathcal{T}_E; E)). \quad (21)$$

For a normalized wavefunction we can simplify by bounding $\|\psi\|_{L^2(\cup_{j=1}^m [b_j, b_j + \ell])}$ above by 1. We caution that, unlike the upper bound of Theorem 3.1, the magnitude of the wave function itself may, and frequently does, change monotonically at an exponential rate throughout a barrier. Of course, if it does so, normalization forces it to be exponentially small on one side or other of the barrier.

In some circumstances, a different choice of F can provide a slightly improved upper bound with Agmon's method.

Now fix some $\delta > 0$, and consider the set $\mathcal{T}_{E+\delta} \setminus \mathcal{T}_{E+2\delta}$. Each connected component of this set contains a vertex-free interval of length $\geq L(\delta)$ for some $L(\delta) > 0$, the value of which we consider among the ‘‘accessible’’ properties of a quantum graph.

Integrating (12) and letting $Q^2 := \left(V - E - \left(\frac{F'_{E-\delta}}{F_{E-\delta}} \right)^2 \right) \geq \delta$, we get

$$\begin{aligned} \int_{\Gamma} (((\eta F_{E-\delta} \psi)')^2 + Q^2 (\eta F_{E-\delta} \psi)^2) &= \int_{\Gamma} Q \left(\frac{((\eta F_{E-\delta} \psi)')^2}{Q} + Q (\eta F_{E-\delta} \psi)^2 \right) \\ &\geq \sqrt{\delta} \int_{I_0} \left(\frac{((\eta F_{E-\delta} \psi)')^2}{Q} + Q (\eta F_{E-\delta} \psi)^2 \right) \\ &\geq \sqrt{\delta} \left| \int_{I_0} ((\eta F_{E-\delta} \psi)^2)' \right|, \end{aligned} \quad (22)$$

where I_0 is any subset of $\mathcal{T}_{E+\delta}$. (The final line used the arithmetic-geometric mean inequality, $a^2 + b^2 \geq \pm 2ab$.) In order to estimate $\psi(x)$ for $x \in \mathcal{T}_{E+2\delta}$, we make a specific choice of $\eta \in C^2$ and I_0 as follows.

- (1) I_0 is a vertex-free interval of length $\geq L(\delta)$.

- (2) $\text{supp}(\eta'(x)) \subset I_0 \cup I_1 \subset \mathcal{T}_{E+\delta} \setminus \mathcal{T}_{E+2\delta}$, where I_1 is a finite (possibly empty) union of disjoint vertex-free intervals, such that any path from x to the complement of $\mathcal{T}_{E+\delta}$ passes through $I_0 \cup I_1$.
- (3) $\eta(x) = 1$
- (4) $\eta(y) = 0$ for all y that cannot be connected to x without passing through I_0 .

Applying the Fundamental Theorem of Calculus to the lower side of (22) and invoking the equivalence of (11) and (12), we see that

$$(F_{E-\delta}(x)\psi(x))^2 \leq \frac{1}{\sqrt{\delta}} \int_{I_0} \psi^2 F_{E-\delta}^2 \left(\eta'^2 + (\eta^2)' \left(\frac{F'_{E-\delta}}{F_{E-\delta}} \right) \right).$$

The smoothness required of η can now be relaxed by passing to a sequence of η_k tending uniformly to linear ramp functions increasing from 0 to 1 on a subinterval of I_0 of length at least $L(\delta)$. Hence we conclude that

$$\begin{aligned} (F_{E-\delta}(x)\psi(x))^2 &\leq \frac{1}{\sqrt{\delta}} \max_{I_0} \left(F_{E-\delta}^2 \left(\left(\frac{1}{L(\delta)} \right)^2 + \frac{1}{L(\delta)} \sqrt{V-E-\delta} \right) \right) \|\psi\|_{I_0}^2 \\ &\leq \frac{1}{\sqrt{\delta}} e^{2\sqrt{\delta}L(\delta)} \left(\left(\frac{1}{L(\delta)} \right)^2 + \frac{\delta}{L(\delta)} \right) \|\psi\|_{I_0}^2. \end{aligned}$$

4. CONSTRUCTION OF LANDSCAPE FUNCTIONS ON A GRAPH VIA A SIMPLIFIED TORSION FUNCTION

Here and in §6 we shall discuss ways to construct landscape functions valid when $E \geq V(x)$ (but not by too much), thus complementary to the bounds of §3.

For scalar Schrödinger operators on domains, a standard choice of a “landscape function” is a sufficiently large multiple of a positive solution $T(x)$ of

$$(-\Delta + V(x))T(x) = 1, \tag{23}$$

e.g., [15, 31]. This is a Schrödinger variant of the *torsion function* (cf. [4, 27, 5, 6]) A sufficiently large multiple of $T(x)$ will provide a pointwise bound on an eigensolution $|\psi(x)|$ on some region R , through a maximum-principle argument. The bound will depend on the eigenvalue and on the values of $|\psi(x)|$ on ∂R .

There are two common drawbacks to landscape functions of torsion-function type. The first is that, typically, such landscape functions become trivial for large eigenvalues E , by which we mean that the upper bound thus obtained may on some regions exceed known uniform upper bounds on $\|\psi\|_\infty$, e.g., as in Theorem 2.1. In this situation the upper bounds usually also lack useful dependence on the position x . This is an intrinsic difficulty for the method in a region where the eigenfunction oscillates. It is hard to see how a necessarily positive upper bound will take full advantage of the fact that such an eigenfunction has zeroes. (An alternative and more effective approach to pointwise control of rapidly oscillating eigenfunctions incorporates their derivatives, cf. Theorem 5.1, below.)

