Predicting High Energy Eigenstates by Coupling Discrete Supersymmetry and the Localization Landscape

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Abstract

Anderson localization, a phenomenon describing "localization" in the lower band of the eigenspectrum of a Hamiltonian was largely observationally confirmed throughout the 20th century. It was not until recently that a formalized method named the "localization landscape" based upon solving a Dirichlet problem corresponding to the Schrodinger equation allows one to derive a "landscape" function that effectively predicts the localization regions of the wave functions. However, as the energy values of the system enlarge, states become essentially delocalized as they get enough energy to surpass the potential barriers, making them difficult to predict. The present work is focused on resolving this difficulty by coupling the formalism with discrete supersymmetry, which allows for generation of a hierarchy of isospectral Hamiltonians, with the ground state removed. Because the ground state is removed every iteration of discrete SUSY, we "climb" the ladder of eigenstates by generating new Hamiltonians whose low energy eigenstates correspond to the high energy eigenstates of the original system. A new landscape formalism was needed, as nearest neighbor hopping values become non-constant throughout iterations of supersymmetry. Limitations including the alteration of eigenstates throughout the supersymmetry process and potential ways to undo the transformation are discussed. Future work and applications include analysis on specific models, like the Andre-Aubry model, and further expansion on the theoretical rigor of the formalism.

1 Introduction

We often encounter cases where we would like to approximate eigenvalues and eigenvectors in the context of an eigenvalue problem instead of directly solving. This problem is common in large systems, such as those that commonly show up in physics, because diagonalizing a matrix becomes inefficient and simply approximating the eigenvectors saves computing time and still satisfies the requirements for analysis.

In the 20th century, Anderson observed electronic states of random potential systems exponentially localizing in tight regions in a phenomenon now called "Anderson Localization" [1]. This is explained due to destructive interference of reflected waves in the random potential. Anderson localization was observationally confirmed multiple times and became an important topic of study [2–5], but it was not until quite recently that a formalized method to derive a function that can predict the localization regions was pioneered, and will be discussed in further detail in Section 1.1 [6, 7]. Arnold *et. al* expanded this formalism to also predicting eigenvalues based on the local minima of the landscape function [8].

However, as we go up to higher energy values, the corresponding states of the system become harder to predict. To see why, imagine the classical example of a ball in a valley; when bounded by high cliffs, it remains localized within the valley. However, given more energy, it can often scale the cliffs and enter new valleys in the domain. Analogously, eigenstates surpass their nearby barriers when they correspond to sufficiently high energy, becoming "delocalized." The approximation in particular of delocalized eigenstates that appear correspondingly to high energy states has always proved difficult,

as the function becomes spread across the domain.

In this work, we aim to develop an iterative coupling algorithm that allows for approximation of these delocalized states. We will discuss each part separately.

1.1 Localization Landscape

There has been a lot of interest in the remarkable "localization landscape" as it is able to predict the localization regions of the eigenfunctions of a Hamiltonian. The concept can be introduced quite simply: in the continuum case, given a Schrodinger equation for one particle, we can define a new function u based on the Green's function $H^{-1}(\boldsymbol{r}, \boldsymbol{r'})$.

$$[\frac{\hbar}{2m}\nabla^2 + V]\psi = H\psi = E\psi, u = \int_\Omega |H^{-1}(\boldsymbol{r}, \boldsymbol{r'})| d\boldsymbol{r'} \tag{1}$$

u is called the localization landscape, as it depends on r. The only constraint we place on our Hamiltonian is that $V \geq 0$. This necessarily results in a positive definite Hamiltonian i.e. $E \geq 0$. Thus, the absolute value bars disappear, and then u simply becomes the solution to a significantly easier Dirichlet problem:

$$[\frac{\hbar}{2m}\nabla^2 + V]u = Hu = 1 \tag{2}$$

It can be shown that u also satisfies the following relationship:

$$|\psi(x)| \leq Eu(x) \tag{3}$$

Due to normalization of the wave function, this constraint is only meaningful when $u \leq 1/E$. Thus, in regions where u satisfies this inequality, we expect

