Abstract. The approximation of the eigenvalues and eigenfunctions of an elliptic operator is a key computational task in many areas of applied mathematics and computational physics. An important case, especially in quantum physics, is the computation of the spectrum of a Schrödinger operator with a disordered potential. Unlike plane waves or Bloch waves that arise as Schrödinger eigenfunctions for periodic and other ordered potentials, for many forms of disordered potentials the eigenfunctions remain essentially localized in a very small subset of the initial domain. A celebrated example is Anderson localization, for which, in a continuous version, the potential is a piecewise constant function on a uniform grid whose values are sampled independently from a uniform random distribution. We present here a new method for approximating the eigenvalues and the subregions which support such localized eigenfunctions. This approach is based on the recent theoretical tools of the localization landscape and effective potential. The resulting methods, which have only been partially justified theoretically, enable the calculation of the locations and shapes of the approximate supports of the eigenfunctions, the approximate values of many of the eigenvalues, and of the eigenvalue counting function and density of states, all at the cost of solving a single source problem for the same elliptic operator. We study the effectiveness and limitations of the approach through extensive computations in one and two dimensions, using a variety of piecewise constant potentials with values sampled from various different correlated or uncorrelated random distributions.

Key words. localization, spectrum, eigenvalue, eigenfunction, Schrödinger operator

AMS subject classifications. 65N25, 81-08, 82B44

1. Introduction. Eigenfunctions of elliptic operators are often widely dispersed throughout the domain. For example, the eigenfunctions of the Laplacian on a rectangle are tensor products of trigonometric functions, while on a disk they vary trigonometrically in the angular variable and as Bessel functions in the radial argument. By contrast, in some situations eigenfunctions of an elliptic operator localize, in the sense that they are practically zero in much of the domain (after normalizing the $L^2$ or $L^\infty$ norm, say, to 1), like the two functions pictured on the right of Figure 1 (which will be explained shortly). Localization may be brought about by different mechanisms including irregular coefficients of the elliptic operator, certain complexities of the geometry of the domain such as thin necks or fractal boundaries, confining potential wells, and disordered potentials. A celebrated example is Anderson localization [2], which refers to localization of the eigenfunctions of the Schrödinger operator on $\mathbb{R}^n$ induced by a potential with random values. The eigenfunctions of the Anderson system model the quantum states of an electron in a disordered alloy, and localization can even trigger a transition of the system from metallic to insulating behavior. Over the past 60 years, analogous phenomena have been observed in many other fields, and...
found numerous applications to the design of optical [21], acoustic [23, 7], electromagnetic [15, 22], and photonic devices [10, 17].

The localized functions shown on the right of Figure 1 are the first and second eigenfunctions of the Schrödinger operator $H = -\Delta + V$ on the square $[0, 80] \times [0, 80]$ with periodic boundary conditions. The potential $V$ is of Anderson type: it is a piecewise constant potential obtained by dividing the domain into $80^2$ unit subsquares and assigning to each a constant value chosen randomly from the interval $[0, 20]$. The reader may consider how to predict the location of the eigenfunctions from an examination of the potential. That is an example of a question addressed here.

![Image of potential and eigenfunctions](image)

**Fig. 1.** A piecewise constant potential with randomly chosen iid values, and the first two eigenfunctions of the corresponding Schrödinger operator.

In this paper we shall focus on the Schrödinger operator $H = -\Delta + V$. The domain $\Omega$ will always be either an interval in one dimension or a square in two, the boundary conditions will be periodic, and the potential $V$ will be piecewise constant with respect to a uniform mesh of $\Omega$ having positive values chosen from some probability distribution, either independently or with correlation. Much of the work can be extended, e.g., to more general domains, potentials, PDEs, and boundary conditions. In particular, we remark that the choice of periodic boundary conditions is for simplicity, and that similar localization occurs with Neumann or Dirichlet boundary conditions. We generally choose unit-sized subsquares for the constant regions of the potential, but this is merely a convenient normalization. For example, instead of considering an $80 \times 80$ square broken into unit subsquares as the domain in Figure 1, we could have chosen instead to take the unit square as the domain, with subsquares of side length $1/80$ for the potential. Had we scaled the potential to take values in the range from 0 to 128,000, we would have obtained the same localization ($128,000$ being $20 \times 80^2$).

There is a large literature concerning the localization of eigenfunctions, approaching the phenomenon from various viewpoints: spectral theory, probability, and quantum mechanics. But there is nothing like a complete explanatory and predictive theory which can quantitatively and deterministically answer such basic questions as:

- How are the eigenvalues and eigenfunctions determined by a particular potential?
- Given a potential, do the eigenfunctions localize, and, if so, how many?
- What are the size, shape, and location of the approximate supports and how do the eigenfunctions decay away from them?
- What are the associated eigenvalues?

The present work aims at providing answers to these questions, based on a theory of
localization recently conceived and under active development [8, 9, 4, 16, 3].

In the next section of the paper, we briefly survey some classical tools used to understand localization. Then, in Section 3, we introduce two more recent tools: the localization landscape function and its associated effective potential, introduced in [8, 4]. These are easily defined. The landscape function \( u \) is the periodic solution to \( Hu = 1 \) and the effective potential \( W \) is its reciprocal. Our approach is guided by estimates and relations between these objects and the spectrum of the Schrödinger operator from [8], [4], and the recent theoretical work of [3]. In Section 4 we show how the structure of wells and barriers of the effective potential can be incorporated into numerical algorithms to predict the locations and approximate supports of localized eigenfunctions. Then, in Section 5, we show how the values of the minima of the effective potential can be used to predict the corresponding eigenvalues and density of states. Throughout, the performance of our algorithms is demonstrated for various types of 1D and 2D random piecewise constant potentials (uniform, Bernoulli, Gaussian, uncorrelated and correlated).

