The landscape of Anderson localization in a disordered medium

Marcel Filoche and Svitlana Mayboroda

Abstract. In quantum systems, the presence of a disordered potential may induce the appearance of strongly localized quantum states (called Anderson localization), i.e., eigenfunctions that essentially "live" in a very restricted subregion of the entire domain. We show here that solving a simple Dirichlet problem reveals a network of interconnected lines which are the boundaries of the localization subregions, and allows one to evaluate the strength of the confinement to these subregions. For each given eigenvalue, only a subset of this network effectively determines the confinement of the corresponding eigenfunction. This subset becomes smaller as the eigenvalue increases, leading to a weaker confinement and finally possibly delocalized states.

1. Introduction

Physical systems characterized by a spatial inhomogeneity of the material or by an irregular or disordered geometry exhibit specific vibrating properties, not found in usual smooth or homogeneous systems. In particular, the stationary vibrations, i.e., the eigenfunctions of the corresponding wave operator, can have extremely uneven spatial distributions of their amplitude. More precisely, for some eigenvalues (or frequencies), most of the vibration energy is concentrated only in one very restricted subregion of the entire domain and remains very low in the rest of the domain [**HS**]. Although still poorly understood, this phenomenon, called *localization*, has been observed in acoustical, optical, mechanical, and quantum systems, and plays an essential role in numerous physical properties [**ERRPS, FAFS, RBVIDCW**].

A particular case of localization introduced in 1958 by Anderson [**A**] is the *disorder-induced* localization. It occurs in systems in which the properties of the material vary spatially. For a large enough amplitude of the variation (i.e. for a sufficiently large disorder), the eigenfunctions of the wave operator are strongly localized inside the system; they mostly "live" in a very small subregion and their

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amplitudes decay exponentially away from this region. In quantum systems it implies that the corresponding electronic states in a disordered enough potential are non conducting, even though the system exhibits statistical translational invariance.

Despite vast literature and numerous important results, many features of the localization of eigenfunctions remain mysterious. In particular, it seems very difficult to predict where to expect localized vibrations, and for which eigenvalues, without having to solve the full eigenvalue problem. We will address in this paper the case of Anderson localization of quantum states, and demonstrate that one can in fact predict the localization subregions by solving only one Dirichlet problem. Further related results can be found in [**FM**].

2. Preliminaries

2.1. The quantum states. The stationary quantum states of a particle in a domain Ω are the eigenfunctions of the Hamiltonian $H = -\dfrac{\hbar^2}{2m}\,\Delta + V$ in the domain, where m stands for the mass of the particle and $V(x)$ is the potential function describing the external forces acting on the particle. The eigenvalues of the Hamiltonian correspond to the energies of these states. The electronic states inside a disordered medium can thus be modeled by introducing a random potential V to account for the material inhomogeneities. For instance, the domain Ω can be divided into elementary cells on which V is piecewise constant. The value of V on each cell is taken at random, uniformly between 0 and a maximum value V_{max}. The goal of this paper is to study the spatial distributions of the localized states in such a potential.

In what follows, we will first present the main inequalities and their proofs in the context of a general second order elliptic operator with bounded measurable coefficients, and in numerical experiments we will come back to quantum mechanics in a disordered medium and, respectively, to the Hamiltonian H.

2.2. The wave operator. Let L be a divergence form elliptic operator or an elliptic system with bounded measurable coefficients. For the sake of simplicity we shall work here with the second order symmetric operators with real-valued coefficients, which already include the main examples in the focus of the present paper: the Laplacian, the Hamiltonian, and their non-homogeneous analogues. It is worth mentioning, however, that an appropriate version of the key inequalities remains valid for much more general elliptic operators, with complex coefficients and/or of higher order.

