Local integrals of motion in the two-site Anderson-Hubbard model

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Abstract

It has been proposed that the states of fully many-body localized systems can be described in terms of conserved local pseudospins. Due to the multitude of ways to define these, the explicit identification of the optimally local pseudospins in specific systems is non-trivial. Given continuing intense interest in the role of disorder in strongly correlated systems, we consider the disordered Hubbard model. By studying a small system we provide concrete examples of the form of local integrals of motion in the Anderson-Hubbard model. Moreover, we are able not only to identify the most local choice but also to explore the nature of the distribution of possible choices. We track the evolution of the optimally localized pseudospins as hopping and interactions are varied to move the system away from the trivially localized atomic limit.

Keywords: localization, strong correlations, disorder, Hubbard model

(Some figures may appear in colour only in the online journal)

1. Introduction

In 1958, Anderson showed that disorder can cause the single-particle states in non-interacting systems to be localized in space [1]. Spurred by the work of Basko et al [2], recent attention has focused on the persistence of this localization in the presence of interactions and the nature of the resulting many-body localized phase [3–5]. In isolated quantum systems, key signatures of this phase include a lack of ergodicity [6, 7] and a logarithmic growth of entanglement entropy at long times [8–10]. Several recent experiments in cold atom and trapped ion systems show evidence of many-body localized states [11–16].

The properties of fully many-body localized systems can be understood as arising from the presence of a macroscopic number of local conserved quantities [7, 17–26]. Most studies have associated these local integrals of motion with spin-\(\frac{1}{2}\) pseudospins [7, 17, 24, 25], although a few have considered more general forms [18, 23]. The Hamiltonian may be written in terms of these pseudospins as [7]

\[ H = \sum_i \alpha_i \tau_i^z + \sum_{ij} \beta_{ij} \tau_i^z \tau_j^z + \sum_{ijk} \gamma_{ijk} \tau_i^z \tau_j^z \tau_k^z + \ldots, \quad (1) \]

where \(\tau_i^z\) is the z-component of the \(i\)th pseudospin. While this is true for any system for which Hilbert-space dimension is a power of two [27], a defining feature of the many-body localized phase is that these pseudospins can be chosen to be local. Indeed choice is involved—LIOM are not uniquely defined, because combinations of conserved quantities are themselves conserved. In non-interacting Anderson localized systems, it is convenient to identify the LIOM as the occupancies of the localized single-particle states such that the Hamiltonian is expressed in the form of (1) with only the \(\alpha_i\) coefficients non-zero [24]. In contrast, a many-body localized insulator will have interactions between the local pseudospins. A variety of different schemes have been proposed for mapping many-body localized systems onto a pseudospin Hamiltonian [7, 17–25, 28–34].

Much of the theoretical work on many-body localization has focused either on spin systems [6, 7, 17, 18, 23,
or equivalently spinless fermions [19, 22, 24]. How the phenomenon of many-body localization manifests in other systems remains less well explored. Hubbard-type systems in particular are of immediate interest due to indications of many-body localization in cold atoms in optical lattices [14]. Moreover, the continuing drive to understand the many fascinating properties of doped transition metal oxides, uniquely associated with the interplay of strong correlations and disorder, points to the importance of a complete picture of many-body localization in the Hubbard model. With distinct charge and spin degrees of freedom, this model presents a richer landscape than spin only models, as highlighted by recent work. [35] However, theoretical work on Hubbard systems to date [35–37] has not focused on identifying LIOMs.

Here we provide a concrete picture of the integrals of motion in the Anderson-Hubbard model and explore how the most local set can be identified. The intent is to build an intuitive framework. Aiming for maximum transparency, we consider the toy system of the two-site Anderson-Hubbard model. Past work has demonstrated that two-site versions of the Anderson [38], Hubbard [39–42], and Anderson-Hubbard model [43–45] can provide insights into the physics of these respective models. For example, Johri and Bhatt [38] used a two site model to provide physical insight into a novel singularity of eigenstates in the Anderson model identified in [46]. Similarly, we take advantage of the simplicity of our system to provide explicit examples of LIOM and to explore all possible choices of pseudospins for which the single-particle eigenstates of the system are connected to the vacuum by a single pseudospin raising operator. We search the tremendous multiplicity of options to identify the most local choice, using a localization measure based on the strength of the support of the pseudospin operator on a single site and focusing on minimizing not the average but the largest localization measure in the set of pseudospins. We present maps of the strength of localization as a function of the on-site interaction strength $U$ and the hopping amplitude $t$. We show explicit expressions for the resulting pseudospin operators in terms of Fock space creation and annihilation operators, and demonstrate the wide distribution of localization strengths which arise for different choices of pseudospin mapping.