Note that the computation of the effective potential involves the solution of a single source problem, and so is far less demanding than the computation of a significant portion of the spectrum by traditional methods. However, a remarkable conclusion of our results is that, for the localized problems studied here, a great deal of information about the spectrum can be extracted easily from the effective potential.

2. Classical confinement. A simple and well-understood example of eigenfunction localization for the Schrödinger equation occurs with a classically confining potential. Such a potential is decisively different and simpler than the highly disordered potentials we consider, but we shall draw a connection in the forthcoming discussion, and for that reason we now briefly review localization by confinement. The basic example is the finite square well potential in one dimension, for which the analytic solution is derived in first courses on quantum mechanics [19, vol. 1, p. 78]. This problem is posed on the whole real line with the potential \( V \) equal to some positive number \( \nu \) for \( |x| > 1 \) and vanishing otherwise. The fundamental eigenfunction is then

\[
\psi(x) = \begin{cases} 
\cos(\sqrt{\lambda}x), & |x| \leq 1, \\
c_{\nu} \exp(-\sqrt{\nu - \lambda} |x|), & |x| > 1,
\end{cases}
\]

where the eigenvalue \( \lambda \) is uniquely determined as the solution to the equation \( \cos(\sqrt{\lambda}) = \sqrt{\lambda/\nu} \) in the interval \((0, \pi^2/4)\) and \( c_{\nu} = \sqrt{\lambda/\nu} \exp(\sqrt{\nu - \lambda}) \). Since \( \lambda < \nu \), the solution decays exponentially as \( |x| \to \infty \), which captures localization in this context. A similar calculation can be made in higher dimensions, for example for spherical wells [19, vol. 1, p. 359-361], in which case the well height \( \nu \) must be sufficiently large to ensure that there exists an eigenvalue.

A fundamental result for the localization of eigenfunctions of the Schrödinger equation with a general confining potential is Agmon’s theory [1], [11, § 3.3], [13, Ch. 3], which demonstrates a similar exponential decay for a much larger class of potentials. In this case the domain is all of \( \mathbb{R}^n \) and the Schrödinger operator is understood as an unbounded operator on \( L^2 \). One requires that the potential be sufficiently regular and bounded below and that there is an eigenfunction \( \psi \) with eigenvalue \( \lambda \) such that \( V > \lambda \) outside a bounded set. In other words, outside a compact potential well where \( V \) dips below the energy level \( \lambda \), it remains above it (thus creating confinement). Agmon defined an inner product on the tangent vectors
at a point \( x \in \mathbb{R}^n \) by

\[
\langle \xi, \eta \rangle_x = \sqrt{\left[V(x) - \lambda\right]_+ \cdot \xi \cdot \eta},
\]

where the subscript + denotes the positive part. This defines a Riemannian metric, except that it degenerates to zero at points \( x \) where \( V(x) \leq \lambda \). Its geodesics define a (degenerate) distance \( \text{dist}_V^\lambda(x, y) \) between points \( x, y \in \mathbb{R}^n \), and, in particular, we may define \( \rho(x) = \text{dist}_V^\lambda(x, 0) \) to be the distance from the origin to \( x \) computed using the Agmon metric. Agmon’s theorem states, with some mild restrictions on the regularity on \( V \), that for any \( \epsilon > 0 \),

\[
\int_{\mathbb{R}^n} |e^{(1-\epsilon)\rho(x)}\psi|^2 \, dx < \infty.
\]

This result describes exponential decay of the eigenfunction in an \( L^2 \) sense in regions where \( \rho(x) \) grows, which expresses localization in this context.

For the random potentials which we investigate in this paper, the Agmon distance is highly degenerate, and, consequently, an estimate like (3) is not generally useful. Consider, as a clear example, the Bernoulli potential shown in Figure 2, in which the values 0 and 4 are assigned randomly and independently to each of the \( 80 \times 80 \) subsquares with probabilities 70\% and 30\%, respectively. As shown in color on the right of Figure 2, the region where the potential is zero has a massive connected component which nearly exhausts it. For any positive \( \lambda \), the Agmon distance between any two points in this connected component is zero, and hence an estimate like (3) tells us nothing. Nonetheless, as exemplified by the first two eigenfunctions shown in the figure, the eigenfunctions do localize, a phenomenon for which we must seek a different justification.

3. The landscape function and the effective potential. An important step forward was made in [8] with the introduction of the landscape function, which is simply the solution to the PDE \( Hu = 1 \) together with, for us, periodic boundary conditions. Note that, as long as the potential \( V \) is a bounded nonnegative function,
nonzero on a set of positive measure, then \( u \) is a strictly positive periodic \( C^1 \) function (indeed, it belongs to \( W^2_p \) for any \( p < \infty \)). The following estimate, taken from [8], relates the landscape function to the eigenvalues.

