Evaluation of the Lanczos algorithm for studying Anderson localization on finite and infinite lattices*

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A method of transforming the tight-binding model into a basis generated by the Lanczos algorithm for tridiagonalization of matrices is investigated as way to derive properties of Anderson localization. The Lanczos algorithm is used analytically and numerically on finite and infinite lattices. Some asymptotic estimates are reported and a perturbation theory approach for single-site disorder is developed. A mobility edge on a finite lattice is computed, and numerical behavior of localized states on the infinite lattice are investigated.

I. INTRODUCTION

Studying the mobility of electrons in materials is one of the central themes of solid state physics. In the conventional model of an ordered periodic lattice, Bloch's theorem states that electron wavefunctions are spatially extended with periodic behavior. Realistic materials, however, do not conform exactly to the picture of a perfectly ordered lattice. Naïvely, one might suppose that the introduction of disorder would simply decrease the conductivity proportionally to the disorder, but this picture is not preferable *a priori* to more complicated possibilities involving phase transitions with respect to a change in disorder. Indeed, Anderson argued in a seminal 1958 paper that with a critical level of disorder, some eigenstates on disordered lattices are spatially localized, decaying exponentially.[1] Since this initial work, a large literature has, with mixed success, attempted to better understand the circumstances under which localization occurs.

Various approaches have been used to study localization including perturbation theory, field theory, and numerical simulations. One recent work[2] has studied localization on an infinite lattice by transforming the problem from a coordinate basis to a basis of extended wavefunctions. We explore a different change of basis, commonly used in numerical analysis, using an algorithm of Lanczos for bringing a Hermitian matrix to tridiagonal form.[3] The advantages of this approach are that the basis is analytically simple and that basis vectors have finite support so that numerical verification is possible. Writing the hamiltonian in tridiagonal form has the effect of mapping a 2D or 3D tight-binding model onto a 1D lattice with nearest neighbor interaction.

II. THE ANDERSON MODEL

The Anderson model is a minimal model for studying phenomena on lattices: it is simple enough to be tractable, complicated enough to contain interesting physics, and easily extensible for modeling more realistic situations. Consider the d-dimensional cubic lattice $\mathbb{Z}^d$. Define the following hamiltonian

$$H = h \sum_{\substack{\mathbf{r}\in\mathbb{Z}^\mathbf{d} \\ \mathbf{r}'\in\mathbf{N}(\mathbf{r})}} |\mathbf{r}\rangle \langle\mathbf{r}'| + \sum_{\mathbf{r}\in\mathbb{Z}^\mathbf{d}} \epsilon_\mathbf{r} |\mathbf{r}\rangle \langle\mathbf{r}| . \tag{1}$$

The first summation is taken over all pairs of nearest neighbor sites on the lattice, with $N(\mathbf{r})$ denoting the set of nearest neighbors: lattice sites distance 1 away from the site $\mathbf{r}$. This term represents the energy associated with "hopping" between sites on the lattice, and the coefficient h is assumed to be constant over all sites. The second term is the energy associated with each site itself, where the sum taken over all sites. To add disorder to the system, we let $\epsilon_\mathbf{r}$ be a random variable chosen from a uniform distribution taking values on the interval $[-W/2, W/2]$. With this choice, the amount of disorder is characterized by the choice of the ratio W/h. A variety of disorder distributions have been studied in the literature, but the uniform distribution is most common and we will restrict ourselves to the uniform case in this paper.

In the case of no disorder, $\epsilon_\mathbf{r} = 0$, and the solutions to equation (1) are simply the familiar Bloch waves

$$\psi(\mathbf{r}) = \sum_{\mathbf{r}\in\mathbb{Z}^\mathbf{d}} \mathbf{e}^{\mathbf{i}\mathbf{k}\cdot\mathbf{r}} |\mathbf{r}\rangle .$$

The introduction of disorder, however, produces destructive interference that causes some eigenstates to have an exponential envelope. With a sufficiently large disorder term, all states may become localized. Previous work has focused on determining the amount of disorder needed to localize all eigenstates, but there are many conflicting numerical and analytic arguments. While few results have been rigorously proven, there is mathematical proof that strong disorder localizes all states in arbitrary dimensions.[4]