To this end, let Ω be a bounded open set in $\mathbb{R}^n$ and denote

$$L = -\mathrm{div}\, A(x)\nabla + V(x), \tag{2.1}$$

where A is an elliptic real symmetric $n \times n$ matrix with bounded measurable coefficients, that is,

$$A(x) = \{a_{ij}(x)\}_{i,j=1}^n,\ x \in \Omega, \quad a_{ij} \in L^\infty(\Omega), \quad \sum_{i,j=1}^n a_{ij}(x)\xi_i\xi_j \geq c|\xi|^2,\ \forall\, \xi \in \mathbb{R}^n, \tag{2.2}$$

for some $c > 0$, and $a_{ij} = a_{ji}$, $\forall i, j = 1, ..., n$, and $V \in L^\infty(\Omega)$ is a non-negative function. The action of the operator L in (2.1) is understood, as usually, in the weak sense. Indeed, recall that the Lax-Milgram Lemma ascertains that for every $f \in (\mathring{H}^1(\Omega))^* =: H^{-1}(\Omega)$ the boundary value problem

$$Lu = f, \quad u \in \mathring{H}^1(\Omega), \tag{2.3}$$

has a unique solution such that

$$\int_{\mathbb{R}^n} (A\nabla u\, \nabla v + Vuv)\, dx = \int_{\mathbb{R}^n} fv\, dx, \quad \text{for every} \quad v \in \mathring{H}^1(\Omega). \tag{2.4}$$

Here $\mathring{H}^1(\Omega)$ is the Sobolev space of functions given by the completion of $C_0^\infty(\Omega)$ in the norm

$$\|u\|_{\mathring{H}^1(\Omega)} := \|\nabla u\|_{L^2(\Omega)}. \tag{2.5}$$

For later reference, we also define the Green function of L, as conventionally, by

$$L_x G(x,y) = \delta_y(x), \quad \text{for all}\, x, y \in \Omega, \quad G(\cdot, y) \in \mathring{H}^1(\Omega) \quad \text{for all}\, y \in \Omega, \tag{2.6}$$

in the sense of (2.4), so that

$$\int_{\mathbb{R}^n} L_x G(x,y) v(x)\, dx = v(y), \quad y \in \Omega, \tag{2.7}$$

for every $v \in \mathring{H}^1(\Omega)$.

Remark. The solution given by the Lax-Milgram Lemma can be thought of as a solution of the Dirichlet problem with zero boundary data, and for relatively nice domains it can be shown that u is a *classical* solution:

$$-\Delta u = f \quad \text{in} \quad \Omega, \qquad u|_{\partial\Omega} = 0, \tag{2.8}$$

where $u|_{\partial\Omega}$ denotes the pointwise limit at the boundary, i.e.,

$$u(x) = \lim_{y \to x,\ y \in \Omega} u(y), \quad x \in \partial\Omega. \tag{2.9}$$

In principle, on "bad" domains the definition (2.9) might not make sense, i.e., such a limit might not exist, and then the solution can only be interpreted in the sense of (2.4). For the Laplacian, and all homogeneous second order operators with bounded measurable coefficients as above it is known which domain are "good" and which are "bad", due to the 1924 Wiener criterion and its generalization by Littman, Stampacchia and Weinberger [**W**], [**LSW**]. The gist of the matter is that the boundary should not have too sharp inward cusps, cracks or isolated points.

3. The control inequalities

3.1. Control of the eigenfunctions by the solution to the Dirichlet problem. Having at hand (2.3)–(2.4), one can consider the eigenvalue problem:

$$L\varphi = \lambda\varphi, \quad \varphi \in \mathring{H}^m(\Omega), \tag{3.1}$$

where $\lambda \in \mathbb{R}$. If for a given $\lambda \in \mathbb{R}$ there exists a non-trivial solution to (3.1), interpreted, as before, in the weak sense, then the corresponding λ is called an eigenvalue and $\varphi \in \mathring{H}^1(\Omega)$ is an eigenvector. Under the assumptions on the operator imposed in the previous section (which, in particular, yield self-adjointness), the standard methods of functional analysis directly apply to show that the eigenvalues of L form a positive sequence going to $+\infty$, and the eigenfunctions of L define a Hilbert basis of $L^2(\Omega)$ (cf. [**E**], [**H**]).