**Proposition 3.1.** If \( \psi : \Omega \to \mathbb{R} \) is an eigenfunction of \( H \) with eigenvalue \( \lambda \), then

\[
\psi(x) \leq \lambda u(x) \| \psi \|_{L^\infty}, \quad x \in \Omega.
\]

If we normalize the eigenfunction \( \psi \) so that \( \| \psi \|_{L^\infty} = 1/\lambda \), then the theorem asserts that \( \psi \leq u \) pointwise, a fact illustrated in Figure 3, which shows the one-dimensional case where the potential has 256 values randomly chosen uniformly iid from \([0,4]\). The argument was made in [8] that if the landscape function \( u \) nearly vanishes on the boundary of a subregion \( \Omega_0 \) of the domain \( \Omega \), then (4) implies that any eigenfunction \( \psi \) must nearly vanish there as well, and so \( \psi \big|_{\Omega_0} \) is nearly a Dirichlet eigenfunction for \( \Omega_0 \) (with the same eigenvalue \( \lambda \)). Similarly \( \psi \) restricts to a near Dirichlet eigenfunction on the subdomain complementary to \( \Omega_0 \). Except for the unlikely case in which these two subdomains share the eigenvalue \( \lambda \), this suggests that \( \psi \) must nearly vanish in one of them, and so be nearly localized to the other. This viewpoint gives an initial insight into the situation illustrated in Figure 3, where it is seen that the eigenfunctions are essentially localized to the subdomains between two consecutive local minima of \( u \). However, it must be remarked, in the case shown in Figure 3 and many other typical cases, the landscape function merely dips, but in no sense vanishes, on the boundary of localization regions, and so a new viewpoint is needed in order to satisfactorily explain the localization which is observed.

**Fig. 3.** The potential on the left gives rise to the landscape function, plotted in blue on the right. The first four eigenfunctions are also plotted, scaled so that their maximum value is the reciprocal of their eigenvalue, illustrating the inequality of (4).

Such a new viewpoint was developed in the paper [4], where the emphasis was placed on the effective potential \( W \), defined as the reciprocal \( 1/u \) of the landscape function. A key property of \( W \) and the explanation for its name, is that it is the potential of an elliptic operator which is conjugate to the Schrödinger operator \( H \) and so has the same spectrum. The following essential identity was derived in [4].

**Proposition 3.2.** Suppose that the potential \( V \in L^\infty(\Omega) \) is nonnegative and positive on a set of positive measure. Let \( u > 0 \) be the landscape function and \( W = 1/u \) the effective potential. Define \( L : H^1(\Omega) \to H^{-1}(\Omega) \) by

\[
L \phi = -\frac{1}{u^2} \text{div}(u^2 \text{grad} \phi).
\]
Then
\[ (-\Delta + V)(u\phi) = u(L + W)\phi, \quad \phi \in H^1(\Omega). \]

In this result, \( H^1 \) denotes the periodic Sobolev space on \( \Omega \) and \( H^{-1} \) its dual. The equation holds in \( H^{-1} \), making sense because \( u \in C^1 \).

**Corollary 3.3.** Let \( V, u, \) and \( W \) be as in the theorem and \( \lambda \in \mathbb{R} \). Then \( \psi \in H^1 \) satisfies \( (-\Delta + V)\psi = \lambda \psi \) if and only if \( \phi := \psi/u \) satisfies \( (L + W)\phi = \lambda \phi \).

Thus the eigenvalues of the operator \( L + W \) (with periodicity) are the same as those of the original Schrödinger operator, and the eigenfunctions are closely related. However the the corresponding potentials \( W \) and \( V \) are very different. The effective potential \( W \) is often much more regular than the physical potential \( V \). More importantly, it has a clear structure of wells and walls. As we shall see, these induce a sort of localization by confinement, which is not evident from the physical potential. For example, for the Bernoulli potential shown in Figure 2, the effective potential is shown in Figure 4. Note that the effective potential contains many wells: small regions where its value is low, but surrounded, or nearly surrounded, by crestlines where its values are relatively high. If we think of a gradient flow starting at a generic point in the domain and ending at a local minimum, thereby associating the point to one of the local minima of \( W \), the crestlines, displayed in green in Figure 4, are the boundaries of the basins of attraction of the local minima. There are several algorithms to compute the precise location of these crestlines. The one used in this case is the watershed transform as described in [5].

![Fig. 4](image)

**Fig. 4.** The effective potential associated to the Bernoulli potential of Figure 2. It is shown with its crestlines which partition the domain into a few hundred basins of attraction surrounding wells.

In recent work [3], we have established a rigorous connection between the well and wall structure of \( W \) and the exponential decay of eigenfunctions. Using the Agmon distance \( \text{dist}_W^\lambda \), defined after (2) in Section 2 but with the potential \( V \) replaced by the effective potential \( W \), we show, roughly speaking, that whenever a well of the effective potential exists with sufficient separation of the well depth from the height of the surrounding barriers, then eigenfunctions \( \psi \) of the operator \( H \) with eigenvalue \( \lambda \) are localized to \( \{ W \leq \lambda \} \) in the sense that they decay exponentially in the Agmon
Theorem 3.4. Suppose \((\psi, \lambda)\) is an eigenpair of the Schrödinger operator \(H = -\Delta + V\). Let \(W\) be the effective potential and \(\text{dist}_W^x(x, y)\) the associated Agmon distance. Let \(\delta > 0\),

\[
S = \{x \in \Omega \mid W(x) \leq \lambda + \delta\},
\]

a sublevel set of \(W\), and \(h(x)\) the Agmon distance from \(x\) to \(S\). Then there exists a constant \(C\) depending only on \(\|V\|_{L^\infty}\) and \(\delta\) (but not the domain \(\Omega\)) such that

\[
\int_\Omega e^{h(x)} \psi^2 \, dx \leq C \int_\Omega \psi^2 \, dx.
\]

This result can be found, stated in considerably more generality and in sharper form in [3, Corollary 3.5]. The dependence of the constant is given there explicitly. It grows at most linearly in \(\|V\|_{L^\infty}\). The same paper also proves exponential decay for the gradient of the eigenfunctions. On the other hand these theoretical results do not capture fully the accuracy with which \(W\) predicts the behavior of the eigenfunctions. Our numerical results show that the eigenfunctions typically occupy a single connected component of the set \(W \leq \lambda\) and decay exponentially across each green crestline of Figure 4, whereas the theorems do not rule out eigenfunctions that have significant mass in several different components of \(W \leq \lambda\).