Consider for instance the simplest situation, an ordinary differential equation with periodic boundary conditions, $\psi(x+L) = \psi(x)$. At large energies

$E \gg V(x)$ we can approximate by dropping V , so that the normalized real-valued eigenfunctions are well approximated by

$$\sqrt{\frac{2}{L}} \cos(\sqrt{E}x - \phi), \quad E = \left(\frac{2\pi m}{L}\right)^2,$$

and by appropriate choice of the phase ϕ the position of the maximal value can be placed at will. In addition to this elementary limitation on the use of landscape functions, when we adapt them to quantum graphs there are further barriers to their use arising from the connectedness of the graph, as shown in Case Studies 1 and 2.

A second drawback to landscape functions based on (23) is that, usually, the torsion function and its variants are only computationally known. As we shall elaborate below in the context of quantum graphs, however, due to the maximum principle it suffices in lieu of (23) to have an inequality

$$HT = (-\Delta + V(x))T(x) \geq 1, \quad (24)$$

The flexibility of an inequality allows more accessible or even explicit choices of landscape functions, without losing qualitative features.

Before showing how to construct explicit, elementary functions satisfying (24) on quantum graphs, which is done below, let us describe how T can be used to provide a landscape function in two different ways.

In both cases we suppose that (24) holds on some $\Gamma_0 \subset \Gamma$, with Kirchhoff conditions at the vertices of Γ_0

We consider

$$W(x, \pm) := \pm\psi(x) - E\|\psi\|_{L^\infty(\Gamma_0)}T(x),$$

where we shall consider both signs in order to bound $|\psi|$. We see that

$$HW(x, \pm) = E(\pm\psi(x) - \|\psi\|_{L^\infty(\Gamma_0)}) \leq 0. \quad (25)$$

We now apply the maximum principle Lemma 2.1 to $W(x, \pm)$ for both signs, concluding that $W(x) := |\psi(x)| - E\|\psi\|_{L^\infty(\Gamma_0)}T(x)$ is maximized on the boundary of the region on which (24) holds. We thus obtain

$$|\psi(x)| \leq \max_{x \in \partial\Gamma_0} W_+(x) + E\|\psi\|_{L^\infty(\Gamma_0)}T(x), \quad (26)$$

and hence if $W = 0$ on $\partial\Gamma_0$ then

$$\Upsilon_{\max \text{ princ.}}(x) := E\|\psi\|_{L^\infty(\Gamma_0)}T(x)$$

is a landscape function in the sense of [15, 31]. Of course, this is only interesting for x such that $ET(x) < 1$ or when ψ is known *a priori* to be small on Γ_0 .

The second way to build a landscape function out of $T(x)$, following ideas of Steinerberger in the case of domains [31], is to use Lemma 2.2. Since

$$\frac{H\Upsilon(x)}{\Upsilon(x)} \geq \frac{1}{\Upsilon(x)}, \quad (27)$$

which is positive, we can use the method of §3 to obtain Agmon-type bounds on parts of Γ_0 that extend beyond the tunneling region. In particular, using

$f = \eta F \psi$ in Lemma 2.2 and inserting (27) into (12), we find that

$$\left(\frac{1}{\Upsilon} - E - \left(\frac{F'}{F} \right)^2 \right) (F \eta \psi)^2 - H'(x) \leq \psi^2(x) \left(\eta'(x) (\eta(x) F^2(x))' \right) - G'(x),$$

where G' and H' will integrate to 0. This allows us to chose

$$F(x) = \exp \left(\int_{x_0}^x \sqrt{\frac{1}{\Upsilon} - E - \delta} \right) \quad (28)$$

on any region where $\frac{1}{\Upsilon} - E \geq \delta$, with η supported in the same region, and proceed as before. In this manner, bounds based on Agmon's method are obtainable in parts of \mathcal{C}_E where $V(x) < E < \frac{1}{\Upsilon(x)}$.

We next turn to the construction of a torsion-type landscape function on a quantum graph, considering first the case of a set of abutting intervals $[x_i, x_{i+1}]$, containing no vertices. Suppose $x_i < y_i < x_{i+1}$ and that on this interval

$$V(x) \geq V_i + b_i^2(x - y_i)^2, \quad (29)$$

with $b_i \geq 0$, $V_i \geq 0$. We can construct a landscape function on this interval in the form of a Gaussian function plus a constant, as follows. We temporarily set $i = 1$, $y_1 = 0$, $b_i = b$ for simplicity. If $b > 0$, define $\Upsilon_0(x) := A \left[\frac{1}{2} + \exp(-bx^2/2) \right]$. Then

$$\begin{aligned} \left[-\frac{d^2}{dx^2} + V \right] \Upsilon_0 &\geq \left[-\frac{d^2}{dx^2} + V_1 + b^2 x^2 \right] \Upsilon_0 \\ &= A \left[\frac{V_1 + b^2 x^2}{2} + (b + V_1) e^{-bx^2/2} \right]. \end{aligned} \quad (30)$$