This paper is structured as follows: In section 2 we introduce the two-site Anderson-Hubbard model, discuss the choices involved in identifying pseudospins and present our method of searching for the most local option. In section 3 we present the results we obtain from numerical optimization of the locality of the LIOMs and in section 4 discuss the implications of our results.

2. Model and approach

In this section we introduce the two-site Anderson-Hubbard model and our approach to obtain optimally localized LIOMs. For context we briefly present natural choices of integrals of motion in two simple limits (no hopping and no interactions), before considering in detail the optimization of the locality of the LIOMs in the general case.

2.1. Two-site Anderson-Hubbard model

The Anderson-Hubbard model is a tight-binding model which combines the on-site Coulomb repulsion of the Hubbard model with the disorder of the Anderson model. For a two-site system, the Hamiltonian takes the form

$$
\mathcal{H} = -t \sum_{\sigma = \uparrow, \downarrow} \left( \hat{c}_{i \sigma}^\dagger \hat{c}_{2 \sigma} + \hat{c}_{2 \sigma}^\dagger \hat{c}_{i \sigma} \right) U \sum_{i = 1, 2} \hat{n}_{i \uparrow} \hat{n}_{i \downarrow} + \sum_{i = 1, 2, \sigma = \uparrow, \downarrow, \tau} \epsilon_{i \sigma},
$$

(2)

where $\hat{c}_{i \sigma}^\dagger$ ($\hat{c}_{i \sigma}$) is the creation (annihilation) operator for an electron with spin $\sigma$ at lattice site $i$ and $\hat{n}_{i \sigma} = \hat{c}_{i \sigma}^\dagger \hat{c}_{i \sigma}$ is the number operator for spin $\sigma$ at site $i$. The site potentials $\epsilon_i$ are randomly chosen from a probability distribution such as a Gaussian or a uniform distribution with fixed width. In the present study our focus is on the properties of individual systems as opposed to disorder-averaged quantities, and we therefore let $\epsilon_1 = 0.5$ and $\epsilon_2 = -0.5$ such that the difference in potential between the two sites $|\epsilon_1 - \epsilon_2|$ sets the energy scale for the hopping amplitude $\tau$ and the interaction strength $U$.

This model is sufficiently simple that analytic expressions for all eigenvalues and eigenvectors can be found, as summarized in appendix A. The dimension of the Hilbert space is $2^4 = 16$ which implies that the Hamiltonian can be mapped to four pseudospins. Our main focus here is exploring the representation of the model in terms of LIOMs, a task for which the analytic solutions are convenient but not required.

2.2. Identifying LIOMs

In this section we discuss the construction of LIOMs for the two-site Anderson-Hubbard model, and the optimization of the locality of these LIOMs. Before tackling the general case, we start with a discussion of the pseudospin representation of the model in two simple limits in which one can immediately identify integrals of motion: the atomic limit ($t = 0, U \neq 0$) and the non-interacting limit ($t \neq 0, U = 0$).

2.2.1. The atomic limit: $t = 0, U \neq 0$. The simplest limit is when hopping $t = 0$ and the system is trivially localized. The Hamiltonian contains only number operators $\hat{n}_{i \sigma} = \hat{c}_{i \sigma}^\dagger \hat{c}_{i \sigma}$ and we can write down pseudospins by inspection. The first can be related to fermion creation and annihilation operators via

$$
\tau_1^+ = \hat{c}_{1 \uparrow}^\dagger \tau_1^- = (\tau_1^+)^\dagger = \hat{c}_{1 \uparrow}, \quad \tau_2^+ = \tau_1^- = \frac{1}{2} m_{1 \uparrow} - \frac{1}{2}.
$$

(3)

Similarly we may define $\tau_2^+ = \hat{c}_{2 \uparrow}^\dagger, \tau_3^+ = \hat{c}_{1 \downarrow}^\dagger$ and $\tau_4^+ = \hat{c}_{2 \downarrow}^\dagger$, which gives

$$
\mathcal{H}_{i = 0} = \epsilon_1 (\tau_1^+ + \tau_3^+) + \epsilon_2 (\tau_2^+ + \tau_4^+) + U\tau_1^+ \tau_2^- + U\tau_3^+ \tau_4^- + \text{constants}.
$$

(4)

In this case the integrals of motion are simply the numbers of particles of each spin at each site, $\hat{n}_{i \sigma}$, up to a constant. These are conserved and maximally local.