4. Eigenfunction prediction. We may apply the theory described in the previous section to predict the location and extent of the supports of localized eigenfunctions. For this we proceed in four steps.

1. Compute the landscape function \(u\) from the PDE \(Hu = 1\), and define the effective potential \(W = 1/u\).

2. To approximate a desired number of localized eigenfunctions, identify the same number of local minima of \(W\), selected in order of increasing minimal value. The location of these minima will be our prediction of the place where the eigenfunctions localize, in the sense that the maximum of the localized eigenfunction will occur nearby there.

3. To each of the selected local minimum we associate an energy level \(E\) given by the minimum value of \(W\) in the well times a constant greater than 1. The constant is chosen so that \(E\) is close to fundamental eigenvalue of the well, or perhaps somewhat larger. (We show in the next section how this may be achieved.)

4. From the corresponding sublevel set, consisting of all \(x\) for which \(W(x) \leq E\), we compute the connected component which contains the selected local minimum. This is the region we predict to be occupied by the eigenfunction.

Figure 5 shows the outcome of applying this approach to the 1D Schrödinger equation with the potential shown in Figure 3. The landscape function was computed using Lagrange cubic finite elements with a uniform mesh of 2,560 subintervals (10 element per constant piece of the potential). The finite element solution was evaluated at 15,360 equally-spaced points (6 per element), with the reciprocals giving the values of the effective potential. The local maxima and local minima of the effective potential were then identified by comparing the value at each point to that of its two immediate neighbors. For comparison, the true eigenvalues and eigenfunctions were computed by using the same finite element discretization and solving the resulting sparse matrix real symmetric generalized eigenvalue problem using a Krylov–Schur
The finite element discretizations were implemented using the FEniCS software environment [18], calling the SLEPc library [12] for the eigenvalue solves. Note that the locations of the four local minima of the effective potential, indicated by small circles in both plots of Figure 5, very nearly coincide with the locations of the maxima of the four corresponding eigenfunctions. Moreover the correspondence respects the ordering of the eigenvalues, in the sense that the $i$th eigenfunction corresponds to the $i$th well for $i = 1, 2, 3, 4$. To predict the extent of the localized eigenfunctions, we use as outer boundaries the level curves of the effective potential at an energy level $E$ set to be 1.875 times the depth of the wells. This is 150% of the value we justify in the next section as an approximation of the eigenvalues. Of course, this choice is somewhat arbitrary, since the effective support of a localized function is not an absolute notion, but must be defined with respect to some tolerance. We could as well have chosen a somewhat larger level to get wider regions incorporating more of the tail of the eigenfunctions, or have chosen a somewhat smaller level to get narrower regions.

Next, we vary this example by increasing the amplitude of the potential by a factor of 64, so that it takes values between 0 and 256, but is otherwise identical to the potential shown on the left of Figure 3. The results analogous to Figure 5 for this potential are shown in Figure 6. Note that, despite the fact that the potentials are proportional in the two cases, the effective potentials look quite different and the eigenfunctions localize in entirely different places. The eigenvalue maxima occur at 17.85, 41.47, 90.75, and 72.92 for the smaller potential and at 90.57, 73.42, 204.5, and 110.5 for the second. These locations again are captured very accurately by the minima of the effective potential, and in the correct order. A crucial difference between the two examples is that the eigenvalues for the problem with the larger potential are much more tightly localized, as predicted by the thinner wells of its effective potential.

We now consider the two-dimensional case where the potential is the random $80 \times 80$ Bernoulli potential shown in Figure 2, for which the effective potential is shown in Figure 4. To compute the landscape function we again used the finite

![Figure 5](image_url)
 element method with Lagrange cubic finite elements on a uniform mesh. The mesh was obtained by dividing each of the unit squares into 10 × 10 subsquares, each of which was further divided into two triangles, resulting in 1,280,000 triangles altogether. We then evaluated the solution at a uniform grid of 400 × 400 points and found the local minima of the effective potential by comparing each of these values to the values at the eight nearest neighbors (horizontally, vertically, and diagonally). In Figure 7 the first plot shows the first four local minima of the effective potential. For each, a corresponding sublevel set of the effective potential is shown. The four minima and sublevel sets are our predictors for the locations of the eigenfunctions. The energy level \( E \) of the sublevel sets was taken as 1.56 times the well depth, just slightly larger than the prediction for the eigenvalue, namely 1.5 times the well depth, which we propose in the next section. Recall that the choice of \( E \) is somewhat arbitrary. This choice gives a good visual match with the apparent support of the eigenfunctions. The second plot in Figure 7 is a plot of the sum of four eigenfunctions, each normalized in the \( L_\infty \) norm. Since they are localized one can easily distinguish the location of each within the sum, which is very close to that predicted. The third plot is a superposition of the first two, to facilitate comparison.

In the three cases just considered, there is a clear correspondence between the first four eigenfunctions and the four deepest wells of the effective potential, with each of eigenfunctions, when ordered as usual by increasing eigenvalue, centered at the corresponding local minimum of the effective potential, ordered by depth of the minimum. However, this ideal situation does not always pertain. When two eigenvalues, or two of the minima, are nearly equal, their ordering may not be respected by the correspondence. Another situation which may arise is that the basin surrounding one of the minima may include another. In that case the second minima does not lead to a separate eigenfunction. Both of these issues arise in the the case of the uniformly random potential of Figure 1. Figure 8 shows the first five local minima of the effective potential, and their basins. The numbers provided show the ordering by the depth of the wells. Note that the third and fourth minima nearly coincide in location, and they only contribute one well, even though they are, technically, two distinct minima. The actual minimum values and eigenvalues are given in Table 1. It reveals that the third and fourth minima are not only close in location, but nearly
The first plot shows the prediction for the location of the first four eigenfunctions for the Bernoulli potential of Figure 2. The second plot shows the actual positions of these eigenfunctions, superimposed. The final plot compares the actual positions to the predictions.

coincide in value as well. Moreover the difference between their value and values of the preceding and following minima is rather small. These close values account for the fact that the correspondence between the eigenfunctions and minima clearly visible in Figure 8 does not respect the precise ordering. Nonetheless, the structure of the effective potential clearly provides a lot of information on the localization structure of the eigenfunctions. To account for such near coincidences we could seek to develop an algorithm to identify clusters of minima with nearly equal values and relate them to clusters of nearly equal eigenvalues. However we shall not pursue this direction here.