One important question that arises in studying localization is how to characterize a localized state as opposed to an extended state. The Green's function for the Anderson hamiltonian contains information on the localization of states, and was one of Anderson's original objects of interest.[5] Green's functions have played a

central role in the study of localization, both in the informal arguments to characterize localization in the physics literature and in the rigorous mathematical studies of the phenomenon. Indeed, the proof of localization by Fröhlich, et al. relies on an estimate of the decay of the Green's function for a Schödinger operator with uniform disorder, as in equation (1).[4]

Recall that the Green's function for the time-dependent Schrödinger equation, or the so-called propagator, gives the probability amplitude for a particle at a position $\mathbf{r}$ and time 0 to be at $\mathbf{r}'$ at a time t, and it is given by

$$\langle \mathbf{r}' | \, G(t) \, | \mathbf{r} \rangle = \langle \mathbf{r}' | \, e^{-iHt/\hbar} \, | \mathbf{r} \rangle \, .$$

The physical meaning of the Green's function immediately suggests its usefulness for studying localization: Green's functions of localized states decay exponentially, while those of extended states do not. Taking the Fourier transform of the operator $G(t)$ recasts Green's function into a more convenient form in terms of the energy.

$$\begin{aligned} G(E) &= \frac{i}{\hbar} \int_0^\infty e^{-iHt/\hbar} e^{iEt/\hbar} dt \\ &= (E - H)^{-1}. \end{aligned}$$

Thus, in addition to representing transition amplitudes between sites, we see the familiar form of the Green's function as a solution to the homogeneous Schrödinger equation $(E - H)G(E) = \mathbf{1}$. If we consider the position-space representation of this object, then we obtain matrix elements between lattice sites

$$G(\mathbf{r}, \mathbf{r}'; E) = \langle \mathbf{r} | \, (E - H)^{-1} \, | \mathbf{r}' \rangle \, .$$

A simple example of Thouless,[6] relevant to our application of the Lanczos algorithm in later sections, illustrates one of several ways that Green's functions can employed in localization theory. Consider a 1-dimensional lattice with N sites. Define a hamiltonian as in equation (1), with the modification that for endpoints $H_{0,1} = H_{N,N+1} = 0$ because the lattice is finite. In the position basis, the hamiltonian takes tridiagonal form with the random onsite energies on the diagonal and the nearest-neighbor hopping amplitudes on the off-diagonals. If an eigenstate is localized then it has a low probability of passing through the entire lattice, and thus we would expect the matrix element representing this probability, $G_{1N}(E)$, to scale with the localization length. In this special case, this matrix element is particularly easy to calculate because $G(E)$ is just the inverse of the matrix $E\mathbf{1} - H$, whose form we know explicitly. We can use the cofactor expansion for the matrix inverse to obtain the desired matrix element. For this tridiagonal matrix, we find that

$$G_{1N}(E) = \frac{\prod_{i=1}^{N-1} V_{i,i+1}}{\det(E\mathbf{1} - H)}. \tag{2}$$

It is clear from equation (2) that G_{1N} has a simple pole at an energy eigenvalue $E = E_\beta$. We also have another expression for this matrix element of the Green's function, obtained by projecting $(E - H)^{-1}$ into the energy eigenbasis, and taking the overlaps with position states $|1\rangle$ and $|N\rangle$,

$$G_{1N}(E) = \sum_{\alpha=1}^{N} \frac{\langle 1|\alpha\rangle \, \langle \alpha|N\rangle}{E - E_\alpha}. \tag{3}$$

Setting equal the residues of equations (2) and (3) at $E = E_\beta$ and taking the logarithm we find

$$\ln |\langle 1|\alpha\rangle \, \langle \alpha|N\rangle| = \sum_{i=1}^{N-1} \ln |V_{i,i+1}| - \sum_{\alpha \neq \beta} \ln |E_\beta - E_\alpha| \, . \tag{4}$$

For extended states, we expect the amplitude $\langle \alpha|i\rangle$ at the i^{th} site to be of order $1/N$, and consequently equation (4) is proportional to $-2 \ln N$. With the ansatz an exponentially localized state with maximum amplitude at the i^{th} site, we have $\langle \alpha|1\rangle = e^{-\lambda(i-1)}$ and $\langle \alpha|N\rangle = e^{-\lambda(N-i)}$, where $\lambda(E)$ is known as the Lyapunov exponent and $\lambda^{-1}(E)$ is the localization length. Since $\lambda(E)$ depends on the particular random disorder terms associated with the realization of the system being considered, it is useful to average this exponent over many realizations of the system. Doing so with equation (4), we obtain

$$\lambda^{-1}(E_\beta) = \lim_{N \to \infty} \frac{1}{N} \overline{\left[\sum_{i=1}^{N-1} \ln |V_{i,i+1}| - \sum_{\alpha \neq \beta} \ln |E_\beta - E_\alpha| \right]}.$$

