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An Agmon estimate for Schrödinger operators on graphs

Stefan Steinerberger[1]

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Abstract
The Agmon estimate shows that eigenfunctions of Schrödinger operators, $-\Delta\phi + V\phi = E\phi$, decay exponentially in the 'classically forbidden' region where the potential exceeds the energy level $\{x : V(x) > E\}$. Moreover, the size of $|\phi(x)|$ is bounded in terms of a weighted (Agmon) distance between x and the allowed region. We derive such a statement on graphs when $-\Delta$ is replaced by the graph Laplacian $L = D - A$: we identify an explicit Agmon metric and prove a pointwise decay estimate in terms of the Agmon distance.

Keywords Agmon estimate · Agmon metric · Schrödinger operator · Graph

Mathematics Subject Classification 31B15 · 35J10 · 35R02

1 Introduction: Agmon estimates

Let $V : \mathbb{R}^n \rightarrow \mathbb{R}$ be a nonnegative potential growing at infinity, i.e., $V(x) \rightarrow \infty$ as $\|x\| \rightarrow \infty$. Agmon estimates are concerned with eigenfunctions of the Schrödinger operator $-\Delta + V$: we study functions $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$ satisfying

$$-\Delta\phi + V\phi = E\phi,$$

where $E \in \mathbb{R}$ is the eigenvalue. Multiplying with ϕ and integrating by parts,

$$\int_{\mathbb{R}^n} |\nabla\phi|^2 dx + \int_{\mathbb{R}^n} V(x) \cdot \phi(x)^2 dx = \int_{\mathbb{R}^n} E \cdot \phi(x)^2 dx.$$

This identity implies that most of the L^2-mass should be contained in the 'allowed' region $\{x \in \mathbb{R}^n : V(x) \leq E\}$ and only very little mass can be in the 'forbidden' region

✉ Stefan Steinerberger
steinerb@uw.edu

1 Department of Mathematics, University of Washington, Seattle, WA 98195, USA

$\{x \in \mathbb{R}^n : V(x) > E\}$. The celebrated Agmon estimate [1] shows that this is indeed the case and, moreover, that ϕ decays exponentially in terms of the distance from the allowed region for a suitable notion of distance. Agmon's estimate can be derived from an explicit integral identity. One way of motivating the estimate (taken from a summary of Deift [8]) is as follows: if

$$-\Delta\phi + V\phi = E\phi,$$

then for any (sufficiently regular) $g : \mathbb{R}^n \to \mathbb{R}$

$$\int_{\mathbb{R}^n} \left|\nabla(e^g\phi)\right|^2 \mathrm{d}x + \int_{\mathbb{R}^n} \left(V - E - |\nabla g|^2\right) e^{2g}\phi^2 \mathrm{d}x = 0.$$

Ignoring the first (positive) term, this implies

$$\int_{\mathbb{R}^n} \left(V - E - |\nabla g|^2\right) e^{2g}\phi^2 \mathrm{d}x \leq 0.$$

We note that e^{2g} and ϕ^2 are positive, $V - E - |\nabla g|^2$ is negative in the allowed region and positive in the forbidden region provided $|\nabla g|$ is sufficiently small. The inequality then naturally implies that there cannot be too much L^2-mass of ϕ in the forbidden region except this is now coupled with an additional exponentially growing term e^{2g}. The statement becomes stronger, the larger we make g; however, we want to maintain the nonnegativity of $V - E - |\nabla g|^2$ in the forbidden region. This then suggests a way of defining g: the *Agmon metric* associated with the energy level E between two points $x, y \in \mathbb{R}^n$ is given as the minimum energy taken

$$\rho_E(x, y) = \inf_{\gamma} \int_0^1 \max\left(\sqrt{V(\gamma(t)) - E}, 0\right) |\dot{\gamma}(t)| \mathrm{d}t,$$

where $\gamma : [0, 1] \to \mathbb{R}^n$ ranges over all paths from $\gamma(0) = x$ to $\gamma(1) = y$. The integral identity can then be used (see for example Carmona and Simon [6]) to derive pointwise statements in the forbidden region along the lines of that for all $\varepsilon > 0$

$$|\phi(x)| \leq c_\varepsilon \sup_{\substack{y \in \mathbb{R}^n \\ V(y) \leq E}} e^{-(1-\varepsilon)\rho_E(x,y)}.$$

We refer to Aizenman and Simon [2], Carmona [5], Dimassi and Sjöstrand [9], Helffer [13], Helffer and Sjöstrand [14, 15], Hislop [16], Simon [23, 24] and references therein for a more complete picture regarding Agmon's estimate in the continuous setting. Our paper is partially inspired by a recent probabilistic approach to obtain sharp pointwise Agmon estimates in the continuous setting [25].