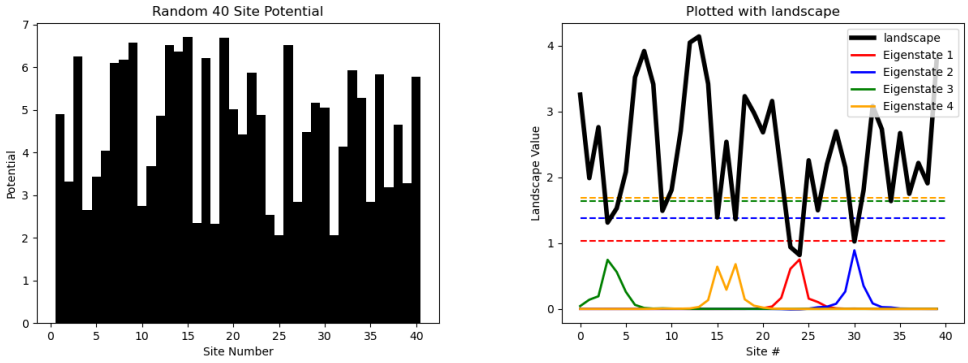

FIGURE 1: A random 40 site potential is plotted on the left. On the right, the corresponding landscape function W, or pseudopotential, is plotted with the 4 lowest eigenstates of a random potential. The eigenvalues are also shown through dashed lines to reveal the predicted localization regions of the respective eigenstates.

the wave function to be localized. The appearance of this relationship motivates us to define a new function $W = 1/u$, so that the relationship becomes when $W \leq E$. W, as plotted on the right in Fig. 1, appears as a smoothed version of the random potential V on the left, and thus is often called the "pseudopotential." We can see from Fig. 1 that the landscape does indeed accurately predict the locations of the eigenstates, and the eigenvalues reveal the locations in which the eigenstates reside. This conclusion has been mathematically and observationally proven to work in many contexts and with various random potentials [7, 9].

This is rather remarkable; instead of having to diagonalize a large matrix to find all eigenvalues and eigenstates, which often takes about $N^2 \log(N)$ time, we simply invert the matrix or solve the linear system of $Hu = 1$, which takes more around $N \log(N)$ time.

However, the limitations of the localization landscape become apparent in higher energy states: as E grows, it surpasses the lower peaks of W and thus adjacent localization regions join together, thus delocalizing the eigenstates. The landscape then becomes pretty poor at predicting the location and decay of the these eigenstates. It has been shown that there is also localization that can be predicted at other parts of the spectrum through a similar formalism [10], but behavior elsewhere still remains unpredictable.

This localization landscape notion has been generalized to discrete lattices, which is our focus in this work since we are working with supersymmetry on a lattice [10]. Assuming a lattice on sites $i = 1, ..., L$ with constant nearest neighbor hopping of t and boundary conditions of $\psi_0 = \psi_{L+1} = 0$ we can reexpress the Schrodinger equation defined in Eq. 1 as the following:

$$-t(\psi_{i-1} + \psi_{i+1}) + V_i(\psi_i) = \lambda_i \psi_i \tag{4}$$

Essentially, this is the discrete version of the Schrodinger equation. Thus, the corresponding Dirichlet problem changes as well:

$$-t(u_{i-1} + u_{i+1} - 2u_i) + (V_i - 2t)u_i = 1 \tag{5}$$

with boundary conditions $u_0 = u_{L+1} = 0$. There is also a corresponding inequality for Eq. 3 in the discrete case ($j = 1, ..., L$):

$$\frac{|\psi_j|}{\max_k |\psi_k|} \leq \lambda u_j \tag{6}$$

Again, the discrete case experiences the same limitations as the the continuum case in predicting delocalized states. In this work, we aim to address this limitation through the coupling.