We want to assign A the minimal possible value so that the right side of (30) ≥ 1 on the interval $[x_1, x_2]$. To do so we find the minimum of

$$f(x) := \frac{V_1 + b^2 x^2}{2} + (b + V_1) e^{-bx^2/2}$$

on $[x_1, x_2]$. Taking the derivative and setting it to 0 we obtain

$$b^2 x - bx(b + V_1) e^{-bx^2/2} = 0$$

Since $b + V_1 > 0$ by assumption, the minima occur at

$$x^2 = -\frac{2}{b} \ln \frac{b}{b + V_1}$$

and the value of such a minimum is $\frac{V_1}{2} - b \ln \frac{b}{b + V_1} + b$. When $-\frac{2}{b} \ln \frac{b}{b + V_1} > 0$ we can obtain a real value for the minimizer, which gives

$$\frac{1}{A} = \min \left\{ \frac{V_1}{2} - b \ln \frac{b}{b + V_1} + b, f(x_1), f(x_2) \right\}.$$

We illustrate this construction in Case Study 6. We also observe that with a slight weakening of the inequality, an explicit value of A can be assigned using the fact that that $e^{-y} + y \geq \max\{1, y\}$ for all $y > 0$, *viz.*,

$$A_0 = \frac{1}{b + \frac{V_1}{2}}. \quad (31)$$

When $b = 0$, Υ_0 can be chosen, for example, as an elementary quadratic of the form $a_1 - b_1 x^2$, such that $V_1(a_1 - b_1 x^2) + 2b_0 \geq 1$ on $[x_1, x_2]$. If V_1 is large it may even suffice for these purposes to choose $b_1 = 0$, i.e., Υ_0 may be constant on $[x_1, x_2]$. In practice, where $b_1 = 0$ the upper bound given by a quadratic Υ_0 will often either be weaker than the Agmon estimate, when applicable, or, as illustrated in Case Studies 1 and 2, no better than the uniform bound of Theorem 2.1. It is included here only to ensure that a single, seamless landscape function can be constructed on a set of concatenated intervals.

Letting $T(x) = \Upsilon_0(x)$ on $[x_1, x_2]$ we obtain from (26) that

$$|\psi(x)| \leq \max\{W_+(x_1), W_+(x_2)\} + E\|\psi\|_{L^\infty([x_1, x_2])} \Upsilon_0(x). \quad (32)$$

For the bound (32) to be nontrivial, we want E to be small in comparison with $b + \frac{V_1}{2}$ and we shall need to address the boundary values at $x_{1,2}$.

First, however, we show how to concatenate the construction of a landscape function in a multiple-well region. Suppose now that $V(x)$ satisfies inequalities of the form (29) on the interval $[x_1, x_2]$ with $y = y_1$, the analogous inequality on the interval $[x_2, x_3]$ with $y = y_2$, etc. The landscape functions as constructed above will be denoted $\Upsilon_0(x; b_i, V_i, y_i)$. They do not *a priori* define a C^1 function at the ends of the intervals x_i , but that problem can be fixed.

- Step 1. Beginning with $\Upsilon_0(x_i; b_i, V_i, y_i)$ as defined above, we first ensure that the derivatives are zero at the end points of its interval by adding functions of the form

$$\frac{\epsilon}{2} |\Upsilon'_0(x_i; b_i, V_i, y_i)| \left(1 - \frac{|x - x_i|}{\epsilon}\right)^2 \chi_{[x_i, x_i + \epsilon]}(x),$$

resp.

$$\frac{\epsilon}{2} |\Upsilon'_0(x_{i+1}; b_i, V_i, y_i)| \left(1 - \frac{|x - x_{i+1}|}{\epsilon}\right)^2 \chi_{[x_{i+1} - \epsilon, x_{i+1}]}(x)$$

for ϵ small enough that the supports of these functions are contained in (x_{i-1}, x_{i+1}) . Evidently, the quantity ϵ may be chosen in some convenient and roughly optimal way, depending on the parameters x_i, y_i, b_i, V_i , and need not have the same value at the two ends. We denote the sum of these two local quadratic functions $\rho_i(x)$.

- Step 2: Add positive constants $c_i \chi_{[x_i, x_{i+1}]}$ on a subset of the intervals $[x_i, x_{i+1}]$ in order make the concatenated function continuous. (Although we are describing here a universal way to piece together the landscape construction, in individual cases a good alternative to adding constants is often to choose the ends of the intervals x_i in advance so that $\Upsilon_0(x_i; b_{i-1}, V_{i-1}, y_{i-1}) = \Upsilon_0(x_i; b_i, V_i, y_i)$, making use of the fact that $\Upsilon_0(x; b_{i-1}, V_{i-1}, y_{i-1})$ decreases as $x \uparrow x_i$, whereas $\Upsilon_0(x; b_i, V_i, y_i)$ increases as x increases beyond x_i .)
- Step 3. If necessary, an overall constant c_0 is also added to ensure that $H\Upsilon \geq 1$ after Step 1 has been carried out.

The explicit expression

$$\Upsilon(x) := c_0 + \sum_i (\Upsilon_0(x; b_i, V_i, y_i) + c_i) \chi_{[x_i, x_{i+1}]} + \rho_i(x) \quad (33)$$

then has all the properties required of a landscape function on a sequence of abutting intervals, in the absence of vertices.

When adapting this construction to quantum graphs, in the vicinity of vertices we use star-graphs instead of intervals. When we overlay a subgraph with abutting intervals and star-graphs, we must take into account the vertex conditions and the possibility of closed loops. For the purpose of constructing a consistent landscape function, we impose additional symmetry conditions on our star-graphs.