III. THE LANCZOS ALGORITHM

The Lanczos algorithm is an iterative technique that brings a hermitian matrix into tridiagonal form. The procedure produces a new basis by choosing an arbitrary initial vector $|0\rangle$, and calculating orthogonal vectors until the set spans the Krylov subspace generated by H and $|0\rangle$. The initial step is given by

$$H \, |0\rangle = a_0 \, |0\rangle - b_0 \, |1\rangle \, , \tag{5}$$

and subsequent iterations for $n > 1$ are given by

$$H \, |n\rangle = -b_{n-1} \, |n-1\rangle + a_n \, |n\rangle - b_n \, |n+1\rangle \, . \tag{6}$$

Requiring the basis vectors to be orthonormal, we can calculate the coefficients a_n, b_n, and basis vectors $|n\rangle$,

$$a_n = \langle n|H|n\rangle \tag{7}$$

$$b_n = |b_{n-1} \, |n-1\rangle - a_n \, |n\rangle + H \, |n\rangle| \tag{8}$$

$$|n+1\rangle = -\frac{1}{b_n} \left(-b_{n-1} \, |n-1\rangle + a_n \, |n\rangle - H \, |n\rangle \right) \tag{9}$$

If carried out in exact arithmetic for a finite matrix M, the Lanczos procedure will terminate after r iterations, where r is the number of distinct eigenvalues of M. On an infinite lattice, however, the hamiltonian does not have a

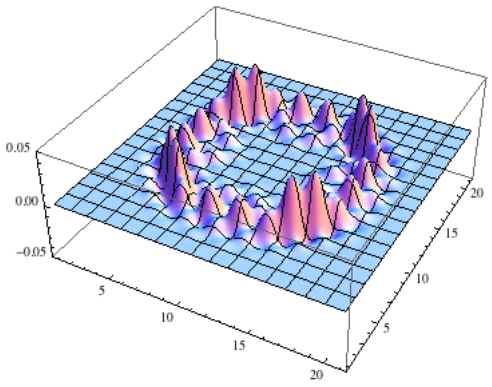

FIG. 1: The square amplitude of the Lanczos basis vector for $n = 10$.

finite number of distinct eigenvalues. Consequently, the Lanczos algorithm will continue indefinitely.

In the situation of finite precision encountered when numerically tridiagonalizing matrices, rounding errors develop in the procedure. This corrupts the orthogonality of the basis states. The violation of orthogonality means that the Lanczos procedure will not necessarily truncate after a number of iterations equal to the number of distinct eigenvalues of the matrix. There are, however, several ways of mitigating this problem. When rounding errors are problematic and memory is plentiful, greater precision can be used in the calculation or states can be reorthogonalized using Gram-Schmidt at each iteration. The latter, however, is quite slow and can be impractical if a large number of iterations is needed. Since a Lanczos procedure with rounding errors will not terminate, one can also continue the iterations to produce a matrix far larger than the original one. C. Paige demonstrated that even with rounding errors, nearly identical eigenvalues of the tridiagonal matrix converge to eigenvalues of the original matrix.[7] Thus by looking for eigenvalues of the tridiagonal matrix that are very closely bunched, one can approximate some eigenvalues of the original matrix. This method is biased toward extremal eigenvalues in the spectrum, and it does not generate all eigenvalues, but it can be useful when only some of the eigenvalues are needed.

IV. APPLICATION OF THE LANCZOS ALGORITHM

The Lanczos algorithm can be applied to the localization problem both analytically and numerically. Analytically, it functions as a change of basis that simplifies a perturbative analysis of disorder. Numerically, it is easy to implement so that it can easily be used to check analytic arguments and as part of numerical simulations of localization.