1.2 Supersymmetry

The other half of the coupling comes from supersymmetry, which provides a method of generating a hierarchy of isospectral Hamiltonians with partner superpotentials [11]. Like in Section 1.1, we will first discuss the continuum case; the discrete case will be detailed as part of the algorithm in Section 2.1. We begin again with the Schrodinger equation of a one particle system like in Eq. 1. Assume $_0 = 0$. We can then factorize the Schrodinger equation in the following ansatz:

$$H = A^\dagger A \tag{7}$$

We can then construct $H' = AA^\dagger$, and upon inspection, it is just another Hamiltonian with a potential V_2:

$$H' = -\frac{\hbar}{2m}\frac{d^2}{dx^2} + V_2(x) \tag{8}$$

It turns out, the eigenvalues and eigenfunctions of H' and H are very related: $E'_n = E_{n+1}$, and $\psi' = A\psi$ [11]. Notice, that the ground state energy of $E_0 = 0$ has been annihilated in the process, resulting in a Hamiltonian in which the lowest energy state is simply E_1. Now, note that this could be done many more times, each time resulting in a Hamiltonian with a higher ground state energy than before.

Motivated by this annihilation of the ground state while preserving the rest of the spectrum and related eigenstates, we aim to couple this with the landscape formalism in order to predict the behavior of the middle-high end of the spectrum of the original Hamiltonian. The proposed algorithm requires discretizing both supersymmetry and the landscape formalism, which the latter proves to be nontrivial. However, the results indicate that this coupling

proves to be a potentially powerful predictor of delocalized eigenstates.

2 Theory

2.1 Discrete Supersymmetry

Discrete quantum supersymmetry begins the same way as continuous supersymmetry, except with a discrete Hamiltonian and Schrodinger equation (Eq. 4). Notice: the left side can easily be expressed as left multiplying by a tridiagonal matrix $\hat{H}$, where $\hat{H}_{i,i} = V_i$, $i = 1, ..., L$, $\hat{H}_{i+1,i} = -t$, $i = 1, ...L-1$, and $\hat{H}_{i,i+1} = -t$, $i = 1, ...L-1$. The energy spectrum is now described by the eigenvalues of the matrix and the corresponding wavefunctions are described by the eigenvectors. Now, we would like to proceed with a factorization/decomposition similar to Eq. 7.

Something already interesting on its own is that when the Hamiltonian is expressed as a matrix, the ansatz in Eq. 7 is the same as a family of algorithms in the computing community; namely, the LR/LU, QR, and Cholesky decompositions/algorithms [12, 13]. Iterating through these algorithms has been shown to converge to a diagonal matrix, thus exposing the eigenvalues [14]. Knowing this connection allows us to both speed up computation time and make some important observations.

Primarily, we notice that our assumption that $E_0 = 0$ necessarily implies our matrix Hamiltonian is now positive semi-definite. Problematically, a Cholesky decomposition is only unique when the matrix is positive definite; however, with a minor alteration, this problem is fixed. If the factors are rectangular instead of square, the decomposition is now unique and we avoid

directly calling it a Cholesky decomposition. In other words, when A and $A^\dagger$ are of dimensions N by $N-1$ and $N-1$ by N respectively, the decomposition in Eq. 7 becomes unique. When the factors were square, they were bidiagonal; that property remains, but in rectangular form. $A^\dagger$ is simply a bidiagonal square matrix but with the last column removed, while A is a bidiagonal square matrix with the last row removed.

Now, we can decompose the matrix , flip the factors, and construct $H' = AA^\dagger$. By properties of matrix algebra, H' is $N-1$ by $N-1$, and correspondingly, only has $N-1$ eigenvalues. This dimensional reduction makes sense, because we want to be removing the ground state in the process of constructing H'. Thus, we still have the previous relations between the eigenvalues and eigenvectors of H and H': $E'_n = E_{n+1}$, and $\psi' = A\psi$. With the newly defined rectangular Cholesky decomposition, we can now construct a hierarchy of discrete isospectral Hamiltonians.