Theorem 4.1. *Any connected subset \mathcal{S} of a quantum graph can be overlaid in an algorithmic manner with abutting intervals and star graphs on which a function of the form (33) can be defined, in terms of which $|\psi(x)| - \Upsilon(x)$ does not have a local maximum on $\text{int}(\mathcal{S})$.*

Remark 4.1. The construction in this theorem will be illustrated on a small scale in Case Study 7. An interesting situation arises when $\partial\mathcal{S} \subset \mathcal{T}_E$, because then the boundary values can be controlled by the Agmon estimates of the previous section.

Proof. The vertices do not pose much difficulty in adapting (33), because the maximum principle of Lemma 2.1 applies with super-Kirchhoff vertex conditions. We can and shall exclude intervals for which vertices occur at the endpoints. Each vertex can thus be regarded as interior to a subinterval of a pair of its edges. If it should happen that the vertex v coincides with a maximal point y_i for which an estimate (29) holds on a set of subintervals of all pairs of the edges incident to v , then $\pm\psi - C\Upsilon_0$ satisfies the Kirchhoff conditions at v , where Υ_0 is defined as above on each of those subintervals. In this circumstance, we can proceed as above. Otherwise, for any given v we privilege one of the adjacent edges, \mathbf{e}_p to contain a value y_i with respect to which an inequality of the form (29) holds on subintervals of $\mathbf{e}_p \cup \mathbf{e}$ uniformly for all edges $\mathbf{e} \neq \mathbf{e}_p$ incident to v . We now choose the function Υ_0 constructed above identically on each of these subintervals of $\mathbf{e}_p \cup \mathbf{e}$. Because Υ_0 decreases outward from v along each $\mathbf{e} \neq \mathbf{e}_p$ and only increases from v along \mathbf{e}_p , any function of the form $\pm\psi - C\Upsilon_0$ satisfies super-Kirchhoff conditions at v , and the maximum principle applies.

Next we arrange that the landscape function constructed on a concatenated set of intervals and star graphs remains C^1 even when the intervals compose a closed cycle.

- Step 1. First, we may restrict ourselves to using star-graphs in the covering of \mathcal{S} that a) contain no more than one vertex, and b) are symmetric with respect to y_i . Consequently, the functions $\Upsilon_0(x; b_i, V_i, y_i)$ on these star-graphs will be symmetric in x with respect to reflection through y_i .
- Step 2. On each star-graph, on neighborhoods of its ends we add quadratic functions ρ_i as defined above, to ensure that $\Upsilon'_0(x; b_i, V_i, y_i) + \rho'_i(x) = 0$ when x is at an endpoint.
- Step 3. We subtract a constant on each star-graph so that $\Upsilon_0(x; b_i, V_i, y_i) + \rho_i(x) - c_i = 0$ at the endpoints. The resulting functions compose a C^1 function on all of \mathcal{S} .

- Step 4. We now add a single constant c_0 on \mathcal{S} sufficiently large to ensure that $H\Upsilon \geq 1$ for all $x \in \mathcal{S}$.

□

5. LANDSCAPE FUNCTIONS IN THE HIGH-ENERGY RÉGIME

A good tool for controlling high-energy eigenfunctions is a theorem of Davies [11] using a differential inequality:

Theorem 5.1 (Davies). *Given a real-valued solution of (1) on an edge \mathbf{e} and $E_m < E$, define*

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

Then for $x, y \in \mathbf{e}$, choosing a parametrization so that $x \geq y$,

$$g(x, E, E_m) \leq g(y, E, E_m) \exp\left(\frac{1}{\sqrt{E - E_m}} \int_y^x |V(t) - E_m| dt\right). \quad (34)$$

We have rewritten this result in a form compatible with our presentation and have inserted a useful parameter E_m not used in [11]. While this bound is universally valid on intervals, it is most striking when E is large, as it implies that g is slowly varying. The shortcoming of Theorem 5.1 is that since it involves the derivative, which is not generally continuous on a path that passes a vertex, it is difficult to adapt to regions containing vertices. That this is a true difficulty is illustrated in Case Studies 1 and 2, in which the magnitude of an eigenfunction differs dramatically on parts of a graph separated by vertices.

For completeness we offer a proof of Theorem 5.1.

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

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

This yields

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

Dividing by g and integrating yields the result. □

In concert with Sturm oscillation theory, Theorem 5.1 can sometimes be used to obtain “landscape functions” that do not contain derivatives explicitly, so long as vertices are avoided.

Corollary 5.1. *Let $\psi(x)$ be a real solution of (1) on an interval \mathcal{I} , and suppose that $E - V(x) \geq k^2 > 0$ on a subinterval $\mathcal{I}_- = (x_1, x_2)$ of length at least $\frac{\pi}{k}$. Then for any $x \geq x_1$ and any $E_m < E$,*

$$\begin{aligned} |\psi(x)| &\leq \sqrt{\psi(x)^2 + \frac{\psi'(x)^2}{E - E_m}} \\ &\leq \|\psi\|_{L^\infty(\mathcal{I}_-)} \exp\left(\frac{1}{2\sqrt{E - E_m}} \int_{x_1}^x |V(t) - E_m| dt\right). \end{aligned} \quad (37)$$

The analogous statement holds for any $x \leq x_2$.

Proof. According to the Sturm Oscillation Theorem, in any closed interval of length $\frac{\pi}{k}$, $\psi'(x)$ must vanish at least once, and at any such point $g(x) = |\psi(x)| \leq \|\psi\|_{L^\infty(\mathcal{I}_-)}$. We now apply the Theorem, taking into account that the location of the maximum of $|\psi(x)|$ in \mathcal{I}_- is not specified and hence extending the range of the integral to begin at x_1 . \square

The usefulness of (34) is illustrated in Case Study 8.