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Table 1

The values of the effective potential at its first five minima, and the first five eigenvalues for the uniformly random potential of Figure 1. Cf. Figure 8.
Thus far we have examined random piecewise constant potentials with values taken independently and identically distributed according to some probability distribution (uniform or Bernoulli). In the final example of this section, we consider a potential for which the values are correlated rather than independent. To generate values for the potential, we use circulant embedding to convert uncorrelated Gaussian $N(0,1)$ random vector samples to correlated Gaussians [14]. We take a 1-dimensional example, in which the potential is piecewise constant with $n$ unit length pieces, with $n$ even. Define $q_i = q_{n-i} = \sigma \exp(-di), \ 0 \leq i \leq n/2$, where $d$ is a positive constant, and let $Q$ be the diagonal matrix with entries $q_0, q_1, \ldots, q_{n-1}$. A sample vector for the values of $V$ is obtained by squaring the components of the vector $F^{-1}QFz$ where $z$ is a vector of length $n$ with components sampled independently from a normalized Gaussian distribution, and $F$ is the discrete Fourier transform on $\mathbb{C}^n$. This type of a random potential is typically created by optical speckles in a Bose-Einstein condensate. See, e.g., [20], [6]. It is quite challenging to derive rigorous probabilistic results when the correlation is not negligibly small, especially in higher dimensions. The landscape theory, however, continues to apply. We consider an example with $n = 1, 024, \ \sigma = 1.0, \ d = 0.01$, shown in Figure 9 along with the corresponding effective potential. Note that, although the potential and effective potential look quite different from the previous examples, the effective potential still has clearly defined wells which allow us to apply our theory. In the final plot in Figure 9 we use the effective potential as before to predict the location and extent of the first seven eigenfunctions. As in the uncorrelated cases, the well minima very nearly coincide with the peak of the eigenfunctions. The first three minima, in order, correspond to the first three eigenfunctions, but after that the order is not the same. The discrepancy in ordering is not very significant, however, since both the minimum values and the eigenvalues are very close to one another, as indicated in Table 2.

5. Eigenvalue prediction. We now turn to the question of predicting eigenvalues of the Schrödinger operator $\hat{H}$ from the effective potential. As a simple illustration of the utility of the effective potential for eigenvalue estimation, we start by recalling
Fig. 9. A correlated potential and the corresponding effective potential with its seven lowest minima marked. On the top left is the original correlated potential, on the top right the corresponding effective potential. On the bottom are the first seven eigenfunctions with the color giving the order as indicated by the inset. A rectangle is superimposed on each eigenfunction. The heights of the rectangles and eigenfunctions are normalized to unity, while each rectangle’s width indicates the extent of the localized eigenfunction as predicted by the effective potential (using a sublevel set at an energy level equal to 1.875 times the depth of the wells as was done for Figure 5). The small yellow circles give the position of the local minima and the numbers over them, the order of the local minima. Notice that the order differs from the order of the corresponding eigenfunctions after the first three.

the basic lower bound on the fundamental eigenvalue in terms of the potential $V$, and show how it can be improved by using the effective potential.

For an eigenfunction $\psi$ of $H$ with eigenvalue $\lambda$, normalized to have $L^2$ norm 1, we have

\begin{equation}
\lambda = (H\psi, \psi) = \| \text{grad } \psi \|^2 + (V\psi, \psi)
\end{equation}

which represents the decomposition into kinetic and potential energy. Dropping the kinetic energy term and replacing $V$ by its infimum gives a lower bound on the eigenvalues:

\begin{equation}
\lambda \geq \inf V.
\end{equation}
Table 2

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The values of the effective potential at its first seven minima, and the first seven eigenvalues for the correlated potential of Figure 9.

Now we use the fundamental identity of Theorem 3.2 to decompose the eigenvalue in terms of the effective potential:

\[(H\psi, \psi) = (u^2L\phi, \phi) + (W\psi, \psi),\]

where \(\phi = \psi/u\). In view of the form of \(L(5)\), the first term on the right hand side is positive, so dropping it and replacing \(W\) by its infimum gives another lower bound:

\[\lambda \geq \inf W.\]

Figure 10 allows one to compare the two bounds for a random potential with 64 values chosen uniformly iid in the range \([0, 8]\). The fundamental eigenvalue for this realization is 1.58, indicated on the plot in red. The infimum of \(V\) is, however, very near zero: 0.00009, and so the bound (7) is nearly worthless. (In this realization \(\inf V\) happens to be particularly small, but the expected value of \(1/65 = 0.015\) is again of little use.) By contrast, \(\inf W = 1.22\), which is a useful lower bound. In fact, the fundamental eigenvalue is equal to about \(1.3 \inf W\). We shall see below that this factor of roughly 1.3 applies for a wide range of random potentials in one dimension.