2.2 Non-constant Hopping Landscape Formalism

Let the number of sites be L throughout the following calculations. A key observation is that throughout iterations of discrete supersymmetry, our assumption that t is constant falls apart. In fact, we cannot even assume that $t_i > 0, i = 1, ...L-1$. Thus, we need to redefine the discrete landscape formalism proposed in Section 1.1.

We first begin with a new Schrodinger equation, defined for hopping t_i that represents hopping from the ith site to the i+1th site, the same boundary conditions as before with the new condition that $t_0 = t_L = 0$, on $i = 1, ..., L$:

$$-t_{i-1}(\psi_{i-1}) - t_i(\psi_{i+1}) + V_i(\psi_i) = E\psi_i \tag{9}$$

Notice that Eq. 9 can be rewritten into the following equation:

$$-t_{i-1}(\psi_{i-1}-\psi_i)-t_i(\psi_{i+1}-\psi_i)+(V_i-t_i-t_{i+1})\psi_i=E\psi_i \tag{10}$$

This reexpression will prove important when we need to derive the necessary constraints for this formalism to work.

u is thus the solution to the corresponding Dirichlet problem:

$$-t_{i-1}(u_{i-1})-t_i(u_{i+1})+V_i(u_i)=1 \tag{11}$$

We can similarly reexpress this equation:

$$-t_{i-1}(u_{i-1}-u_i)-t_i(u_{i+1}-u_i)+(V_i-t_i-t_{i+1})u_i=1 \tag{12}$$

We now define $\boldsymbol{t}=[t_1,...,t_{L-1}]$, and notice how Eqs. 9 and 11 can then be written as $H\psi=E\psi_i$ and $Hu=1$, respectively, with $H_{i,i}=Vi$ and both off diagonals of H as $-\boldsymbol{t}$. For ease, define $V-t_i-t_{i-1}=Q$.

We are still missing the analogous inequality presented in Eqs. 6 and 3 that allows us to impose restrictions on the localization region of the eigenstates. The inequality is the most important part of the landscape formalism and deriving it proves to be nontrivial when the constant hopping constraint is relaxed.

To generalize the discrete landscape formalism to a non-constant t, we need to first prove some lemmas. We follow logic very similar to the proofs and lemmas demonstrated in the appendix of [10]. One of our assumptions will be that $\boldsymbol{t_i}>0, i=1,...,L-1$. On face, this looks like a clear violation of our idea of generalizing to a variable hopping because we are assuming all the t_is are of the same sign; however, this condition is valid because the supersymmetry process we will end up coupling with is only affected by the

absolute value of t_i and is not affected by the sign. Therefore, we can begin with the following statement:

Lemma 2.1. *For* $\boldsymbol{t_i} > 0, i = 1, ..., L-1, t_0 = t_L = 0, Q > 0$, *if* $-t_{i-1}(u_{i-1}) - t_i(u_{i+1}) + V_i(u_i) \geq 0, i = 1, ..., L$, *and boundary conditions* $u_0 = u_{L+1} = 0$, *then* $u_i > 0$, $i = 1, ..., L$.