2.2.2. The non-interacting limit: $t \neq 0, U = 0$. A second case which provides useful context is the non-interacting limit (i.e. $U = 0$). Here we know that the many-body states can be
expressed in the terms of the occupancies of a set of single-particle states, which for the two-site system are just the bonding and anti-bonding orbitals with corresponding creation operators
\[ \hat{a}_{+\sigma}^\dagger = \alpha \hat{c}_{1\sigma}^\dagger - \beta \hat{c}_{2\sigma}^\dagger, \quad \hat{a}_{-\sigma}^\dagger = \beta \hat{c}_{1\sigma}^\dagger + \alpha \hat{c}_{2\sigma}^\dagger. \]

The coefficients \( \alpha \) and \( \beta \) as well as the corresponding energies \( E_{1\sigma} \) and \( E_{2\sigma} \) can be determined by diagonalizing equation (2) with \( U = 0 \) and are listed in appendix A. If we let
\[ \tau_{1}^+ = \hat{a}_{+\uparrow}^\dagger, \quad \tau_{2}^+ = \hat{a}_{-\downarrow}^\dagger, \quad \tau_{3}^+ = \hat{a}_{-\uparrow}^\dagger \text{ and } \tau_{4}^+ = \hat{a}_{+\downarrow}^\dagger, \]
then the Hamiltonian can be written as
\[ \mathcal{H} = E_{1\uparrow} \tau_{1}^+ + E_{2\downarrow} \tau_{2}^+ + E_{1\downarrow} \tau_{3}^+ + E_{2\uparrow} \tau_{4}^+ + \text{constants.} \]

These integrals of motion are (up to a constant) the number of particles of each spin in each orbital. Although in the thermodynamic limit all states are localized by disorder in 1D when \( U = 0 \), there is nothing inherently local about this set of integrals of motion in our finite system. When \( t \ll |\epsilon_1 - \epsilon_2| \) most of the weight for a given \( \tau \) will be on a single site, but in the limit \( t \to \infty \) the states are as delocalized as they can be in a two-site system, having equal weight on the two sites.

When both \( t \) and \( U \) are non-zero, the choice of \( \tau \) operators is less clear, and we address both how to define them in general and how to choose them to ensure that they are as local as possible.

2.2.3. The general case: \( t \neq 0, U \neq 0 \). In the cases considered in sections 2.2.1 and 2.2.2 the many-body eigenstates either correspond to occupied sites \((t = 0)\) or occupied bonding/anti-bonding orbitals \((U = 0)\). The pseudospin raising operators \( \tau_i^+ \) may thus be chosen to equal the corresponding fermion creation and annihilation operators. When both hopping and interactions are present, the single-particle eigenstates are the same as in the non-interacting case, and so the raising operators chosen in (6) connect the vacuum to the single-particle eigenstates. However, applying two such raising operators will not result in the correct interacting two-particle eigenstates. This implies that pseudospin raising operators need to be modified by including terms which have no effect on the vacuum, but have non-trivial effects on occupied states. Given the many possible options, a more systematic approach is required than that used in sections 2.2.1 and 2.2.2.

The eigenstates of the Hamiltonian are also eigenstates of the \( \tau_i^+ \) operators. This informs our approach to identifying pseudospins, which relies on having all the energy eigenstates and proceeds in five steps. First, list the eigenstates of the \( \tau_i^+ \) operators. These are obtained by acting on the vacuum with all possible combinations of the \( \tau_i^+ \) operators, as shown in the right column of table 1. These states, including their signs and the order in which they are listed, define what we call the \( \tau \) basis.

Second, match each of these states to one of the eigenstates of the system. A particular choice of match, match 1, is shown in table 1. In this choice, \( n \)-particle states are connected to the vacuum by \( n \tau_i^+ \) operators. We emphasize that there is no requirement that such an identification is made. Instead, for example, the four-particle state could be connected to the vacuum by a single \( \tau \) operator if one so chose. The correspondence in table 1 was chosen to align with the pseudospin choice for the non-interacting case discussed above.

Third, write a particular pseudospin operator, e.g. \( \tau_1^+ \) (which we use below to illustrate the approach), in the \( \tau \) basis. Fourth, perform the unitary transformation from the \( \tau \) basis to the Fock basis using the matrix of eigenvectors, \( Q \), that diagonalizes the Hamiltonian in the Fock basis. When the eigenstates are ordered as in table 1 the matrix \( Q \) takes the form
\[
Q = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & Q_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & Q_1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & Q_3 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & Q_3 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix},
\]