![Figure 10. A random potential (in shaded gray), the corresponding effective potential (the solid blue line), and the fundamental eigenvalue (the horizontal red line).](image)

In the remainder of this section, we shall consider two approaches to eigenvalue prediction, one based solely on the local minima values of the effective potential, and the other based on a variant of Weyl’s law utilizing the effective potential. Although we shall explain the thinking behind these approaches, it has to be noted that neither has yet been justified rigorously.

5.1. Eigenvalues from minima of the effective potential. In this section we discuss the approximation of the eigenvalues of the Schrödinger operator \(H\) using the
effective potential \( W \). We shall be interested in both the approximation of individual eigenvalues, and in the distribution of the eigenvalues. The latter is captured by the density of states (DOS). Defined precisely, the DOS is the distribution on \( \mathbb{R} \) obtained by summing the delta functions centered at each eigenvalue. For visualization, it is often converted to a piecewise constant function with respect to a partition of the real line into intervals of some length \( \epsilon > 0 \), with the value over any interval being the integral of the DOS over the interval (so a plot of this function is a histogram of the eigenvalues using bins of width \( \epsilon \)). The integrated density of states (IDOS) is the integral of the DOS from \(-\infty\) to a real value \( E \). The resulting function \( N : \mathbb{R} \to \mathbb{N} \) is simply the eigenvalue counting function, with \( N(E) \) defined as the number of eigenvalues \( \leq E \).

To motivate our first approach to eigenvalue prediction, consider again the potential shown in Figure 1, a piecewise constant function with \( 80 \times 80 \) pieces and constant values chosen randomly and independently from \([0, 20]\). In the first plot of Figure 11 we have computed the values of the effective potential \( W \) at its local minima and compared the first 100 of these, in increasing order, to the first 100 eigenvalues of \( W \). Just below we plot the quotients of each of these eigenvalues divided by the corresponding local minimum value of \( W \). Observe that the quotient is quite constant, taking on a value of roughly 1.5. We shall endeavor to explain this value below, but first we observe that this ratio of roughly 1.5 between the \( m \)th eigenvalue and the \( m \)th minimum value of the effective potential holds over a wide range of random potentials in two dimensions. In the remainder of the first two rows of Figure 11 we show the same results also for the Bernoulli potential of Figure 2 and the correlated potential shown in Figure 12. (The correlated potential was constructed with circulant embedding as discussed above for one dimension, except that we of course used the two-dimensional discrete Fourier transform, and we took as aperture function \( \sigma \chi(d|t|) \) with \( \sigma = 4 \) and \( d = 0.05 \), where \( \chi \) is the characteristic function of the unit interval, instead of \( \sigma \exp(-d|t|) \) as we took previously.) The three pairs of plots in the final two rows of the figure show the case of a uniformly random \( 40 \times 40 \) potential with values taken between 0 and 4, 16, and 64, respectively. The quotient is quite close to being constant with value 1.5, particularly in the last two cases. In the first case, with the lowest disorder, the ratio drifts away from 1.5 to about 1.75 after approximately 50 eigenvalues.

In Table 3 we display the mean and standard deviation of these ratios computed for the first 10, 50, and 100 eigenvalues for each of the six potentials. The main observation is that, across all this range, the ratio stays quite close to 1.5.

Table 4 is similar, but shows the results for a variety of potentials in one dimension. Again, we see that the ratio of the eigenvalue to the corresponding minimum values of the effective potential is roughly constant, as it was in two dimensions. However the constant value we find in one dimension is about 1.25 or 1.3 rather than the value of 1.5 we saw in two dimensions.

Finally, in Figures 13 we plot the 1st, 10th, and 25th eigenvalues versus the corresponding minima values of \( W \) for numerous different realizations of a random potential. The first figure displays 64 realizations of a 1D potential on \([0, 256]\) with 256 values selected uniformly iid from \([0, 16]\), while the second figure displays 64 realizations of a 2D potential on \([0, 40] \times [0, 40]\) with 1,600 random values again chosen uniformly iid from \([0, 16]\). We see that in the first case the points line up well along the line \( \lambda = 1.25W_{\min} \), and in the second along the line \( \lambda = 1.5W_{\min} \).
Fig. 11. A comparison of 100 eigenvalues with the corresponding minimum values of $W$ for six different potentials with the ratio of the two shown beneath each one. Top two rows: (left) random $80 \times 80$ piecewise potential with values chosen uniformly in $[0, 20]$; (center) Bernoulli potential of Figure 2; (right) correlated potential of Figure 12. Bottom two rows: random $40 \times 40$ piecewise potential with values chosen uniformly in (left) $[0, 4]$, (center) $[0, 16]$, (right) $[0, 64]$. In all these cases, one can notice that the ratio of the minimum values of $W$ to the corresponding eigenvalues remains remarkably close the value 1.5.

From this and other evidence, we conclude that in many cases

$$\lambda \approx (1 + \frac{n}{4}) W_{\min}.$$  

Here $\lambda$ is one of the lower eigenvalues of $H$, for which the corresponding eigenfunction is localized to a subdomain $\Omega_0$, $W_{\text{min}}$ is the minimum value of the effective potential on that subdomain, and $n$ is the number of dimensions (thus far 1 or 2). The constant $1 + n/4$, i.e., 1.25 in 1D and 1.5 in 2D, is a rough approximation in accord with our observations and which we now further justify heuristically. It is remarkable that this constant, though dimension-dependent, is independent of the specific realization.
of the potential and of the parameters of its probability distribution, the size of the
domain, etc.