Proof. The logic is almost exactly the same as [10], with minor changes in the setup. We prove by contradiction. Begin by assuming the existence of a minimum "in" the domain; in other words, $\exists i_0$ s.t. $u_{i_0} \leq u_{i_{0+1}}$ and $u_{i_0} \leq u_{i_{0-}}$. Combining these inequalities into one vector expression, we have $\begin{bmatrix} u_{i-1} - u_i \\ u_{i+1} - u_i \end{bmatrix} \geq \begin{bmatrix} 0 \\ 0 \end{bmatrix}$. However, notice we can reexpress our condition with a vector dot product: $\begin{bmatrix} -t_{i-1} \\ -t_i \end{bmatrix} \cdot \begin{bmatrix} u_{i-1} - u_i \\ u_{i+1} - u_i \end{bmatrix} + (Q)u_i \geq 0$, and thus $\begin{bmatrix} t_{i-1} \\ t_i \end{bmatrix} \cdot \begin{bmatrix} u_{i-1} - u_i \\ u_{i+1} - u_i \end{bmatrix} \leq (V_i - t_i - t_{i+1})u_i$. We can say $\begin{bmatrix} 0 \\ 0 \end{bmatrix} \leq \begin{bmatrix} u_{i-1} - u_i \\ u_{i+1} - u_i \end{bmatrix} \leq \begin{bmatrix} \frac{1}{t_{i-1}} \\ \frac{1}{t_i} \end{bmatrix} \cdot Q(u_i)$, and then if $Q \geq 0$, clearly $u_{i0} \geq 0$ because we have assumed $t_i \geq 0$ and $Q \geq 0$. However, our initial assumption was that u_{i0} was a minimum, meaning that it had to be lower than the boundary conditions of $u_0 = u_{L+1} = 0$. This is a contradiction, so we conclude that there cannot exist a minimum "inside" the domain and thus all values of u are non-negative.

To show strict positivity, the logic is simple: notice if $\exists i_0$ s.t. $u_{i0} = 0$, $u_{i0+1} = u_{i0-1} = 0$ as well because u_{i0} cannot be a local minima. This pattern continues, and we simply conclude that if one value of u is equal to 0, all values of u must be 0 as well, and thus $-t_{i-1}(u_{i-1}) - t_i(u_{i+1}) + V_i(u_i) = 0, i =$

$1, ..., L$. □

Previously, our condition for positivity of u was that $V > 2t$, but notice that Lemma 2.1 reveals the condition is now altered to $V - t_i - t_{i-1} = Q > 0$.

Lemma 2.2. *For matrix H as defined earlier to express the Dirichlet problem as $Hu = 1$, there exists $H^{-}1$ and every entry is strictly positive.*

The proof for Lemma 2.2 is exactly the same as in [10], so we choose not to include it here. However, we now have the necessary proofs to derive the inequality.

Theorem 2.3. *Given $-t_{i-1}(\psi_{i-1}) - t_i(\psi_{i+1}) + V_i(\psi_i) = \lambda\psi_i, i = 1, ..., L$ with boundary conditions $\psi_0 = \psi_{L+1} = 0$ and $t_0 = t_L = 0$, $Q = V_i - t_i - t_{i-1} \geq 0$, and $t_i \geq 0 i = 1, ..., L-1$, then:*

$$\frac{|\psi_i| \max(t)}{\max_k(|\psi_k)|} \geq \lambda u_i \quad \forall i = 1, ..., L$$

Proof. Using Lemma 2.2, this proof is straightforward:

$$\psi_i = (\lambda A^{-1}\psi)i = \lambda \sum_{k=1}^{L} A_{i,k}^{-1}\psi_k$$

Then, we can make a generalization to get our upper bound:

$$\psi_i \leq \frac{\lambda \max_k(|\psi_k|)}{\max(t)}$$

The max(t) in the denominator has yet to be fully justified, but in numerical results, it works well as a method of scaling by t. A more rigorous scaling method is a part of future work. □

2.3 Coupling

Coupling discrete supersymmetry and the new landscape formalism was not difficult, however some nuance was required due to technology limitations. We begin with a randomly generated $N = L$ site potential $V > 0$ (whether or not this has constant t does not matter), and utilize the matrix representation described in Section 2.1. In order to reproduce results, the randomness was generated using md5 hashes with a random seed.

$$H\psi = E\psi \tag{13}$$

Then, we can apply the appropriate landscape formalism to predict the eigenstates, as shown in Fig 1.