Goldenfeld and Haydock[2] were motivated by a similar idea, but they chose to change to a basis of distorted extended states in a so-called augmented space often used to study electronic states of disordered alloys. Their idea was to incorporate the disorder of the Anderson hamiltonian into the definition of the new basis vectors, rendering the transformed hamiltonian nonrandom. Consequently, the basis vectors had some randomness and had infinite support. The obvious advantage of this approach is that eliminating the randomness of the hamiltonian causes its asymptotic analysis to be much more tractable. On the other hand, since the basis vectors are extended states with infinite support, this method cannot be numerically simulated alongside the analytic work.

The Lanczos approach begins with an arbitrarily chosen initial vector. While the initial vector can be arbitrary, the simplest choice is a vector with amplitude 1 at the origin and amplitude 0 everywhere else. In the case of no disorder, the Anderson hamiltonian in equation (1) has $\epsilon_{\mathbf{r}} = 0$ and therefore $a_n = 0$ for all n in equation (5). The hamiltonian thus represents a random walk, starting at the origin, with equal probability of hopping to any nearest neighbor site. For such a model, the amplitude at a given site after n iterations, or the probability of a particle starting at the origin to reach a given site after n steps, is simply proportional the number of paths to the given point divided by the total number paths. If we wish to consider a point on the perimeter of the support of some $|n\rangle$, this amplitude takes a particularly nice form. In order to reach the perimeter of supp $|n\rangle$ in n iterations, the steps must all be taken in the same direction in each coordinate. In two dimensions, for example, the amplitude on the perimeter is given by the binomial coefficient, and for even n this attains a maximum at the site $(n/2, n/2)$ where

$$\psi(n/2, n/2) = A\frac{n!}{(n/2)!(n/2)!} = O(n^{-1/2}),$$

and A is a constant of proportionality.

Analytically, we expect that the Lanczos basis vectors without disorder should be peaked at points $(n/d, n/d, ..., n/d)$ on the perimeter of support, and that the states should increase in perimeter like a wave moving outward from the origin. Numerical simulation confirms this expectation, as shown in figure 1. The introduction of weak disorder into the hamiltonian changes the picture of figure 1 slightly, by increasing the amplitude in the center of the region of support by random amounts.

There are several quantities of interest that can be calculated numerically from this approach. We can calculate, for example, the asymptotic behavior of the localization length as introduced in the section II. Since the area of support of the Lanczos basis vectors increases with the number of iterations, exponentially localized states in the position basis should be exponentially localized in the Lanczos basis. In other words, if the amplitude of an eigenstate decays exponentially far from the origin, then the coefficients of Lanczos basis vectors with nonzero amplitude there–all $|n\rangle$ for n greater than some

fixed M–should be exponentially small. This allows us to calculate the localization length in the same way that we calculated it in II: replace the $V_{i,i+1}$ by b_n, since the hamiltonian has been transformed to tridiagonal form. Thus we expect

$$\lambda = \lim_{N\to\infty} \frac{1}{N} \overline{\left[\sum_{n=1}^{N-1} \ln|b_n| - \sum_{\alpha\neq n} \ln|E_\beta - E_\alpha| \right]}. \quad (10)$$

The first case of interest is the case of no disorder, for which the Lanczos basis vectors are described above. From equation (7), the coefficients a_n are all equal to 0 in the absence of disorder. Less obvious, but easy to calculate is the fact that the b_n converge rapidly to the dimension of the system.[8] Noting these facts and the fact that the spectrum of a d-dimensional, ordered, tight-binding hamiltonian is $E(k_1, ..., k_d) = 2(\cos k_1 + ... + \cos k_d)$, we expect $\lambda(E) = 0$ for $E \in [-E, E]$. This agrees with the expectation that the absence of disorder should only produce extended states.

For the purpose of an analytic calculation, the simplest way to introduce disorder into the system is to calculate the behavior of the coefficients a_n and b_n due to the presence of a single disordered site, representing an impurity, located near the origin. This can be done perturbatively, so that we can reuse our information on the unperturbed basis states. We attempt to convert the new hamiltonian to tridiagonal form by writing each matrix element as the sum of the unperturbed matrix element with a correction. We then use the corrected matrix elements in equation (10) to compute the localization length. The hamiltonian in this situation is $H = H_0 + \epsilon H_1$, where $H_1 = |\mathbf{r}\rangle\langle\mathbf{r}|$. We divide the Lanczos basis vectors into a sum $|n\rangle = |n^0\rangle + \epsilon|n^1\rangle$, where $|n^0\rangle$ is the unperturbed basis vector and $|n^1\rangle$ is the correction due to the impurity. In a similar manner, we write $a_n = a_n^0 + \epsilon a_n^1$ and $b_n = b_n^0 + \epsilon b_n^1$. We then divide the recurrence relation into a 0^{th}-order equation and a 1^{st}-order equation. The 0^{th}-order equation is identical to the unperturbed recurrence relation in equation (6). The 1^{st}-order equation for the initial vector is formally given by

$$H_0|0^1\rangle + H_1|0^0\rangle = a_0^0|0^1\rangle + a_0^1|0^0\rangle - b_0^0|1^1\rangle - b_0^1|1^0\rangle.$$