Proposition 3.1. *Let L be an arbitrary elliptic operator as defined by* (2.1) – (2.5)*, and assume that λ is an eigenvalue L and $\varphi \in \mathring{H}^m(\Omega)$ is the corresponding eigenfunction, i.e.,* (3.1) *is satisfied. Then for every $x \in \Omega$*

$$\frac{|\varphi(x)|}{\|\varphi\|_{L^\infty(\Omega)}} \leq \lambda u(x), \quad \textit{for all}\, x \in \Omega, \tag{3.2}$$

where u is the solution of the boundary problem

$$Lu = 1, \quad u \in \mathring{H}^m(\Omega). \tag{3.3}$$

Proof. By (3.1) and (2.6) (with the roles of x and y interchanged), for every $x \in \Omega$

$$\varphi(x) = \int_\Omega L_y \varphi(y)\, G(x,y)\, dy = \int_\Omega \lambda\, \varphi(y)\, G(x,y)\, dy, \tag{3.4}$$

and hence,

$$|\varphi(x)| \leq \lambda\, \|\varphi\|_{L^\infty(\Omega)} \int_\Omega |G(x,y)|\, dy, \quad x \in \Omega. \tag{3.5}$$

The Green function is positive in Ω and eigenfunctions are bounded for all second order elliptic operators (2.1) in all dimensions due to the strong maximum principle (see, e.g., [**GT**], Section 8.7). Hence,

$$\int_\Omega |G(x,y)|\, dy = \int_\Omega G(x,y) \cdot 1\, dy, \quad x \in \Omega, \tag{3.6}$$

which is by definition a solution of (3.3). □

The inequality (3.2) provides the "landscape of localization", as the map of u in (3.2) draws the lines separating potential subdomains. The exact meaning of this statement is to be clarified below.

3.2. Analysis of localized modes on the subdomains. The gist of the forthcoming discussion is that, roughly speaking, a mode of Ω localized to a subdomain $D \subset \Omega$ must be fairly close to an eigenmode of this subdomain, and an eigenvalue of Ω for which localization takes place, must be close to some eigenvalue of D.

Assume that φ is one of the eigenmodes of Ω, which exhibits localization to D – a subdomain of Ω. This means, in particular, that the boundary values of φ on ∂D are small. The "smallness" of φ on the boundary of D is to be interpreted in the sense that an L-harmonic function, with the same data as φ on ∂D, is small. More precisely, let us define $\varepsilon = \varepsilon_\varphi > 0$ as

$$\begin{aligned} &\varepsilon = \|v\|_{L^2(D)}, \text{ where } v \in H^1(D) \text{ is such that} \\ &w := \varphi - v \in \mathring{H}^1(D) \text{ (that is, } \varphi \text{ and } v \text{ on } \partial D \text{ coincide),} \\ &\text{and } Lv = 0 \text{ on } D \text{ in the sense of distributions.} \end{aligned} \tag{3.7}$$

Proposition 3.2. *Assume that Ω is an arbitrary bounded open set and that L is an elliptic operator defined in* (2.1) – (2.5)*. Let $\varphi \in \mathring{H}^1(\Omega)$ be one of the eigenfunctions of L in Ω and denote by λ the eigenvalue corresponding to φ. Suppose further that D is a subset of Ω and denote by ε the norm of the boundary data of φ on ∂D in the sense of* (3.7)*. Then either λ is an eigenvalue of D or*

$$\|\varphi\|_{L^2(D)} \leq \left(1 + \frac{\lambda}{d_D(\lambda)}\right) \varepsilon \tag{3.8}$$

Here, $d_D(\lambda)$ is the distance from λ to the spectrum of the operator L in the subregion D (defined as: $d_D(\lambda) = \min_{\lambda_{k,D}} \{|\lambda - \lambda_{k,D}|\}$, the minimum being taken over all eigenvalues $(\lambda_{k,D})$ of L in D).

PROOF. If λ is the eigenvalue of L in Ω corresponding to φ, then we have

$$(L - \lambda)w = \lambda v \quad \text{on } D, \tag{3.9}$$

as usually, in the sense of distributions.