6. TRANSITION RÉGIME ESTIMATES

In the section we provide a final set of upper bounds on $|\psi(x)|$, which have advantages when $V(x) - E$ is small, which we refer to a the *transition régime*. We begin with the Agmon method, but make different choices of the functions that appear. In particular we will choose $F \equiv 1$ in the basic identities (11)–(12), and choose η to be supported in some region where the negative part of $V - E$ is small. We think of this set as a particular “window” and find that the value of $\psi(x)$ is controlled by its values around the border of the window.

Theorem 6.1. *Consider a region $W \subset \Gamma$ such that for some $\ell > 0$, $B_\ell := \{x \in W : \text{dist}(x, \partial W) \leq \ell\}$. If B_ℓ contains no vertices, then for all $x \in W$ such that $\text{dist}(x, \partial W) \geq \ell$,*

$$|\psi(x)|^2 \leq \left(\frac{1}{\ell^2} \int_{B_\ell} \psi^2 + \int_W (E - V(x))_+ \psi^2 \right) \text{dist}(x, \partial W). \quad (38)$$

Here $z_+ := \max(z, 0)$. An obvious simple upper bound for a normalized eigenfunction is

$$|\psi(x)|^2 \leq \left(\frac{1}{\ell^2} + \max_W (E - V(x))_+ \right) \text{dist}(x, \partial W).$$

Hence, if we can choose ℓ large on a transition régime or we have information that $|\psi|$ is small near its boundary, e.g., because of an Agmon estimate, we are ensured that ψ remains small on the window W .

Proof. We set $F \equiv 1$ in (11)–(12) and choose $\eta(x) = 1$ for $\text{dist}(x, \partial W) \geq \ell$, $\eta(x) = 0$ on W^c , and interpolate with a linear ramp on B_ℓ , hence $|\eta'(x)| = \frac{1}{\ell}$ on B_ℓ . By integrating (11)–(12), we find that

$$\int_W (((\eta(x)\psi(x))')^2 + (V(x) - E)(\eta(x)\psi(x))^2) dx = \frac{1}{\ell^2} \int_{B_\ell} \psi(x)^2 dx. \quad (39)$$

For $x \in W \setminus B_\ell$, choosing a parametrization so that $x = 0$ corresponds to the nearest point on a path to x for which $\eta(0) = 0$, we can write

$$\begin{aligned} \psi(x)^2 &= \left(\int_0^x (\eta(t)\psi(t))' dt \right)^2 \\ &\leq x \int_0^x ((\eta(t)\psi(t))')^2 dt \\ &\leq \text{dist}(x, \partial W) \int_W ((\eta(t)\psi(t))')^2 dt \\ &\leq \text{dist}(x, \partial W) \left(\frac{1}{\ell^2} \int_{B_\ell} \psi(x)^2 dx + \int_W (E - V(x))_+ - \psi(x)^2 dx \right), \end{aligned}$$

as claimed. \square

An alternative on an edge where $|V(x) - E|$ is small and no vertices are encountered, good pointwise control of eigenfunctions can be obtained with Gronwall's inequality. Using the Fundamental Theorem of Calculus we write

$$\psi(x) = \psi(x_0) + (x - x_0)\psi'(x_0) + \int_{x_0}^x (x - t)(V(t) - E)\psi(t)dt,$$

so

$$|\psi(x)| \leq |\psi(x_0) + (x - x_0)\psi'(x_0)| + \int_{x_0}^x (x - t)|V(t) - E||\psi(t)|dt,$$

to which Gronwall's inequality as stated in [19] applies, yielding

$$|\psi(x)| \leq |\psi(x_0) + (x - x_0)\psi'(x_0)| \exp\left(\int_{x_0}^x (x - t)|V(t) - E|dt\right). \quad (40)$$

The bound (40) is of a similar type to (34), one being more useful when $E \gg V(x)$ and the other when $E \approx V(x)$.

7. CASE STUDIES

- (1) Our first two case studies show that a wavefunction ψ can be concentrated to an arbitrarily large extent, even completely, in subsets of \mathcal{C}_E , the part of the graph where $E > V(x)$, while being small or even vanishing in other subsets of \mathcal{C}_E which do not differ in any meaningful way from the sets on which ψ is concentrated. Consider a quantum graph with a constant potential $V = 0$ which includes several circles \mathcal{C}_j of length $2\pi/k$, which have been connected by edges. We assume two edges per circle and use a coordinate system on each \mathcal{C}_j so that the edges connect at $x = 0, \pi$. Letting $E = k^2$, on the j -th circle we can have an eigenfunction $\mu_j \sin(kx)$, which vanishes at the nodal points $x = 0, \pi$. We suppose that the connecting edges are attached at these nodal points and that the eigenfunction equals 0 on every connecting edge. The numbers μ_j can be assigned arbitrarily, showing that there is no control whatsoever of the magnitude of the eigenfunction on a given circle in terms of its values elsewhere! We can even shrink the edges in this example so that pairs of circles are in direct contact.
- (2) As a variant of the previous case study, we show that the problem is not that the eigenfunctions can vanish. On the same graph, let the eigenfunctions have the form $\kappa_j \cos(kx) + \mu_j \sin(kx)$ on the circles \mathcal{C}_j . We equip the connecting edges with any set of Sturm-Liouville eigenfunctions having the eigenvalues k^2 and Neumann conditions at the ends. We choose κ_j to guarantee continuity of the eigenfunctions at the vertices where the circles meet the edges, and observe that the Kirchhoff conditions are satisfied at those vertices by construction.
- (3) It is also possible for an eigenfunction ψ to concentrate on \mathcal{T}_E , the part of the graph where $E < V(x)$, as shown by the example of a half line with a little circle attached at the origin. The potential is a constant on the circle, 0 on $[0, a)$, and some other constant on $[a, \infty)$. The constants and the eigenvalue are chosen so that that

the eigenfunction is constant on the circle. We can take a and the size of the circle small and show explicitly that almost all of the L^2 norm of ψ arises from the part of ψ supported in the tunneling region. In contrast to the situation where $E > V(x)$, however, the magnitude of the eigenfunction must be small in the interior of \mathcal{T}_E , in accordance with Proposition 3.1.