To proceed to the next iteration, we first subtract away the ground state energy. This is done by computing $H' = H - E_0 I$. Importantly, this operation only shifts the eigenvalues, but does not alter the eigenstates. We can then proceed with a rectangular Cholesky decomposition, as previously detailed, and generate a new $N - 1$ by $N - 1$ Hamiltonian. We choose to implement this quite primitively, because there is no direct method that can compute a rectangular decomposition. We utilize the fact that the factors A and $A^\dagger$ are bidiagonal, and symbolically define all necessary elements. We then minimize the Frobenius norm of $H - A^\dagger A$ to be as close to 0 as possible instead of just directly solving $H - A^\dagger A = 0$, as data beyond 6 decimal points is inaccurate. After solving for A, we flip the factors and generate a new isospectral H' matrix. We ensure that $V_i - t_i - t_{i-1} \geq 0$ for all i to ensure strict positivity of our u function. A transformation of the u function across iterations of discrete supersymmetry is discussed in Section 4.1.

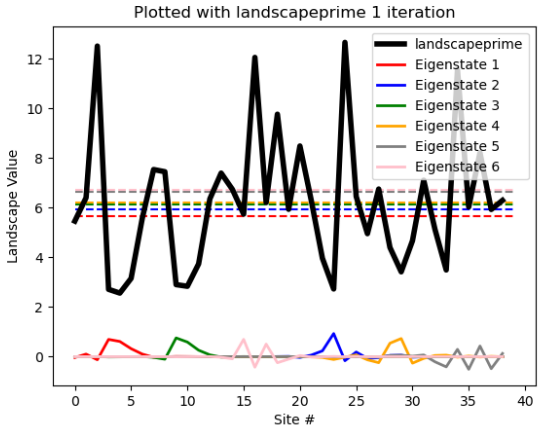

FIGURE 2: The landscape function W is plotted after one iteration of the algorithm. The dotted lines represent the boundaries of the localization regions of the corresponding eigenstates.

We can then apply the non-constant hopping landscape formalism to predict the eigenstates. Based on the same random potential as in Fig. 1, we can perform one iteration of this process. It is important to remember that the eigenstates look different because they are transformed from ψ to $A\psi$. That alteration would appear problematic on face, but A is actually a "local" operator, meaning that localized functions transformed by A tend to remain localized. In fact, this transformation in it of itself is very interesting because it means that A is an operator that can be used to, with enough applications, change delocalized states into localized states.

The landscape function and eigenstates after one iteration are displayed in Fig. 2. We observe that the altered localized eigenstates are still well predicted by the landscape, and the localization regions provide bounds on the spread of the eigenstate before it begins exponentially decaying. Beyond

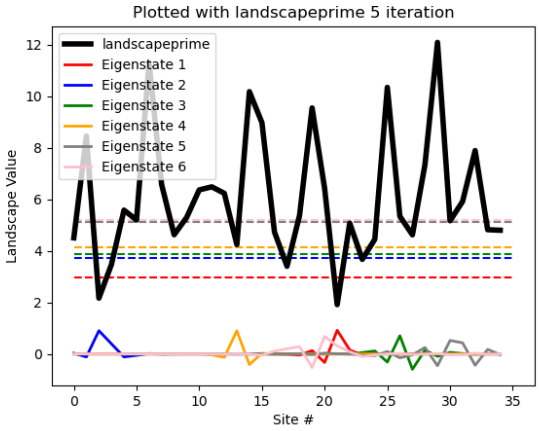

FIGURE 3: The landscape function and lowest eigenstates are plotted after 5 iterations of the algorithm. The horizontal lines represent the t-scaled eigenvalues.

eigenstate 4, our wave functions clearly become delocalized, and more difficult to predict.