2 An Agmon estimate on graphs

2.1 Setup

Let $G = (V, E)$ be a finite, connected graph with $V = \{v_1, \dots, v_n\}$. We introduce the diagonal matrix $D \in \mathbb{R}^{n \times n}$ satisfying $d_{ii} = \deg(v_i)$ and the adjacency matrix $A \in \mathbb{R}^{n \times n}$ given by

$$A_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{otherwise.} \end{cases}$$

There is a natural notion of a discrete Laplacian acting on functions $f : V \to V$ given by the linear operator $L = D - A \in \mathbb{R}^{n \times n}$. We observe that L can be interpreted as the discrete analogue of $-\Delta$ as both are positive semi-definite and allow for integration by parts: for $f : V \to \mathbb{R}$

$$\langle f, Lf \rangle = \sum_{(v_i, v_j) \in E} (f(v_i) - f(v_j))^2.$$

Given an arbitrary potential $W : V \to \mathbb{R}$, our goal is to understand the behavior of eigenfunctions $\phi : V \to \mathbb{R}$ satisfying

$$L\phi + W\phi = E\phi$$

for some eigenvalue $E \in \mathbb{R}$. Multiplying with ϕ and integrating by parts

$$\sum_{(v_i, v_j) \in E} (\phi(v_i) - \phi(v_j))^2 + \sum_{v \in V} W(v) \cdot \phi(v)^2 = \sum_{v \in V} E \cdot \phi(v)^2.$$

This suggests, just as in the continuous case above, that there should be relatively little ℓ^2-mass in the ‘classically forbidden’ region $\{v \in V : W(v) > E\}$. The question is now whether, just as in the continuous case, one can expect exponential decay in the forbidden region and how this can be quantified.

2.2 Main result

We define a notion of Agmon distance $\rho_E : V \to \mathbb{R}$ as the cost of the cheapest path starting in $v \in V$ and ending in any arbitrary vertex in the allowed region where ‘cheap’ refers to an explicit cost function on V depending on the potential W, the energy E and the degree of the vertex. Formally,

$$\rho_E(v) = \inf \left\{ \sum_{i=1}^{\ell} \log\left(1 + \frac{(W(v_i) - E)_+}{\deg(v_i)}\right) : v = v_1 \to \cdots \to v_\ell \text{ and } W(v_\ell) \le E \right\},$$

where the infimum is taken over all paths that start in v and end in a vertex v_ℓ in the allowed region. As usual, $(W(v_i) - E)_+ = \max\{W(v_i) - E, 0\}$. Note that $\rho_E \equiv 0$ in the allowed region and $\rho_E > 0$ in the forbidden region.

Theorem *We have, for all $v \in V$,*

$$|\phi(v)| \le e^{-\rho_E(v)} \cdot \|\phi\|_{\ell^\infty}.$$

The maximum principle shows that $|\phi|$ assumes its maximum in the allowed region and thus $\|\phi\|_{\ell^\infty} = \|\phi\|_{\ell^\infty(W(v)\le E)}$. Since $\rho_E \equiv 0$ in the allowed region, the inequality is sharp in the maximum and the implicit constant 1 in front cannot be improved any further. In terms of the exponential decay, there are graphs where the inequality is asymptotically optimal: such examples are constructed in §3.2.

2.3 Related results

There is relatively little work regarding Agmon estimates on graphs. However, we emphasize one recent result which is close in spirit to our result. Filoche, Mayboroda and Tao [11] study eigenvector localization for a fairly general class of matrices $A \in \mathbb{R}^{n\times n}$. They obtain an integrated exponential estimate in terms of an explicit Agmon-type distance. Considering $A = D - A + W$ and $u = (1, 1, \dots, 1)$ in their approach, one arrives at a notion of distance

$$\rho(v, w) = \inf \left\{ \sum_{i=1}^{\ell} \log \left(1 + \sqrt[4]{(W(v_i) - E)_+ (W(v_{i+1}) - E)_+} \right) \right\},$$

where the infimum ranges over all paths that start in $v = v_1$ and end in $w = v_{\ell+1}$ (and, as in our approach, traveling through the allowed region is free which we suppress in the equation above for simplicity of exposition). This is very similar in flavor to our distance above: using this, they then obtain an integrated estimate also involving a landscape-type potential $A^{-1}\mathbf{1}$ [11, Theorem 2.5] as well as more general integrated estimates [11, Theorem 2.7]. A main difference is the dependency on the degree of a vertex which is locally built into our distance while arising in the integrated estimates of [11] more globally (somewhat unsurprisingly: integrated estimates themselves are global). Both our estimate and the estimates in [11] are complementary: which one ends up being better will depend (among other things) on whether there is a lot of variation in the degrees of the vertices.