We now give some heuristic support of the eigenvalue approximation (9). Our
argument will be rather crude, and we do not claim it fully explains the numerical
evidence presented above. Let \( \psi \) denote one of the eigenfunctions associated to a
smaller eigenvalue. We assume \( \psi \) to be localized, i.e., essentially supported in a
small subdomain \( \Omega_0 \), for which it is the fundamental Dirichlet eigenfunction. We
also assume that on the subdomain \( \Omega_0 \) the landscape function \( u \) is well approximated
by a constant multiple of the fundamental eigenfunction \( \psi \) of the subdomain. This
is roughly supported by experimental results such as shown in Figure 3. Another
supporting argument comes from the expansion of the constant 1 on \( \Omega_0 \) in terms
of the Dirichlet eigenfunctions of the domain, retaining only the first term \( c_0 \psi \), and
dropping the terms coming from the eigenfunctions which change sign. Then \( u \approx (c_0/\lambda)\psi \), indeed a multiple of \( \psi \). We may use these two assumptions, together with
The mean and standard deviation for the ratio of first 10, 25, and 50 eigenvalues to the corresponding minima values of $W$, tabulated here for 8 different types of random potentials in one dimension.

<table>
<thead>
<tr>
<th>potential</th>
<th>$n_c$</th>
<th>mean</th>
<th>SD</th>
<th>mean</th>
<th>SD</th>
<th>mean</th>
<th>SD</th>
</tr>
</thead>
<tbody>
<tr>
<td>uniform [0, 4]</td>
<td>256</td>
<td>1.303</td>
<td>0.026</td>
<td>1.321</td>
<td>0.029</td>
<td>1.300</td>
<td>0.067</td>
</tr>
<tr>
<td></td>
<td>1024</td>
<td>1.302</td>
<td>0.019</td>
<td>1.301</td>
<td>0.020</td>
<td>1.304</td>
<td>0.022</td>
</tr>
<tr>
<td>uniform [0, 16]</td>
<td>256</td>
<td>1.322</td>
<td>0.023</td>
<td>1.308</td>
<td>0.031</td>
<td>1.240</td>
<td>0.099</td>
</tr>
<tr>
<td></td>
<td>1024</td>
<td>1.274</td>
<td>0.018</td>
<td>1.296</td>
<td>0.031</td>
<td>1.294</td>
<td>0.027</td>
</tr>
<tr>
<td>Bernoulli</td>
<td>256</td>
<td>1.301</td>
<td>0.033</td>
<td>1.316</td>
<td>0.050</td>
<td>1.296</td>
<td>0.130</td>
</tr>
<tr>
<td></td>
<td>1024</td>
<td>1.262</td>
<td>0.014</td>
<td>1.272</td>
<td>0.026</td>
<td>1.266</td>
<td>0.073</td>
</tr>
<tr>
<td>correlated</td>
<td>256</td>
<td>1.335</td>
<td>0.055</td>
<td>1.404</td>
<td>0.090</td>
<td>1.310</td>
<td>0.171</td>
</tr>
<tr>
<td></td>
<td>1024</td>
<td>1.280</td>
<td>0.018</td>
<td>1.286</td>
<td>0.017</td>
<td>1.303</td>
<td>0.042</td>
</tr>
</tbody>
</table>

Fig. 13. The 1st, 10th, 25th, and 50th eigenvalues versus the corresponding minima values of the effective potential, for 64 independent realizations of a random potential. Left in 1D where the black line shown is $\lambda = 1.25W_{\text{min}}$, right in 2D with $\lambda = 1.5W_{\text{min}}$.

the definition $Hu = 1$ of the landscape function, to approximate the Rayleigh quotient:

$$\lambda = \frac{\int_{\Omega} \psi H \psi \, dx}{\int_{\Omega} \psi^2 \, dx} \approx \frac{\int_{\Omega_0} \psi H \psi \, dx}{\int_{\Omega_0} \psi^2 \, dx} \approx \frac{\int_{\Omega_0} Hu \, dx}{\int_{\Omega_0} u^2 \, dx} = \frac{\int_{\Omega_0} u \, dx}{\int_{\Omega_0} u^2 \, dx}.$$  

Next we assume that on $\Omega_0$ the landscape function $u$ (or $\psi$ which we are supposing is a constant multiple of $u$ there) can be approximated by the simplest sort of positive bump-like function, the positive part of a concave quadratic function. After rotating and translating the coordinate system, this means that

$$u \approx u_{\text{max}} \left[ 1 - \sum (x_i / a_i)^2 \right]$$

on $\Omega_0 \approx \{ x \in \mathbb{R}^n \ | \ \sum (x_i / a_i)^2 \leq 1 \}$, for some positive constants $a_i$. Thus our approximation to the eigenvalue is

$$\lambda \approx \frac{\int_{\Omega_0} u \, dx}{\int_{\Omega_0} u^2 \, dx} = \frac{c}{u_{\text{max}}}, \quad c = \frac{\int_{\Omega_0} \left[ 1 - \sum (x_i / a_i)^2 \right] \, dx}{\int_{\Omega_0} \left[ 1 - \sum (x_i / a_i)^2 \right]^2 \, dx}.$$
Finally, we compute $c$ using the change of variables $\hat{x}_i = x_i/a_i$ to convert the integrals in the numerator and denominator into integrals over the unit ball $B$ which can be computed with polar coordinates. This gives $c = 1 + n/4$ (independent of the values of the $a_i$ and so of the size and shape of the ellipsoid). Since $1/u_{\text{max}} = W_{\text{min}}$, this indeed gives the approximation (9).