We arbitrarily set $|0\rangle$ regardless of the impurity. So $|0^1\rangle = 0$, and we reduce the initial equation to

$$H_1|0^0\rangle = a_0^1|0^0\rangle - b_0^0|1^1\rangle - b_0^1|1^0\rangle.$$

The general recurrence relation is given by

$$\begin{aligned} H_0|n^1\rangle + H_1|n^0\rangle = -b_{n-1}^0|n-1^1\rangle - b_{n-1}^1|n-1^0\rangle \\ +a_n^0|n^1\rangle + a_n^1|n^0\rangle - b_n^0|n+1^1\rangle - b_n^1|n+1^0\rangle. \end{aligned}$$

After a moment of reflection on the recurrence relations, it is clear that all corrections to the unperturbed system vanish until the outgoing wave of the basis vectors has nonzero overlap with the site of the impurity.

In order to calculate expressions for the a_n^1, b_n^1, and $|n+1^1\rangle$, we proceed in the same manner as in the unperturbed case, exploiting normalization and orthogonality relations to perform the calculation. The normalization and orthogonality relations chosen are only approximate, but this choice simplifies the problem considerably. The conditions that we demand are

$$\langle n|m\rangle = \delta_{nm} \quad (11)$$

$$\langle n^0|m^0\rangle = \delta_{nm}. \quad (12)$$

By substituting $|n^0\rangle + \epsilon|n^1\rangle$ into equation (11), using equation (12), and carrying the result to first order, we obtain

$$\langle n^1|n^0\rangle + \langle n^0|n^1\rangle = 0$$

$$\langle n^1|m^0\rangle + \langle n^0|m^1\rangle = 0 \text{ for } n \neq m.$$

Since all entries of $|n\rangle$ are real, we deduce

$$\langle n^1|n^0\rangle = 0, \quad (13)$$

and we record

$$\langle n^1|m^0\rangle = -\langle n^0|m^1\rangle \text{ for } n \neq m. \quad (14)$$

Taking inner products between the general recurrence relations and the proper choice of vectors, and then applying equations (13) and (14), we find that

$$\begin{aligned} a_0^1 &= \langle 0^0|H_1|0^0\rangle, \\ b_0^1 &= 0, \\ |1^1\rangle &= \tfrac{1}{b_0^0}\left(a_0^1|0^0\rangle - H_1|0^0\rangle\right). \end{aligned}$$

In the general recurrence relation, we have

$$\begin{aligned} a_n^1 = \langle n^0|H_0|n^1\rangle + \langle n^0|H_1|n^0\rangle + b_{n-1}^0\langle n^0|n-1^1\rangle \\ +b_n^0\langle n^0|n+1^1\rangle, \\ b_n^1 = -\langle n+1^0|H_0|n^1\rangle - \langle n+1^0|H_1|n^0\rangle \\ -b_{n-1}^0\langle n+1^0|n-1^1\rangle + a_n^0\langle n+1^0|n^1\rangle, \\ |n+1^1\rangle = \tfrac{1}{b_n^0}(-b_{n-1}^0|n-1^1\rangle - b_{n-1}^1|n-1^0\rangle + a_n^0|n^1\rangle \\ +a_n^1|n^0\rangle - b_n^1|n+1^0\rangle - H_0|n^1\rangle - H_1|n^0\rangle). \end{aligned}$$