Whenever λ is, in addition, an eigenvalue of a subdomain D, there is nothing to prove. Otherwise we proceed as follows. The eigenfunctions of L on D, $\{\psi_k\}$, form an orthogonal basis of $L^2(D)$. In particular, for every $f \in L^2(D)$ there are constants $c_k(f)$ such that $f = \sum_k c_k(f)\psi_k$ in $L^2(D)$ and $\|f\|_{L^2(D)} = \left(\sum_k c_k(f)^2\right)^{1/2}$. Therefore, for every λ not belonging to the spectrum of L on D and for every $f \in L^2(D)$

$$\begin{aligned} \|(L-\lambda)f\|_{L^2(D)} &= \left\|(L-\lambda)\sum_k c_k(f)\psi_k\right\|_{L^2(D)} = \left\|\sum_k (\lambda_k(D) - \lambda)c_k(f)\psi_k\right\|_{L^2(D)} \\ &= \left(\sum_k (\lambda_k(D)-\lambda)^2 c_k(f)^2\right)^{1/2} \\ &\geq \min_k |\lambda_k(D) - \lambda| \left(\sum_k c_k(f)^2\right)^{1/2} \\ &= \min_k |\lambda_k(D) - \lambda| \, \|f\|_{L^2(D)}, \end{aligned} \tag{3.10}$$

which leads to

$$\|w\|_{L^2(D)} = \|(L-\lambda)^{-1}\lambda v\|_{L^2(D)} \leq \max_{\lambda_k(D)} \left\{\frac{1}{|\lambda - \lambda_k(D)|}\right\} \|\lambda v\|_{L^2(D)}, \tag{3.11}$$

where the maximum is taken over all eigenvalues of L in D.

Going further, (3.11) yields

$$\|w\|_{L^2(D)} \leq \max_{\lambda_k(D)} \left\{\left|1 - \frac{\lambda_k(D)}{\lambda}\right|^{-1}\right\} \|v\|_{L^2(D)} \leq \max_{\lambda_k(D)} \left\{\left|1 - \frac{\lambda_k(D)}{\lambda}\right|^{-1}\right\} \varepsilon, \tag{3.12}$$

and therefore,

$$\|\varphi\|_{L^2(D)} \leq \left(1 + \max_{\lambda_k(D)} \left\{\left|1 - \frac{\lambda_k(D)}{\lambda}\right|^{-1}\right\}\right) \varepsilon. \tag{3.13}$$

The inequality (3.13) then immediately yields (3.8). □

The presence of $d_D(\lambda)$ in the denominator of the right-hand side of Eq. (3.8) assures that whenever λ is *far* from any eigenvalue of L in D in relative value, the norm of φ in the entire subregion, $\|\varphi\|_{L^2(D)}$, has to be smaller than $2\|\varepsilon\|$. Consequently, such a mode φ is expelled from D and must "live" in its complement, exhibiting weak localization. Conversely, φ can only be substantial in the subregion D when λ almost coincides with one of local eigenvalues of the operator L in D. Moreover, in that case φ itself almost coincides with the corresponding eigenmode of the subregion D.

3.3. The definition of the valleys. Note that $|\varphi|\Big|_{\partial D}$ is majorized pointwise by $u\Big|_{\partial_D}$ according to the inequality (3.2). In fact, without loss of generality we can assume that all φ are normalized so that $\|\varphi\|_{L^\infty(\Omega)} = 1$, so that, in particular, $|\varphi(x)| \leq \lambda u(x)$ for every $x \in \partial\Omega$. The normalization clearly does not affect the statement of the Proposition 3.2, one just has to make sure to use the same normalization in the definition (3.7). Then, according to the maximum principle, the L^2 norm of the L-harmonic extension of $(|\varphi|)\Big|_{\partial D}$ to D, that is, $\|v\|_{L^2(D)}$, is majorized by λ times the L^2 norm of the L-harmonic extension of $u\Big|_{\partial D}$ to D. The latter is, in turn, controlled in the appropriate sense by $u\Big|_{\partial_D}$.

These observations, together with Proposition 3.2, suggest that the localization will take place in the subregions delimited by curves where $u\Big|_{\partial_D}$ is minimal, in the exact sense described above. These lines will be called *valleys* of the landscape.

One yet has to stress that the values of the control landscape u have to be significantly small in the valleys (i.e. much smaller that $1/\lambda$ where λ is a typical eigenvalue of the localized eigenfunction) for the inequality (3.2) to be effective. To this day, it still remains to be investigated under which circumstances this condition is fulfilled, and why these circumstances occur in Anderson localization.

4. Numerical simulations

We have tested the above theory by numerically solving the Schrödinger equation which is the eigenvalue problem associated to the Hamiltonian H. The domain Ω has been chosen as the unit square. This domain Ω is divided into 20×20 elementary square cells, and the potential $V(x)$ is defined as a piecewise constant function on each of these cells. The values of the potential on the cells are independent random variables uniformly distributed between 0 and a maximum value (here 8,000, see Figure 1).