where the \( \phi \)s are defined in appendix A. Hence we may write, e.g. \( \tau_1^+ \) in the Fock basis as
\[
\tau_1^+ \big|_{\text{Fock basis}} = Q \tau_1^+ \big|_{\text{\tau basis}} Q^\dagger.
\]
Fifth, project the \( \tau^+_1 \) operator, written in the Fock basis, onto all possible combinations of \( c_i \sigma \) and \( \tilde{c}_{i\sigma}^\dagger \) operators. These include the identity operator, the single operators \( c_{i\uparrow} \) and \( \tilde{c}_{i\uparrow}^\dagger \), etc, and all possible combinations of two, three and four annihilation and creation operators, up to and including the four fermion operator \( n_1 \hat{r}_{22} \hat{r}_{12} \). There are 256 unique combinations, consistent with the number of independent quantities in a \( 16 \times 16 \) matrix. One can construct matrix representations of all of these operators, starting from the eight single c-operators in the Fock basis. We choose this matrix representation to be orthonormal in the following sense:

\[
\sum_{i,j=1}^{16} A_{ij} B_{ij} = \begin{cases} 1 & \text{for } A = B \\ 0 & \text{for } A \neq B \end{cases}
\]

(12)

where \( A \) and \( B \) are any of the matrices that represent c-operators. For terms involving the number operators orthogonality is achieved by working with \( n_{\uparrow\uparrow} \equiv n_{\downarrow\downarrow} = \frac{1}{2} \).

There is an additional subtlety in the atomic limit. When \( t = 0 \), the triplet state \( |t\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2} \) is degenerate with the singlet state \( |s\rangle = (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2} \). In this case any arbitrary orthogonal superposition of \( |t\rangle \) or \( |s\rangle \) may be assigned as \( \tau \) states. We then search over all matches to find the most local possibility for site 2. When weight shifts off the primary site, there can be a shift of weight from single-site operators on one site to single-site operators on another site, and in addition there can be a shift of weight to operators which act on multiple sites. We use a simple measure which treats both of these possibilities on equal footing. Consider a specific \( \tau^+_1 \) operator from a specific match between \( \tau \) states and eigenstates. Let \( w_1 \) be the sum of the squares of the coefficients of all c-operators which act only on site 1 (e.g. \( c_{1\uparrow}, c_{1\downarrow}, \text{etc} \)). Let \( w_2 \) be the same quantity for site 2. And finally let \( w_b \) be the sum of the squares of the coefficients of all c-operators which act on both sites (e.g. \( c_{1\uparrow} c_{2\uparrow}, c_{1\downarrow} c_{2\downarrow}, \text{etc} \)).

We define

\[
\xi_{m1} = \frac{1 - w_1}{w_1}, \quad \text{and} \quad \xi_{m2} = \frac{1 - w_2}{w_2},
\]

(13)

from which we obtain

\[
\xi_{mi} = \min(\xi_{m1}, \xi_{m2}).
\]

(14)

\( \xi_{mi} \) is a measure of locality for the \( m \)-th pseudospin in match \( m \). When all the weight is on site 1, \( \xi_{m1} = \xi_{m2} = 0 \), and likewise for site 2. When weight shifts off the primary site, \( \xi_{mi} \) becomes nonzero. Only values \( \xi_{mi} \leq 1 \) can be considered localized. In particular, if \( w_b = 0 \) and \( w_1 = w_2 \), \( \xi_{mi} = 1 \). Meanwhile, as \( w_b \to 1 \), \( \xi_{mi} \to \infty \).

For a specific choice of the match between eigenstates and \( \tau \) states, there will be a \( \xi_{mi} \) corresponding to each \( \tau^+_i \). We characterize the match by \( \xi_{m} = \max_{i} \{ \xi_{mi} \} \), the maximum \( \xi_{mi} \) value. We then search over all matches to find the most local set of pseudospins, which we characterize with

\[
\xi = \min_{m} \{ \xi_{m} \}.
\]

(15)

We also explored alternative measures of localization, such as \( \xi_{m} = \text{avg}_{i} \{ \xi_{mi} \} \) defined as the average for each match. Our results were not significantly different, but we feel that using...
the extrema in the definition more accurately reflects the most local choice.

3. Results

In this section we present first our numerical results for the evolution of the localization measure $\xi$ with the parameters $t$ and $U$ in the two-site Anderson-Hubbard model. We then show the explicit form of some of the resulting LIOMs, and finally we display the distribution of $\xi_m$ values obtained from the many possible matches explored.

Figure 1 shows the value of $\xi$ obtained as a function of $t$ and $U$ at fixed disorder strength $|\epsilon_1 - \epsilon_2 | = 1$. Figure 1(a) covers a wide range of values in both $t$ and $U$, while figure 1(b) provides detail for values between zero and one for both parameters. As discussed in section 2.2.1, in the atomic limit ($t = 0$), the system is maximally localized, independent of $U$, as reflected in the figure. The general trend illustrated in the figure is that $\xi$ increases both with increasing hopping amplitude and with increasing interaction strength. We find that $t$ has a stronger delocalizing effect than $U$, with $\xi$ depending on $U$ very weakly for $t > 2|\epsilon_1 - \epsilon_2 |$.