Although it is not immediately obvious from the form of the recurrence relations, numerical calculation to be discussed in the next section shows that in this approximation we actually have $b_n^1 = 0$ for all n. In this setting, the localization length for the perturbed system in the Lanczos basis becomes

$$\lambda'^{-1}(E_\beta) = \lim_{N\to\infty} \frac{1}{N} \overline{\left[\sum_{i=1}^{N-1} \ln|b_i^0| - \sum_{\alpha\neq\beta} \ln|E_\beta - E'_\alpha| \right]}, \quad (15)$$

where the prime indicates that we are considering the perturbed system. To obtain the perturbed localization length completely in terms of unperturbed quantities, we need to calculate the perturbed energy eigenvalues. To do this, note that the tridiagonal form of the perturbed hamiltonian is

$$H' = H_0 + \epsilon V, \tag{16}$$

where V is a diagonal matrix with entries of a_n on the diagonal. Calculating the energy shift from 1^{st}-order perturbation theory is thus trivial. If $|\psi_n\rangle$ are the energy eigenvectors with coefficients c_n in the Lanczos basis, then the energy shift is

$$\begin{aligned} E'_\alpha - E_\alpha &= \epsilon \langle\psi_n| V |\psi_n\rangle \\ &= \epsilon \sum_n |c_n|^2 V_{nn}. \end{aligned}$$

All the variables in equation (15) for the perturbed localization length are now determined in terms of the unperturbed quantities. It is far from clear, however, where to proceed analytically from here. While equation (15) can be calculated numerically, it is quite difficult to determine the limiting behavior of the a_n and b_n from analytic arguments. Moreover, taking the necessary limit requires knowledge of the density of states, and integrating against a logarithm. While the densities of states for the 1D and 2D ordered tight-binding models are known, the Lanczos algorithm does not map the 2D tight-binding model onto an exact 1D tight-binding model because of the oscillation in the b_n. Moreover, integrating the density of states against a logarithm is tricky because of singularities in 1D and 2D expressions.

V. NUMERICAL STUDIES

In parallel with the analytic calculations, a variety of numerical studies were performed on both finite and infinite lattices. All results discussed here were performed in 2 dimensions. Calculations were performed in Mathematica using machine-precision arithmetic with 15.9546 significant figures on a 2GHz Core Duo MacBook running Mac OS 10.5.8. Mathematica carries out internal calculations with 50 significant figures, and it uses a large number of optimization schemes. These features of Mathematica increase the effective precision beyond the reported machine-precision.

The primary disadvantage of the Lanczos method, is the accumulation of rounding errors discussed earlier. Our experience and the experience of others suggest that the size of rounding errors with the Lanczos method can range from negligible[9] to very large[10], depending on the particular form of the Hamiltonian and the number of iterations used. With no disorder, the maximum overlap between Lanczos basis states produced by 80 iterations of the procedure was about $3.1 \cdot 10^{-15}$. Other situations had worse rounding errors, but the precision of the arithmetic in Mathematica was increased when necessary to maintain a maximum overlap of order 10^{-5} or less between states that were supposed to be orthogonal.

In the infinite case, simulations were initially performed in the absence of disorder. As expected in the previous section, $a_n = 0$, $b_n \to d$ rapidly, and the basis vectors appeared as outgoing waves from the origin. Moreover, direct calculation indicates that $\lambda(E) \to 0$, albeit at a somewhat slow rate of convergence. Unfortunately, an analytic calculation of the localization length is extremely difficult since the density of states in two dimensions is an complete elliptic integral of the first kind.

There are two ways to proceed with the addition of disorder. Disorder can be added at a single site, or at all sites. While it was hoped that the convergence of energy eigenvalues would provide a criterion for the localization of states, this method turns out to be infeasible.

Nevertheless, at least some localized eigenvalues do converge for another reason. Since the Lanczos basis vectors have the property that their support increases in size with the number of iterations, and since localized states have an exponentially small contribution from sites far from the origin, localized states should have small contribution from Lanczos basis vectors for large values of n. In other words, states localized in the coordinate basis should be localized in the Lanczos basis. In practice, this does not always occur for localized states, or at least localization lengths in the Lanczos basis tend to be much longer than in the position basis. Although some eigenvalues do converge near the band edge, the eigenvalues in the center of the energy band take much longer to converge if they converge at all. The question of convergence is also complicated by the fact that new eigenvalues are introduced as the number of iterations increases, so it is difficult to numerically separate genuine convergence from random lingering of an eigenvalue around a newly introduced eigenvalue. In short, this behavior is not well-understood, and it is not clear that it is useful as a localization criterion.

With disorder at a single site and using the perturbative approximation scheme discussed in the previous section, the corrections $b_n^1 = 0$ for all n. The corrections a_n^1 gradually converge to 0 after the basis vectors cross the site of the impurity. The convergence of the a_n^1 is show in figure 2.