The simulations have been carried out on two different realizations of the random potential. First, the landscapes u have been computed by numerically solving (3.3) using second order rectangular Hermite elements. Figure 2 displays level set representations of both landscapes. For the purposes of numerical simulations we use as *valleys* the lines of steepest descent starting from the saddle points of the landscape. The deepest valleys (hence leading to the stronger confinement) are drawn in thick white lines while the higher valleys are plotted in thiner white lines.

One can observe that the valley lines form in each case a complicated and interconnected network. Both networks are very different but still exhibit similar features, dividing the unit square into a partition of much smaller subregions of various shapes and sizes. The eigenvalue problems associated to the two different potentials are then numerically solved using the same finite elements scheme. Figure 3 displays 8 eigenfunctions (the corresponding eigenvalues are found above each graph) for both potentials. One can observe in both cases that the subregions of the domain Ω delimited by the corresponding networks indeed extremely accurately predict the localization regions of the eigenfunctions.

However, for higher eigenvalues, the control achieved by the valleys lines on the eigenfunctions through (3.2) becomes weaker. Due to the presence of the $L^\infty(\Omega)$-norm in (3.2), the control partially disappears in a subregion when the eigenvalue

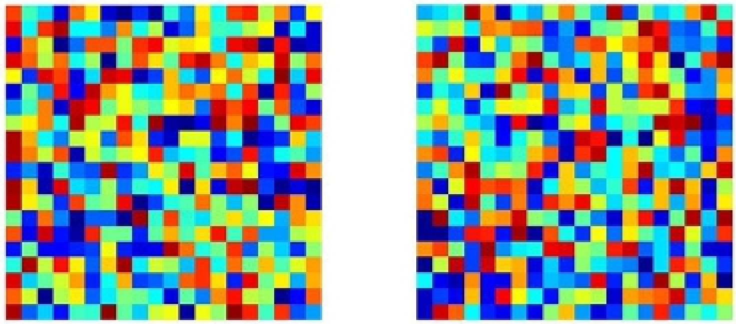

Figure 1. Level set representation of two realizations of a random potential V. The domain Ω is divided into 20×20 elementary square cells. The potential is piecewise constant, and on each cell, the value of the potential is is a uniform random variable between 0 (dark blue) and $V_{max} = 8000$ (red).

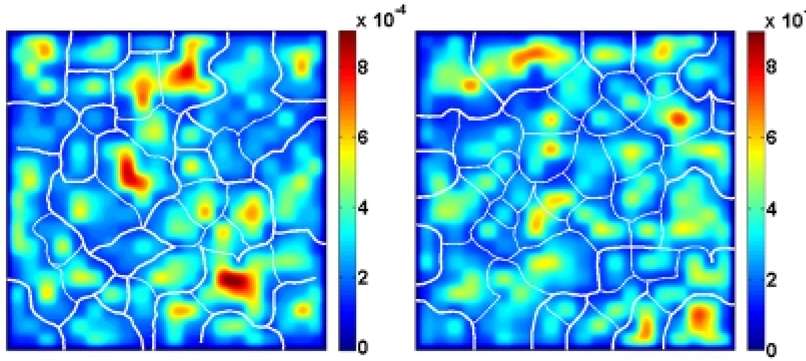

Figure 2. Level set representation of two landscapes, solutions of $Lu = 1$, for the two different realizations of the random potential $V(x)$ given in Figure 1. The thick white lines delineate the deepest valleys of the landscapes while the thinner white lines show the higher valleys.

λ is such that $u(x) \geq 1/\lambda$ along the valley lines surrounding the subregion. To illustrate this, we superimpose over each representation of an eigenfunction the corresponding valley network (deduced from Figure 2) from which we have removed the segments where $\lambda u(x) \geq 1$. One can now observe how the progressive fading of the remaining valley network for higher eigenvalues coincides with the emergence of less localized eigenfunctions. Yet, the spatial structures of these higher order eigenfunctions is still dictated by the remaining network.

5. Conclusion

The theory and the numerical experiments presented in this paper show that the strong localization of eigenfunctions of the Hamiltonian H in a random potential (also called Anderson localization) is the consequence of two control inequalities.