For almost all parameter values shown in figures 1(a) and (b), the optimal match (match 1) is that shown in table 1. There are three exceptions. (i) For $t = 0$ and $U > 1$, the lowest energy 2-particle eigenstate is $|2\rangle$, whereas for $U < 1$ it is $|02\rangle$, the state with both particles on site 2. The optimal correspondence (match 4) switches accordingly. (ii) For $t > 0$ and $0 < U \leq U_1$ the optimal match (match 2) switches the sign of $|\psi_2\rangle$ from that in match 1. (iii) For $t = 1$, when $U \geq 4$, the optimal correspondence (match 3) is significantly rearranged from that shown in table 1. Match 3 is similar to match 4 but with many signs reversed.

At $t = 1$, $\xi$ has a non-monotonic variation with $U$. To explore this in more detail, in figure 1(c) we plot $\xi_m$ values obtained from matches 1, 2 and 3. While match 1 is optimal in the non-interacting limit, it is abruptly usurped by match 2 for nonzero $U$ up to $U = 1$. Meanwhile match 3 gives much larger values of $\xi_m$ than the first two for small $U$ values, but unlike the other matches the $\xi_m$ values decline with increasing $U$ such that match 3 becomes optimal above $U \approx 4$.

In addition to studying the evolution of $\xi$ we investigated the nature of the resulting $\tau_1^+$ operators. We illustrate this with a detailed decomposition of the operator $\tau_1^+$. In the parameter range we have considered, only 24 of the 256 possible combinations of $c$ operators contribute to $\tau_1^+$, and these are listed in table 2. Figure 2 shows the weight of the contribution each

![Figure 1. Plot of $\xi$ for each choice of $t$ and $U$ in units of the site potential difference $|\epsilon_1 - \epsilon_2 |$. (a) Shows the range 0 to 8 for both parameters and (b) expands the region 0 to 1. The color scale is the same for both figures. (c) Shows $\xi_m$ as a function of $U$ for three different matches when $t = 1$.](image1)

![Figure 2. The weights of the coefficients of the normalized Fock-space creation and annihilation operators which make up $\tau_1^+$ for different parameter values. The operator indices are as defined in table 2.](image2)

| Table 2. Fock space operators contributing to $\tau_1^+$ and their indices. Weights are shown in figure 2. Note that $\hat{n}_i \equiv \hat{n}_i - \frac{1}{2} I$. |
|-------|-----|-----|
| 1     | 13  | 12  |
| $\hat{c}_{1\uparrow}$ | $\hat{c}_{2\uparrow}$ | $\hat{c}_{1\downarrow}$ |
| $\hat{n}_{1\uparrow}\hat{c}_{1\uparrow}$ | $\hat{n}_{1\uparrow}\hat{c}_{2\uparrow}$ | $\hat{n}_{1\downarrow}\hat{n}_{1\uparrow}$ |
| $\hat{n}_{1\uparrow}\hat{c}_{1\downarrow}$ | $\hat{n}_{1\downarrow}\hat{n}_{1\uparrow}$ | $\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}$ |
| $\hat{n}_{1\downarrow}\hat{n}_{1\uparrow}$ | $\hat{n}_{1\downarrow}\hat{n}_{1\downarrow}$ | $\hat{n}_{1\downarrow}\hat{n}_{1\uparrow}$ |
| $\hat{n}_{1\downarrow}\hat{n}_{1\downarrow}$ | $\hat{n}_{1\downarrow}\hat{n}_{1\downarrow}$ | $\hat{n}_{1\downarrow}\hat{n}_{1\downarrow}$ |
of these (normalized) operators makes to $\tau_{1}^\tau$ for a range of different parameters.