There is also a recent work of Keller and Pogorzelski [18] who study Agmon estimates in the more general setting of weighted, infinite graphs where the Agmon distance is given in terms of Hardy weights. There is a philosophical overlap with work of Dodziuk [10]. We also note the work of Akduman and Pankov [3, 4] on metric graphs, the work of Harrell and Maltsev [12] on quantum graphs, Damanik, Fillman and Sukhtaiev [7] on tree graphs, results of Hua and Lu [17] and Wojciechowski [27] as well as work of Klein and Rosenberger [19, 20], Mandich [22] and Wang and Zhang [26] on $\mathbb{Z}^d$.

3 Proof

3.1 Proof of the Theorem

Proof Note first that the eigenfunction satisfies

$$(D - A)\phi = (E - W)\phi.$$

Considering this linear system of equations in a fixed vertex $u \in V$ one obtains

$$\deg(u)\phi(u) - \sum_{(u,w)\in E} \phi(w) = (E - W(u))\phi(u).$$

This equation can be rewritten as

$$\left[1 + \frac{W(u) - E}{\deg(u)}\right]\phi(u) = \frac{1}{\deg(u)} \sum_{(u,w)\in E} \phi(w).$$

We observe that if $\phi(u) = 0$, then the theorem is trivially true in u. It thus suffices to prove it for vertices $u \in V$ where $\phi(u) \neq 0$. Note, moreover, that in the forbidden region $\{u \in V : W(u) > E\}$, one trivially has

$$1 + \frac{W(u) - E}{\deg(u)} \geq 1$$

and thus, for $u \in V$ in the forbidden region, it is possible to divide and

$$\phi(u) = \left[1 + \frac{W(u) - E}{\deg(u)}\right]^{-1} \frac{1}{\deg(u)} \sum_{(u,w)\in E} \phi(w).$$

Taking absolute values on both sides, we have

$$\begin{aligned} |\phi(u)| &\leq \left[1 + \frac{W(u) - E}{\deg(u)}\right]^{-1} \frac{1}{\deg(u)} \sum_{(u,w)\in E} |\phi(w)| \\ &\leq \left[1 + \frac{W(u) - E}{\deg(u)}\right]^{-1} \max_{(u,w)\in E} |\phi(w)|. \end{aligned}$$

Since $\phi(u) \neq 0$, we deduce

$$\max_{(u,w)\in E} |\phi(w)| > |\phi(u)|.$$

We can now move from u to its neighbor w maximizing $|\phi(w)|$ and then apply the very same argument again in w. The argument can be applied iteratively as long as the new vertex is still in the forbidden region. Note that $|\phi|$ is increasing along the way which implies that the arising path can never cross itself and must eventually end up in the allowed region $\{v \in V : W(v) \leq E\}$. Altogether, this results in a path

$$u = v_1 \to v_2 \to \cdots \to v_m \to v_{m+1} \quad \text{where} \quad W(v_{m+1}) \leq E$$

since otherwise the path could be further extended. Collecting all the factors

$$\begin{aligned}|\phi(u)| &\leq \left(\prod_{i=1}^{m}\left[1+\frac{W(v_i)-E}{\deg(v_i)}\right]^{-1}\right)\cdot|\phi(v_{m+1})| \\ &\leq \left(\prod_{i=1}^{m}\left[1+\frac{W(v_i)-E}{\deg(v_i)}\right]^{-1}\right)\cdot\|\phi\|_{\ell^\infty}\end{aligned}$$

Note that

$$\prod_{i=1}^{m}\left[1+\frac{W(v_i)-E}{\deg(v_i)}\right]^{-1} = \exp\left(-\sum_{i=1}^{m}\log\left(1+\frac{W(v_i)-E}{\deg(v_i)}\right)\right).$$

By definition of ρ_E, we have

$$\exp\left(-\sum_{i=1}^{m}\log\left(1+\frac{W(v_i)-E}{\deg(v_i)}\right)\right) \leq \exp\left(-\rho_E(v_1)\right)$$

and this concludes the proof. □

Remark We note that the final estimate in the argument implies

$$|\phi(u)| \leq \exp\left(-\sum_{i=1}^{m}\log\left(1+\frac{W(v_i)-E}{\deg(v_i)}\right)\right)\cdot|\phi(w_{m+1})|$$

for any path starting in $u = v_1$ and ending in the vertex v_{m+1} in the allowed region. This would imply a slightly refined estimate where one is not only interested in minimizing the Agmon metric but also wants to end up in a vertex in the allowed region such that $|\phi(w_{m+1})|$ is not too small.