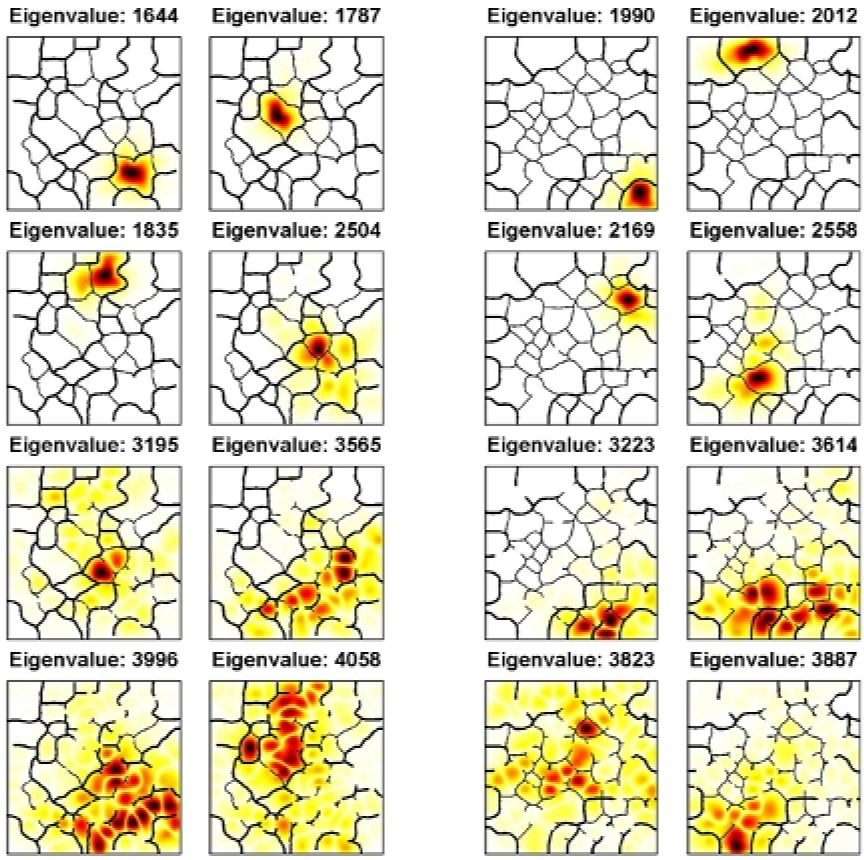

FIGURE 3. Left: Level set representation of 8 eigenfunctions (number 1, 2, 3, 11, 31, 45, 56, and 59) of the Hamiltonian with the first realization of the random potential. The corresponding eigenvalue is displayed above the eigenfunction. Right: Level set representation of 8 eigenfunctions (same numbers as before) of the Hamiltonian with the second realization of the random potential. The thicker dark lines delineate the deepest valleys of the landscapes while the thinnest represent the highest valleys. One can observe how accurately these lines predict the main existence regions of the localized eigenfunctions.

All eigenfunctions of a given elliptic operator, e.g., , the Hamiltonian, are controlled by the same function u, called here the *landscape*. This landscape is obtained by solving the Dirichlet problem $Hu = 1$.

The valley lines of this effective landscape divide the entire domain into an invisible partition of disjoint subregions which correspond to the localization subregions of the eigenfunctions. The control achieved by the function u locally disappears when λ is such that $\lambda u(x) \geq 1$ along a given closed curve of the network. As a consequence, the relative number of localized modes decreases at higher eigenvalues.

The network of valleys of the landscape therefore appears as a geometrical object that plays a major role in understanding the spatial distribution and the localization properties of the eigenfunctions of the Hamiltonian, hence the physical properties that depend on the quantum states. In the limit of a Brownian potential, one may conjecture that both the landscape and its valley network become statistical objects with fractal properties.

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Physique de la Matière Condensée, Ecole Polytechnique, CNRS, 91128 Palaiseau, France

E-mail address: marcel.filoche@polytechnique.edu

School of Mathematics, University of Minnesota, 127 Vincent Hall, 206 Church Street SE, Minneapolis, Minnesota 55455

E-mail address: svitlana@math.umn.edu