In the top panel of figure 2, the black line corresponds to $U = 0$ and $t = 0$. The first operator has weight one and no others contribute, corresponding to $\tau_{1}^\tau = \hat{c}_{1\uparrow}^\dagger$, as discussed in section 2.2.1. As $t$ is increased for $U = 0$, weight shifts from $\hat{c}_{1\uparrow}^\dagger$ (operator 1) to $\hat{c}_{2\uparrow}^\dagger$ (operator 13) consistent with the discussion in section 2.2.2. The second panel of figure 2 shows the same sequence of $t$ values with $U = 1$. The $t = 0$ configuration is identical to the non-interacting case, and even with hopping, while other operators begin to contribute, $\hat{c}_{1\uparrow}^\dagger$ and $\hat{c}_{2\uparrow}^\dagger$ remain dominant. The third and fourth panels of figure 2 show instead a range of $U$ values at fixed $t$. For low $t$ and $U$ values, these maximally localized LIOMs have strong overlap with single-particle occupation numbers obtained in the absence of interactions, a result also noted in other systems [33]. For higher $U$ values, when the optimal match switches to match 3, there is a qualitative change as $\hat{n}_{1\downarrow}\hat{c}_{1\uparrow}^\dagger$ (operator 2) replaces $\hat{c}_{1\uparrow}^\dagger$ as the primary contribution. Not shown, when $t$ is large, independent of $U$, the structure is similar to the atomic limit, with roughly equal weight on $\hat{c}_{1\uparrow}^\dagger$ and $\hat{c}_{2\uparrow}^\dagger$. The construction of figure 2 is reminiscent of the idea of localization in Fock space [47], in which single particle excitations of a many-body occupation numbers can be written in terms of only a finite number of other many-body eigenstates. Indeed, in the atomic limit our construction is the same as Fock-space localization, because in this case the optimal $\tau_{1}^\tau$ operators are equal to the single-particle eigenstate creation operators $\hat{c}_{j\sigma}^\dagger$. However, when $t$ is nonzero, the two pictures diverge as we consider the projection onto $\hat{c}_{i\sigma}^\dagger$ as opposed to the new single-particle eigenstate creation operators $\hat{c}_{j\sigma}^\dagger$.

The $\tau_{1}^\tau$ operators shown in figure 2 are the most local by the criterion that for these matches, $\xi_{m} = \xi$. This most-localized choice is highly non-generic. Figure 3 illustrates this point by showing the distribution of $\xi_{mi}$ values for two different parameter sets: $(t, U) = (0, 1.0)$ and $(t, U) = (0.2, 1.0)$. When either $U$ or $t$ is zero, the distribution has sharp peaks separated by wide gaps. While the distribution is always discrete when viewed with perfect resolution, when $U$ and $t$ are both non-zero, it is more convenient to view the binned distribution. The inset shows the low end of the distribution of $\xi_{mi}$ values, highlighting the point that the most localized match is usually considerably more localized than the next best match.

We note that the peaks of these distributions are at considerably larger values than the optimum, and that they have very long tails at large values of $\xi_{mi}$. We show in figure 3 a comparison of the distribution of $\xi_{mi}$ values (for $t = 0.2$, $U = 1.0$) to a Gaussian and a Gumbel distribution, neither of which is a particularly good fit for large values of $\xi_{mi}$, although the Gumbel distribution is certainly a better fit and fits the data over a large range of $\xi_{mi}$ values for larger $t$. The strength of the tail of the distribution at large $\xi_{mi}$ is particularly notable, since even the Gumbel distribution, which arises in extreme value statistics, is insufficient to capture the tail. The origin of this long tail is the fact that combinations of conserved quantities are also conserved. It is therefore possible to create integrals of motion which are highly nonlocal even in an intrinsically localized case such as the atomic limit. The key point learned from this distribution is that a generic set of integrals of motion is likely to have extremely different localization properties from the most local set.

4. Discussion

In this work we considered the two-site Anderson-Hubbard model as a toy model of interacting electrons in the presence of disorder. We constructed LIOMs for this model, and searched through possible matches between energy eigenstates and $\tau$ basis states to obtain the most local choice of LIOMs as defined by our localization measure (15). We mapped the degree of localization of this most local choice as a function of parameters $t$ and $U$, noting the variation not only in the localization measure but also in the optimal match. We explicitly presented the composition of the optimal LIOMs in terms of standard creation/annihilation operators, and explored the distribution of locality obtained in all matches in our search.

Since the observation that properties of fully many-body localized systems could be described in terms of conserved pseudospins, numerous schemes have been suggested to identify LIOM in particular systems. The use of a direct unitary transformation to map from the energy eigenbasis to a basis of local operators has been raised but rarely implemented [7, 18, 23, 25, 31, 32]. Other proposals include renormalization [17, 25, 28] and perturbative approaches [20, 21, 24] as well as a displacement operator method [22, 33], minimizing the commutator of approximate LIOM with the Hamiltonian [30, 31] and identifying ‘natural orbitals’ from the one particle density matrix [19, 34]. Concurrent with the effort to identify LIOMs is exploration of their optimization. While Rademaker et al [33] recently suggested that one may wish to optimize from alternative perspectives (e.g. information theory might...
suggest minimizing the number of couplings between pseudospins), the primary focus has been on identifying a localization length which diverges at the many-body localization transition, analogous to the localization length defined by the size of single-particle states in Anderson localization. The most direct analogy is to measure the size of the LIOMs themselves. Examples include the inverse participation ratio [19], the support [23, 30], and the overlap with local operators in Fock space [33]. Other work has focused on the length associated with the interactions between pseudospins ($\beta_{ij}$, $\gamma_{ijk}$, ... in (1)) [7, 22, 23, 25]. As shown by Rademaker and Ortiz [22], the lengthscales for pseudospins and interaction parameters can be quite different, even when both exhibit exponential decay with distance.