The key feature of the algorithm is that it is iterative, meaning we can simply apply it however many times we want. Fig. 3 displays the results after 5 iterations. This figure is incredibly significant, as it demonstrates that the formalism continues to work even after iterating all the way into the middle of the spectrum, revealing states that would have previously been delocalized across the sites.

As a sidenote, it is interesting to note that we can run this algorithm until the Hamiltonian matrix becomes 1 by 1, then disappears (although it would not prove very meaningful at that point).

3 Conclusions

We can observe that the powerful relationship between the landscape and the corresponding eigenstates still exists. The numerics reveal that this coupling works well at predicting the low energy eigenstates at each iteration using the new non-constant hopping landscape formalism. One problem appears to be that the landscape valleys become out of order. For instance, the lowest valley is meant to correspond to the lowest energy eigenstate. This problem can likely be solved through some sort of scaling by the hopping, either on the landscape or the eigenvalues.

In [10], a formalism was devised for predicting both very low energy eigenstates and high energy eigenstates. However, with this new promising discrete SUSY and landscape coupling, we can use the localization in exclusively the lower states and predict behavior and localization of eigenstates throughot the entire spectrum. 40-site systems are still very small, but they show promise for running the algorithm on larger systems.

However, there are various limitations to this method: first, we can see that the eigenstates are significantly altered, including dipping into negative values. The main location is preserved, but in order to have meaningful results, it is necessary that we can invert the transformation on the eigenstates: recall that through iterations of discrete supersymmetry, ψ becomes $A\psi$, where A is the right rectangular factor. A has been shown to be invertible when square, but because the inverse definition differs when A is rectangular, guaranteeing A^{-1} or some other inverse operation exists is more difficult.

Finally, predicting the highest energy eigenstates (ex. the top 4 eigen-

states) proves to be less meaningful, as the Hamiltonian's size becomes small and so does the u. Valleys/local minima require 3 points, so once our Hamiltonain is only 2 by 2, and we cannot use this method well anymore. But, at that point, it may be more efficient to simply diagonalize the matrix, because the added complexity coming from coupling with discrete supersymmetry results in a less significant difference between simply diagonalizing a matrix or running our algorithm. At low dimensions this difference is negligible.

Future work in this area of research will include investigating specific Hamiltonian systems which have interesting eigenstate behavior in the middle of the spectrum that could not have previously been accessed. One such model is the Aubry-Andre model, which includes a mobility edge that can be tuned to produce an exact solution to the Schrodinger equation [15]. It might also be interesting to see what happens when the entire spectrum is preserved, as in generating a new Hamiltonian using N by N square factors A and $A^\dagger$ to preserve the ground state.

4 Appendix

4.1 u Transformation

Similar to how eigenstates have a transformation through iterations of discrete supersymmetry, a transformation for u can also be derived between the nth and $n+1$th iteration. Let 1_n denote a vector of length n of all ones. We have the two following equations, taking into account the dimensional

reduction:

$$Hu = \mathbf{1_n} = A^\dagger Au \tag{14}$$

$$H'u' = \mathbf{1_{n-1}} = AA^\dagger u' \tag{15}$$

We can see that we could have just set the two LHS equal to each other if the 1 vectors were the same length. Thus, we simply define the matrix B to be an N by $N-1$ matrix with all 1's in the first column, for simplicity. It could have been any N by $N-1$ matrix with one 1 in each row. This allows us to have a matrix that transforms 1_n to 1_{n-1}. With some additional manipulation after setting the equations equal, we get our relationship:

$$u' = \boxed{(AA^\dagger)^{-1}BA^\dagger Au} \tag{16}$$

We can also express the transformation through a Hadamard or element-wise product.

$$\begin{aligned} AA^\dagger Au &= A\mathbf{1_n} \\ H'Au &= A\mathbf{1_n} \\ u' &= H^{-1}\mathbf{1_{n-1}} = \boxed{Au \circ \frac{1}{A\mathbf{1_n}}} \end{aligned} \tag{17}$$

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