- (4) Since a landscape function is supposed to be an upper bound for *any* eigenfunction of a given value of E , we must accept that some eigenfunctions will be quite small in a region where the appropriate landscape function is large. We recall the analysis of perturbed double-well models, which Simon has called “the flea on the elephant” in [29]. As described in that work, a Schrödinger operator containing a classic double-well potential with a reflection symmetry will have a ground-state eigenfunction that is symmetric and equally concentrated near the bottoms of the two wells, and an anti-symmetric eigenfunction with very nearly the same eigenvalue, likewise equally concentrated near the bottoms of the two wells except for a difference of sign. By making a very small perturbation that is not symmetric, the ground state eigenfunction will be concentrated in only one of the wells, and smaller by an exponential factor in the other well. The next state will be concentrated in the other well, and smaller by an exponential factor in the well where the first eigenfunction resides. Meanwhile, at the level of generality of a landscape function, the upper bounds we wish to create will be virtually the same for the first two eigenfunctions for either the strictly symmetric potential or the slightly perturbed potential. Mathematical details are to be found in [29].
- (5) An oscillatory example. Let us consider $V(x) = \sin(2x)$ on $[-\pi/2, \pi/2]$ and we take periodic boundary conditions so we are effectively on a circle. The Agmon region is therefore on $[0, \pi/2]$. Using (16) and the fact that we are working on S^1 we get that

$$\psi(x) \leq \sqrt{\frac{(x + \pi/4)(3\pi/4 - x)}{\pi}} \frac{2\|\psi\|_{L^2([-\pi/2, 0])}}{\pi/2} \times e^{-\min\{\int_0^x \sqrt{\sin(2t)} dt, \int_x^{\pi/2} \sqrt{\sin(2t)} dt\}}$$

To make sense of this bound we note that $e^{-\min\{\int_0^x \sqrt{\sin(2t)} dt, \int_x^{\pi/2} \sqrt{\sin(2t)} dt\}}$ provides exponential decay into the Agmon region. The square root prefactor $\sqrt{\frac{(x + \pi/4)(3\pi/4 - x)}{\pi}}$ is maximized at $x = \pi/4$ with a maximum value of $\sqrt{\pi}/2$. The remaining factor is double the averaged L^2 norm of ψ on the landscape region.

- (6) Upper bounds based on the maximum principle may or may not include the value of $|\psi|$ at the boundary of the region on which they apply, depending on the sign of W on the boundary in expressions like (26). A case study to illustrate the possible dependence on boundary values can be based on the classic square-well example. Thus let $V(x) = M > 0$ when $|x| > 1$, and $V(x) = 0$ when $|x| \leq 1$. If as in §4 we wish to bound $V(x)$ from below by a convex quadratic,

the symmetric choices would be

$$V(x) \geq b^2(x^2 - 1)$$

on the interval $[-1, 1]$. This is not a positive function, but we can fix that by adding b^2 to V if we likewise replace E by $E + b^2$ in all subsequent formulae.

Since $V(x)$ is symmetric, the eigenfunctions are even or odd, in particular, on $[-1, 1]$ they are proportional to

$$\cos(\sqrt{E}x) \text{ or } \sin(\sqrt{E}x),$$

and they make a C^1 matching with a multiple of

$$\exp(-\sqrt{M - E}x)$$

for $|x| \geq 1$. By a standard calculation of elementary quantum mechanics, the eigenvalues are determined by one of the following conditions

$$\tan(\sqrt{E}) = \sqrt{\frac{M}{E} - 1}$$

or

$$-\cot(\sqrt{E}) = \sqrt{\frac{M}{E} - 1}.$$

As a variant, this example can be modified to a quantum graph by replacing the interval $[-1, 1]$ with n copies of the interval, and imposing Kirchhoff conditions. By again exploiting the symmetry, the eigenfunctions are as before and the eigenvalues are determined by

$$\tan(\sqrt{E}) \text{ or } -\cot(\sqrt{E}) = \frac{1}{n} \sqrt{\frac{M}{E} - 1}.$$

The factor $\frac{1}{n}$ will make no qualitative difference.

The lowest eigenvalue will lie in the interval $(0, \frac{\pi^2}{4})$ (see Figure 2) and by a choice of M can take on any value in this range.

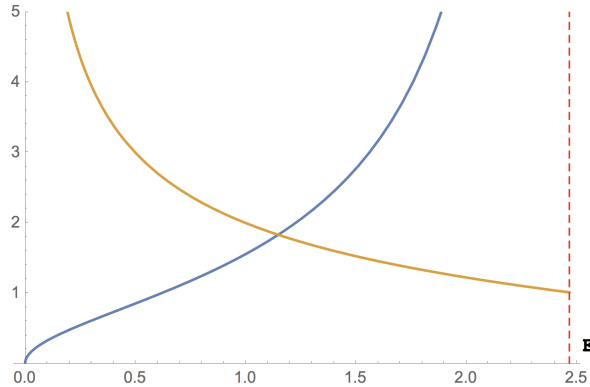


FIGURE 2. The lowest eigenvalue in Case Study 6.