Two advantages of the unitary mapping approach to identifying integrals of motion used here are (i) that it is effective and equally efficient independent of the level of localization in the system, and (ii) that it makes obvious the fact that choice is involved in identifying LIOM. Perturbative schemes break down as the transition is approached and the displacement operator method, while still applicable, requires increasing numbers of transformations. Moreover, these methods focus on a systematic progression towards a single set of LIOMs and do not provide perspective on the discarded alternatives.

A general challenge for any scheme trying to optimize the locality of LIOMs is the choice of measure of localization to use to discriminate between matches. The measure (15) that we used focuses on the extent of the LIOMs themselves as opposed to the range of their interactions and aims to treat delocalization in both a single-particle and many-body sense on the same footing. The need to have access to a complete set of eigenstates as well as the logistics of the search through options, both limit the system sizes for which this approach is practical as discussed further below. Nonetheless, given that the goal of our work is to demonstrate the choices inherent in identifying the most local set of integrals of motion in a situation where the choices can be enumerated and made explicit, working with a small system is itself an advantage. Moreover, we believe the insights gained into how the LIOMs vary with system parameters and the nature of the distribution of non-optimal LIOMs will inform the development of more widely applicable methods for optimizing LIOMs.

We remark here on the potential for generalizing our work to larger systems. A feature of the analysis shown here is access to an analytic solution to the model. This will not hold in general when one considers larger system sizes. However, in treating larger systems, the procedure outlined in section 2.2.3 for identifying LIOMs can be followed identically once all eigenstates of the system have been obtained numerically, which like any exact diagonalization technique scales poorly with system size. The feature of our work which would be more difficult without an analytic solution is the tracking of specific matches. A numerical algorithm may not consistently assign the same sign to a particular eigenvector as parameters are varied. This will not affect the optimal value of $\xi$ obtained for any given parameter set, provided the search through matches allows for all sign options. However, identifying whether the chosen match is the same or different from matches at other parameter values may be more difficult. Another approach to obtain results on larger system sizes could be to use the results we have obtained here to develop a real space renormalization group (RG) method. We note that the real-space RG approach developed by Johri and Bhatt [48] for non-interacting disordered systems is an important example of how knowledge of the localized state can be used to build a more effective RG strategy. Recognizing that eigenstate energy is not uniquely correlated with eigenstate size in the Anderson model, they designed a RG process guided not by energy but by localization length. Similarly, applying the insight we gain here on the nature of the LIOMs toward building an RG procedure for the interacting case is a promising direction for future investigation.

The importance of the Hubbard model as a minimal model of strongly correlated electrons motivates extending our work to larger system sizes using numerical and recently developed tensor network methods [32]. In addition, recent work [35] has suggested that only charge, and not spin, localizes in disordered Hubbard chains, so that many-body localization in the Anderson-Hubbard model may have a different character than in other commonly studied many-body localized systems. The addition of a random magnetic field can lead to localization of spin as well as charge degrees of freedom [35, 36] and should be explored further. Before the current framework for many-body localization was developed, significant effort was invested in calculating a phase diagram of the Anderson-Hubbard model using various adaptations of dynamical mean field theory for disordered systems [49–54]. Now that there is new understanding of the meaning of localization in interacting systems, it is important to determine whether the measures used in these past studies are consistent with this new framework.

In summary, the work presented here provides researchers in strongly correlated electrons with a concrete picture of the form of the LIOMs in a Hubbard system, and it provides the many-body localization community with an exploration of the full range of options for LIOMs in a toy system, offering perspective on the evolution of the nature of the pseudospin operators away from the fully localized limit.