Remark We quickly note a part in the derivation where the argument can be lossy: the main inequality is

$$\begin{aligned}|\phi(u)| &\leq \left[1+\frac{W(u)-E}{\deg(u)}\right]^{-1}\frac{1}{\deg(u)}\sum_{w\sim u}|\phi(w)| \\ &\leq \left[1+\frac{W(u)-E}{\deg(u)}\right]^{-1}\max_{(u,w)\in E}|\phi(w)|.\end{aligned}$$

This inequality could also be interpreted as a type of martingale inequality and can be exploited in this sense. Let us define a sequence of random vertices given by $X_0 = u$ and such that X_{k+1} is a randomly chosen neighbor of X_k and that this random walk is continued until $W(X_k) \leq E$. We will denote the smallest such k by the stopping time τ. Assume furthermore that

$$\frac{W(u) - E}{\deg(u)} \geq \delta \qquad \text{for all } u \in V \text{ in the forbidden region.}$$

An iterative application of the inequality then implies

$$|\phi(u)| \leq \left(\sum_{\ell=0}^{\infty} \frac{\mathbb{P}(\tau = \ell)}{(1+\delta)^{\ell}} \right) \cdot \|\phi\|_{\ell^\infty}.$$

We note that this inequality can lead to improved results in settings where a random walk needs a very long time before arriving in the allowed region. Observe that the sum can be interpreted as an exponential moment $\mathbb{E} \exp(\tau/(\delta+1))$ of the stopping time τ which is a well-studied object. We refer to [25] for the derivation of Agmon estimates via this more stochastic perspective in the continuous setting.

3.2 An Example

The purpose of this section is to construct a graph where the inequality is nearly sharp. One example of such graphs is given by $q-$regular trees of a certain depth where the final layer of vertices is then additionally connected to another vertex v_* (see Fig. 1, for an example). We consider the potential given by $W(v_*) = 0$ and, for all other vertices $v \neq v_*$, we choose the potential to be constant and $W(v) = W \gg q^k \gg 1$ for some very large constant $W \in \mathbb{R}$ where k is the depth of the tree. The function we will consider is the first eigenfunction of $L + W$.

By Rayleigh–Ritz, the smallest eigenvalue of $-\Delta + W$ satisfies

$$\lambda_1 = \inf_{f: V \to \mathbb{R}} \frac{\sum_{(v_i, v_j) \in E} (f(v_i) - f(v_j))^2 + \sum_{v \in V} W(v) f(v)^2}{\sum_{v \in V} f(v)^2}.$$

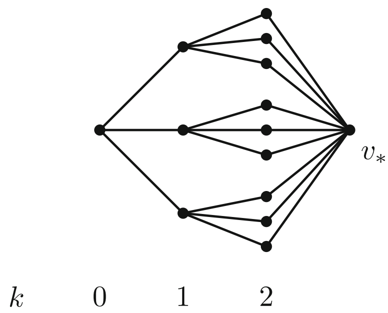

Fig. 1 A $q-$regular tree (here, $q = 3$) of depth k (here, $k = 2$) with final layer being connected to a single additional vertex v_*

Taking $f : V \to \mathbb{R}$ given by $f(v_*) = 1$ and $f(v) = 0$ for all $v \neq v^*$, we deduce that

$$E = \lambda_1 \leq q^k \qquad \text{independently of } W.$$

We can now use the equation

$$\phi(u) = \frac{E - W(u)}{\deg(u)} \phi(u) + \frac{1}{\deg(u)} \sum_{w \sim u} \phi(w)$$

and we shall restrict its use to vertices in the $q-$regular tree. The value of ϕ then only depends on the level. We shall therefore write $\phi(v) = \phi_i$ whenever the vertex v is in the $i-$th level where $1 \leq i \leq k - 1$ (the case $i = 0$ and $i = k$ will be ignored since the algebra is slightly different). The equation then simplifies to

$$\phi_i = \frac{\lambda_1 - W}{q + 1} \phi_i + \frac{1}{q + 1} (q \cdot \phi_{i+1} + \phi_{i-1}).$$

This can be rewritten as

$$(W - \lambda_1 + q + 1) \cdot \phi_i = q \cdot \phi_{i+1} + \phi_{i-1}.$$

For fixed q and $W \gg q^k \geq E$, this implies that approximately $\phi_i \sim (q/W) \cdot \phi_{i+1}$ as $W \to \infty$ which implies exponential decay. Conversely, we have

$$\log\left(1 + \frac{W - E}{\deg(v)}\right) \sim \log\left(\frac{W}{q}\right)$$

which implies, to leading order, the same kind of decay.

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Declarations

Conflict of interest There are no associated data produced and there are no conflicts of interest to declare.

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