Let us compare the corresponding eigenfunction for fixed values of $x \in [-1, 1]$ with the landscape function of §4, *viz.*,

$$\frac{E + b^2}{b} \left(\frac{1}{2} + e^{-\frac{bx^2}{2}} \right) \|\psi\|_{L^\infty[-1,1]}.$$

Minimizing the first factor with the choice $b = \sqrt{E}$, for a normalized eigenfunction we get

$$\begin{aligned} |\psi(x)| - 2\sqrt{E} \left(\frac{1}{2} + e^{-\frac{\sqrt{E}x^2}{2}} \right) \|\psi\|_{L^\infty[-1,1]} \\ \leq \left(|\psi(1)| - 2\sqrt{E} \left(\frac{1}{2} + e^{-\frac{\sqrt{E}}{2}} \right) \|\psi\|_{L^\infty[-1,1]} \right)_+ \end{aligned}$$

for $x \in [-1, 1]$. Equivalently,

$$|\psi(x)| \leq \max \left((\psi(1) + 2\sqrt{E} \left(e^{-\frac{\sqrt{E}x^2}{2}} - e^{-\frac{\sqrt{E}}{2}} \right)) \|\psi\|_{L^\infty[-1,1]}, \sqrt{E} \left(1 + 2e^{-\frac{\sqrt{E}x^2}{2}} \right) \|\psi\|_{L^\infty[-1,1]} \right). \quad (41)$$

The first choice in the maximum is operative for small E , whereas the second is operative for larger values. For yet larger values of E , however, the uniform bound of Theorem 2.1 is better. The situation is depicted in Figure 3.

- (7) Mathieu functions. Our goal in this case study is to provide evidence that the construction in §4 is of interest for some range of parameter values. The Mathieu equation in standard form is 2π -periodic, and conventionally the coefficient of the cosine potential is denoted $2q$. We shift that upwards to ensure our convention of a nonnegative potential and this consider

$$-\psi'' + 2q(1 + \cos(2x))\psi = E\psi \quad (42)$$

on a circle of length 2π . We note that the tunneling and classically allowed régimes each have two connected components, and therefore construct a global of Υ as in §4 by concatenating truncated Gaussians and adding a constant. We set $q = 10$ and used Mathematica to calculate an even and an odd eigenfunction with eigenvalues computed as 6.0630... and, respectively, 6.0634... In Figure 4 the eigenfunctions are compared with an upper bound of torsion type, using the computed L^∞ norm of the normalized Mathieu eigenfunctions. For comparison, on the intervals where $|x - n\pi| < 1$ an Agmon-type upper bound derived from Theorem 3.1. Here we incorporated the L^2 norm of the Mathieu eigenfunctions on intervals such as $1, \frac{\pi}{3}$, but did not attempt to optimize this interval (used as the support of our η') or other details of the Agmon-type estimate. Meanwhile, the uniform hypercontractive bound of Theorem 2.1 was computed as 1.87124, which in this case is not competitive with the other upper bounds.

Although this case study does not have vertices, since the odd Mathieu eigenfunction has zeroes at 0 and π , we could attach an edge, or even a complicated graph, linking these two points on the

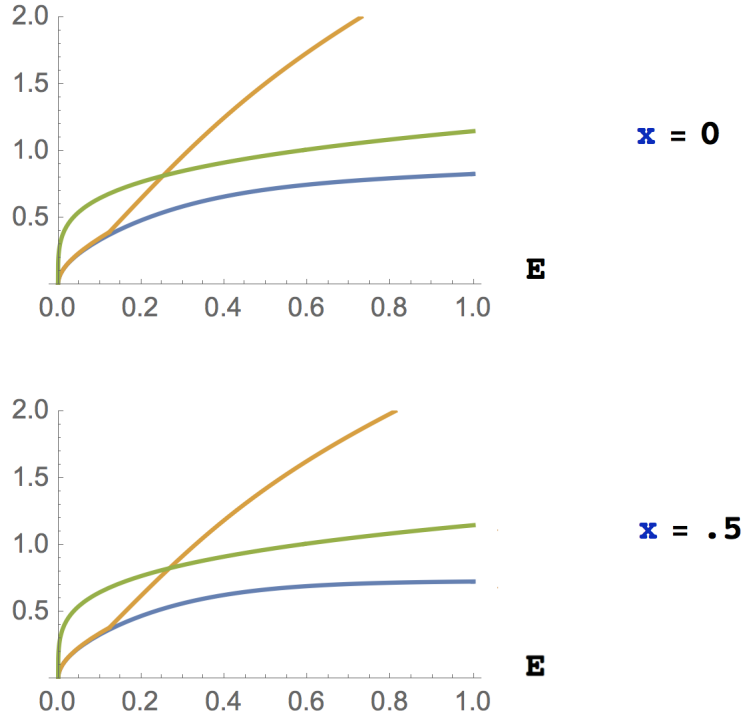


FIGURE 3. Landscape bounds for Case Study 6 with two fixed values of x as functions of E , calculated with *Mathematica*. The eigenfunction is in blue, a torsion-type bound in gold, and the uniform bound from Theorem 2.1 in green. In illustrating the torsion-type bound we have used the maximum of the exact eigenfunction and its value at $x = 1$ (both of which can be calculated in closed form in terms of E), rather than approximations.

circle and extend that ψ by 0, converting this into an example on a more complex graph.