Numerical simulations were also performed on finite lattices with periodic boundary conditions to determine the behavior of the unperturbed basis vectors and to reproduce an earlier study calculating the mobility edge of the system.[10] In the case of no disorder, the Lanczos method is not useful because the spectrum of the hamiltonian is $E(k_1, ..., k_d) = 2(\cos k_1 + ... + \cos k_d)$ with $k_i = 2\pi n_i / N$, which has a large degeneracy. Since the Lanczos algorithm does not detect degenerate eigenvalues, the basis produced by the iterative process is not a complete basis for the lattice, and it leads to a biased density of states.

The introduction of disorder breaks the degeneracy in

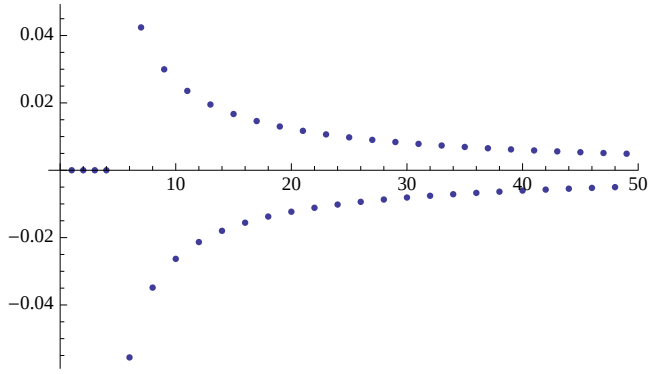

FIG. 2: Plot of the values of a_n^1 in the perturbative approximation. The first nonzero value occurs for the smallest n for which $|n\rangle$ has overlap with the impurity.

the spectrum, and it is a straightforward exercise to calculate a so-called "mobility edge" using a method developed by Thouless, Edwards, and Licciardello[10]. These authors noted that a localized state should be insensitive to a change in boundary conditions due to the exponentially small amplitude on the boundary of the system. More precisely, for an extended state, we expect that the amplitude at a site should be, on average, proportional to the number of sites in the system. So if we calculate the shift in energy of a state when switching from periodic to antiperiodic boundary conditions, ΔE, we should find that $N\overline{\Delta E}dn/dE$ is independent of the size of the system. For the exponentially decaying localized states, we should find that $N\overline{\Delta E}dn/dE$ decreases with the size of the system. Since the energy shifts ΔE vary considerably for different realizations of the system, the geometric mean $\overline{\Delta E}$ over many realizations is used. We plot this number in various energy bins with increasing N. The energy at which this product begins to decrease with the size of the system is the critical energy between localized and extended states. This exercise is shown in Figure 3, with a mobility edge between $E = 3$ and $E = 3.5$. The eigenvalues are sorted into energy bins of width 0.5, the geometric mean of the energy shifts for all eigenvalues in each bin is computed, and the procedure is averaged over 40 realization of the disorder.

VI. CONCLUSIONS

The Lanczos algorithm was used analytically as a change of basis to study localization. A perturbative transformation of single-site disorder was developed. Future work may be able to extend this approach to single-site disorder to disorder at all sites on the infinite lattice. Numerical results were also studied on finite and infinite lattice. The results on finite lattices reproduce older work. The numerical results on infinite lattice are complicated by difficulties regarding the convergence of eigenvalues. In particular, it is not clear that all eigenvalues of localized states should converge, and it is not clear how to determine when an eigenvalue has converged.

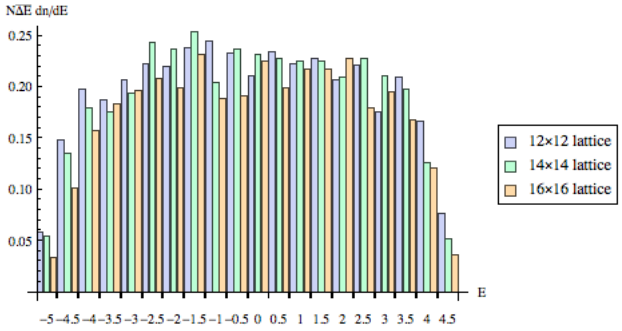

FIG. 3: Plot of the energy shift method showing a mobility edge around $E = 3.5$ for $W/h = 6$.

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