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Appendix A. Eigenvalues and eigenvectors of the two-site Anderson-Hubbard model

In this appendix we summarize the analytic expressions for the eigenvalues and eigenvectors of the two-site Anderson-Hubbard model. In table A1 we first list the basis which we use to express the eigenstates—this is a slightly modified Fock basis in which the states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ are combined to form spin singlet and triplet states.
The eigenvalues and eigenvectors of the two-site Anderson-Hubbard model are summarized in Table A2, where we defined

\[
x = \frac{\epsilon_1 + \epsilon_2}{2}, \quad y = \frac{\epsilon_1 - \epsilon_2}{2}.
\]  

(Note that these definitions differ by a factor of \(\sqrt{2}\) from the definition of \(x\) and \(y\) in [38].) The coefficients \(\alpha\) and \(\beta\) are given by:

\[
\alpha = \frac{1}{\sqrt{t^2 + (y + \sqrt{y^2 + t^2})^2}} \left( y + \sqrt{y^2 + t^2} \right), \quad \beta = \frac{1}{\sqrt{t^2 + (y + \sqrt{y^2 + t^2})^2}} \left( y - \sqrt{y^2 + t^2} \right).
\]  

The eigenvalues for the \(|w_1\rangle, |w_2\rangle\) and \(|w_3\rangle\) states are

\[
E_{w_i} = 2x + \frac{2U}{3} - \frac{2}{3} \sqrt{U^2 + 12(y^2 + t^2)} \cos \left( \frac{\theta_i}{3} \right),
\]

where

\[
\theta_i = \begin{cases} 
\theta + 2\pi, & i = 1, \\
\theta - 2\pi, & i = 2, \\
\theta, & i = 3
\end{cases}
= \cos^{-1} \left[ \frac{U(U^2 - 36y^2 + 18t^2)}{(U^2 + 12y^2 + 12t^2)^2} \right].
\]  

The coefficients in the expressions for the \(|w_1\rangle, |w_2\rangle\) and \(|w_3\rangle\) states in terms of the modified Fock basis are:

\[
\begin{align*}
\phi_{\alpha i} &= \frac{\text{sgn}(4y^2 - B_i^2)}{\sqrt{4y^2 - B_i^2 + 4t^2(4y^2 + B_i^2)}} \left( \sqrt{2t(2y - B_i)} \right), \\
\phi_{\beta i} &= \frac{\text{sgn}(4y^2 - B_i^2)}{\sqrt{4y^2 - B_i^2 + 4t^2(4y^2 + B_i^2)}} \left( -\sqrt{2t(2y + B_i)} \right),
\end{align*}
\]

where

\[
B_i = \frac{U}{3} + \frac{2}{3} \sqrt{U^2 + 12(y^2 + t^2)} \cos \left( \frac{\theta_i}{3} \right).
\]  

\[
\begin{array}{|c|c|c|}
\hline
| State | Eigenvalue | Eigenvector |
\hline
| p \uparrow | E_{1p} = x + \sqrt{x^2 + t^2} & \alpha \uparrow 0 \rangle - \beta \uparrow 0 \rangle | \downarrow 0 \rangle |
\hline
| m \uparrow | E_{1m} = x - \sqrt{x^2 + t^2} & \beta \uparrow 0 \rangle + \alpha \uparrow 0 \rangle | \downarrow 0 \rangle |
\hline
| p \downarrow | E_{1p} = \beta \downarrow 0 \rangle - \beta \downarrow 0 \rangle | \uparrow 0 \rangle |
\hline
| m \downarrow | E_{1m} = \beta \downarrow 0 \rangle + \alpha \downarrow 0 \rangle | \uparrow 0 \rangle |
\hline
| t \uparrow | E_{2t} = 2x | \uparrow \uparrow \rangle |
\hline
| t \downarrow | E_{2t} = 2x | \downarrow \downarrow \rangle |
\hline
| w_1 | E_{w_1} & \phi_{w_1} | 20 \rangle + \phi_{w_1} | \uparrow \rangle |
\hline
| w_2 | E_{w_2} & \phi_{w_2} | 20 \rangle + \phi_{w_2} | \uparrow \rangle |
\hline
| w_3 | E_{w_3} & \phi_{w_3} | 20 \rangle + \phi_{w_3} | \uparrow \rangle |
\hline
| 3p \uparrow | E_{3p} = E_{1p} + 2x + U & \alpha \uparrow \uparrow \rangle + \beta \uparrow \uparrow \rangle |
\hline
| 3m \uparrow | E_{3m} = E_{1m} + 2x + U & -\beta \uparrow \uparrow \rangle + \alpha \uparrow \uparrow \rangle |
\hline
| 3p \downarrow | E_{3p} = E_{1p} & \alpha \downarrow \downarrow \rangle + \beta \downarrow \downarrow \rangle |
\hline
| 3m \downarrow | E_{3m} = E_{1m} & -\beta \downarrow \downarrow \rangle + \alpha \downarrow \downarrow \rangle |
\hline
| 4 \rangle | E_4 = 4x + 2U & | 2 \rangle |
\hline
\end{array}
\]
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