The results we have shown in Figure 11 and Tables 3 and 4 demonstrate that the approximation (9) can be used to estimate 100 eigenvalues with errors of a few percent. Note that it is nonetheless very cheap to apply (9), the cost being that of solving a single source problem and the extraction of some maxima, much less than the cost of computing many eigenvalues. As another example of the utility of (9) we now use it to approximate the density of states in the interval $[0, 1]$ of the 1D Schrödinger operator for which the piecewise constant potential has $2^{19} = 524,288$ pieces. (Specifically, we compute on the interval $[0, 2^{19}]$ and assign the random values to unit subintervals uniformly iid in $[0, 4]$.) We display the DOS as a histogram with 100 bins. The top left plot in Figure 14 shows the actual density of states, requiring the computation of all 7,122 eigenvalues in $[0, 1]$. This is a very large computation: it required about 40 CPU hours on a workstation with an Intel Core i7-4930K processor. Very similar results are displayed in the top right plot, which is a histogram of the values of $1/\sqrt{\text{max}}$ which do not exceed 1 (8,800 in all). This computation is much less demanding. It required slightly over 5 minutes of CPU time of the same workstation, i.e., was about 480 times faster. The two histograms are compared in the bottom plot.

5.2. Eigenvalues from a variant of Weyl’s law. The approximation (9) can be used to predict, at most, one eigenvalue per local minimum of $W$. Intuitively, it approximates a localized eigenfunction by the fundamental mode of the well around the local minimum. Now we present an alternative approach, which again relies on the effective potential $W$, but which gives some sort of prediction for all the eigenvalues. For large eigenvalues, it provides information similar to Weyl’s law. Recall that Weyl’s law for the Schrödinger equation is an asymptotic formula for the eigenvalue counting function:

$$ N(E) \sim N_V(E) := (2\pi)^{-n} \text{vol} \{ (x, \zeta) \in \Omega \times \mathbb{R}^n \mid V(x) + |\zeta|^2 \leq E \} \quad \text{as } E \to \infty, $$

where the volume term is the $2n$-dimensional measure of the indicated subset of the phase space $\Omega \times \mathbb{R}^n$. Assuming smoothness and growth conditions for the potential, Weyl’s law holds asymptotically as $E$ tends to $+\infty$ and so for a large number of eigenvalues [24, Theorem 6.8]. Inverting the counting function, we can thus view Weyl’s law as furnishing an approximation of the $n$th eigenvalue, which is asymptotically valid for $n$ large. Weyl’s law is generally not expected to be accurate for a small number of eigenvalues. However, experimentally we have found that, for the sorts of random potentials considered in this paper, a variant of Weyl’s law invoking the effective potential $W$ gives very good results right down to the first few eigenvalues, while remaining asymptotically correct. The variant, which we shall refer to as the effective Weyl’s law is obtained by simply replacing the potential $V$ in (10) by the effective potential $W$:

$$ N_W(E) = (2\pi)^{-n} \text{vol} \{ (x, \zeta) \in \Omega \times \mathbb{R}^n \mid W(x) + |\zeta|^2 \leq E \}. $$

Figure 15 compares the true eigenvalue counting function $N$ (shown in black), Weyl’s law (green), and the effective Weyl’s law (red), for four different types of potential.
The first is uniformly random iid with 512 pieces and values in $[0, 1]$. The second is Bernoulli potential where the 512 random values are either 0 or 1, each with probability $1/2$. The third is a correlated Gaussian squared potential like that of Figure 9. The fourth is the only deterministic potential treated in the paper: one in which the 512 Boolean values 0 and 1 are assigned alternately. We see that, in each case, Weyl’s law becomes a good approximation only after 100 or so eigenvalues and, in every case, it incorrectly predicts many eigenvalues in the interval from 0 to the least eigenvalue. By contrast, the effective Weyl’s law provides a very good approximation of the counting function for many eigenvalues, starting from the first. It is revealing to compare the two potentials which take on only Boolean values (the second and the fourth). Because the classical Weyl’s law is unaffected by rearrangement of the potential, it gives the same prediction for the counting function in both cases. But the actual counting functions differ very significantly, a fact which is well captured by the effective Weyl’s law. (Similar results were published in [4].)

Finally, in Figure 16 we show similar results for a single 2D potential, namely the uniformly random $80 \times 80$ potential of Figure 1. The first plot shows the first 100 eigenvalues, while the second zooms in on the first 10 eigenvalues. The predictive power of the effective Weyl’s law does not seem to be as great as in one dimension, but again it displays a great improvement over the classical Weyl’s law for small eigenvalues.
Fig. 15. The eigenvalue counting function $N$, the Weyl’s law approximation $N_V$, and the effective Weyl’s law approximation $N_W$ for some potentials in one dimension. Top row: uniform and Boolean random potentials. Bottom row: correlated and periodic Boolean potential.

Fig. 16. The eigenvalue counting function $N$, the Weyl’s law approximation $N_V$, and the effective Weyl’s law approximation $N_W$ for a 2D potential.

6. Conclusion. We have demonstrated numerically that the effective potential, defined as the reciprocal of the localization landscape function, accurately captures a great deal of information about the localization properties of a random potential, and shown how to employ it to predict eigenvalues and eigenfunctions. These predictions are attained by solving a single PDE source problem, without the direct solution of any eigenvalue problems, and so at a very low computational price. The wells of the effective potential reveal the main localization subdomains, and the values of
its minima are found to be very good predictors of the corresponding fundamental eigenvalues. We have tested this approach on piecewise constant potentials with several types of random distributions, uniformly random and Bernoulli, and with a certain correlated distribution, both in one and two dimensions. We have further used the effective potential to predict the density of states and obtain good precision even for small eigenvalues, something which is not attained by the classical Weyl law asymptotics. In highly demanding computations where the Schrödinger equation has to be solved for a large number eigenfunctions and eigenvalues (as for instance in semiconductor physics), the resulting computational efficiency makes it now possible to reproduce numerically, to analyze, and to understand the behavior of quantum disordered materials.

REFERENCES