- (8) Our final case study shows the kind of eigenfunction control that can be achieved when $E - V(x)$ is large and an edge is long enough for the eigenfunction to oscillate many times. In this situation the best options are the bounds of Theorem 2.1 (uniform) and 5.1 (with an exponential integral). Consider a regular tetrahedral graph with four edges of length 2π . On three edges connected to the top vertex we will place a large, positive constant potential, while on each of the other three edges we place a Mathieu potential of the same type as in Case Study 7, with coordinate $x = 0$ at the centers of the latter edges. Using the symmetries of the tetrahedron, we can find some explicit eigenfunctions (with some constants determined numerically), consisting of hyperbolic cosines on the edges connecting to the top vertex and even-symmetry Mathieu functions on the

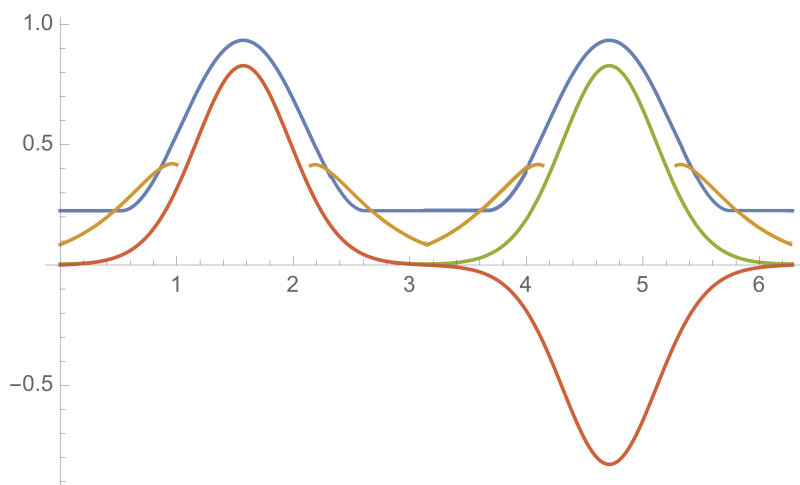


FIGURE 4. The first two Mathieu eigenfunctions for $q = 10$ (green and red), along with landscape bounds using a simplified torsion function (blue) and Agmon's method (gold) (Case Study 7), calculated with *Mathematica*. In the torsion-type bound we have used a numerical calculation of the maximum of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

other edges. Some Mathieu parameter values for which this is possible turned out to be $q = 10$, $E = 72$ and the even more highly oscillatory $q = 5$, $E = 300$. As shown in Figures 5 and 6, when E is only a few times the maximum value of the potential (72 vs. $2q = 20$), these upper bounds are of the right order of magnitude but rather crude, whereas the variable bound becomes much tighter when the ratio of E to the maximum value of the potential is made larger (300 vs. $2q = 10$).

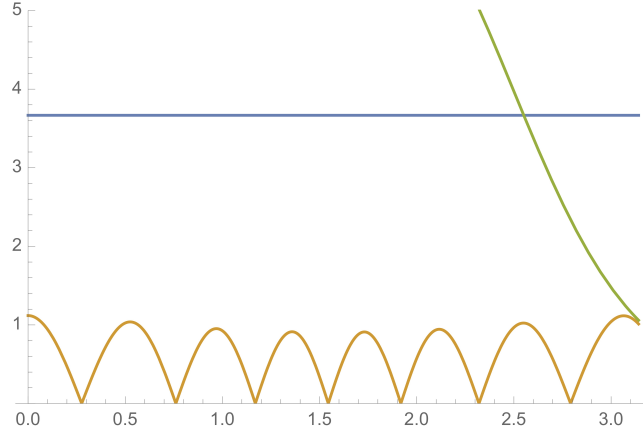


FIGURE 5. An even Mathieu-type eigenfunction on an edge of a tetrahedron, with $q = 10$, $E = 72$ (red), along with the uniform upper bound of Theorem 2.1 and the upper bound from Theorem 5.1 (green). (Case Study 8).

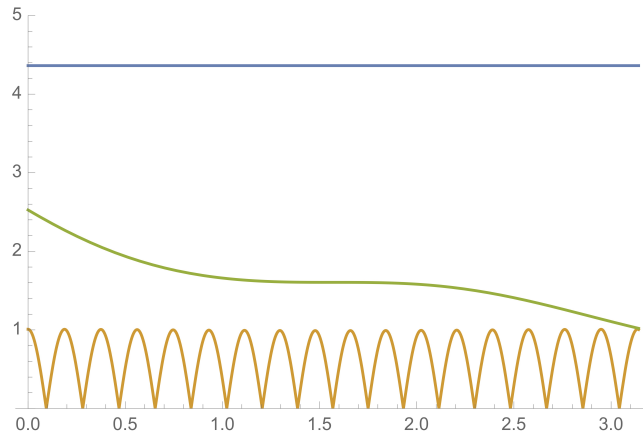


FIGURE 6. An even Mathieu-type eigenfunction on an edge of a tetrahedron, with $q = 5$, $E = 300$ (red), along with the uniform upper bound of Theorem 2.1 and the upper bound from Theorem 5.1 (green). (Case Study 8).

Figures 5 and 6 depict the eigenfunctions on the outer edges of the tetrahedral model, along with the associated uniform upper bound and the upper bound of Theorem 5.1. Since the eigenfunctions are even, only the interval $[0, \pi]$ is shown on the edge, which has total length 2π .

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