Charge and spin-specific local integrals of motion in a disordered Hubbard model

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Abstract While many-body localization has primarily been studied in systems with a single local degree of freedom, experimental studies of many-body localization in cold atom systems motivate exploration of the disordered Hubbard model. With two coupled local degrees of freedom it is natural to ask how localization in charge relates to disorder in spin and vice versa. Most prior work has addressed disorder in only one of these sectors and often has not used measures of localization which distinguish between charge and spin. Here we explore localization in the Hubbard model with a wide range of independent values of charge and spin disorder, using measures of localization based on charge and spin-specific integrals of motion. Our results show a symmetry between the response of the charge to spin disorder and vice versa, and we find very weak disorder in one channel, so long as the disorder in the other channel is sufficiently strong, results in localization in both channels. Further, the weaker the disorder in the less-disordered channel, the longer the time scale at which localization appears in the dynamics of this degree of freedom.

I. INTRODUCTION

How isolated quantum systems reach thermal equilibrium is a long standing question of continuing interest. The absence of equilibration in some systems is also well known, notably Anderson localization in noninteracting systems with quenched disorder. The recent demonstration that the absence of equilibration can persist in the presence of interactions has launched the study of many-body localization (MBL). Most of the theoretical work in this area has focused on charge disorder, or equivalently spinless fermions, in which there is just one local degree of freedom. However, interest in systems with multiple coupled degrees of freedom is growing because of the rich variety of new behavior produced by their added complexity, because of the question of how localization is affected by coupling to a bath, and most directly because of significant experimental studies of MBL using cold atoms which are described by the Hubbard model. Indeed, the influence of disorder on Hubbard systems has a long history of study given its relevance to the doping of high temperature superconductors and other transition metal oxides. The Hubbard model contains two coupled local degrees of freedom, charge and spin. A natural question to ask is how disorder in one of these effects the dynamics of each. Most work to date has focused on charge disorder alone, by including randomly distributed site potentials in the model. One study concluded that for sufficient charge disorder strength the average energy gap ratio is consistent with a Poisson distribution, characteristic of localization, while another study of conserved quantities obtained through time averaging concluded instead that the system was neither localized nor generically ergodic. Other studies have used dynamical properties to gain charge and spin-specific information suggesting that the charge is localized but the spin is neither localized nor generically ergodic. There has also been a study on the case of spin disorder alone, adding a random magnetic field to the Hubbard model. Both conclude the system is fully localized with on, providing charge and spin-specific measures. These measures used to gain information specific to charge and spin have been dynamical quantities. However, a number of authors have noted the potential for relevant time scales to be widely separated, resulting in debate over whether numerics have captured the full dynamics.

A number of questions emerge from this context. Broadly, what is the localization behavior across the full spectrum of charge and spin disorder strengths? In particular, is the level of localization in a given sector—charge or spin—simply a function of the disorder strength in that sector, or is there communication between them? To address this, are there alternatives to dynamical measures which nonetheless provide charge and spin-specific information on localization?

In this work we introduce a method for constructing local conserved quantities from the local charge and spin degrees of freedom. We then measure the level of localization of the charge and spin using two approaches—one based on the local conserved quantities and the other on the dynamics—finding qualitative agreement between them. We conclude that, while disorder in both channels is needed to achieve full localization, very weak disorder in one channel can result in nearly equal localization in both channels so long as the disorder in the dominant channel is sufficiently strong. In addition, we find symmetry between the spin response to charge disorder and vice versa.

In Section we describe the model we study and
provide details on (i) the definition and optimization of charge and spin-specific integrals of motion and (ii) the localization measures built from these integrals of motion as well as the dynamical quantities calculated for comparison. Section II presents our results, which are discussed further in Section IV.

II. MODEL AND METHOD

We study a one-dimensional Hubbard model with nearest-neighbour hopping and on-site interactions, including both charge and spin disorder.

\[
H = -t_h \sum_{\langle ij \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \epsilon_id_i + \sum_i h_im_i
\]

where \(d_i \equiv n_{i\uparrow} + n_{i\downarrow}\) is the local charge density operator and \(m_i \equiv n_{i\uparrow} - n_{i\downarrow}\) is the local magnetization operator. The charge and spin disorders are generated by randomly choosing \(\epsilon_i\) and \(h_i\) from uniform distributions \([-W_{ch}, W_{ch}]\) and \([-W_{sp}, W_{sp}]\), respectively. We use open boundary conditions, and set the hopping amplitude as the unit of energy \(t_h = 1\) so time is measured in units of \(h/t_h\). We focus here on \(U = 1\), half-filling, and total spin zero. At \(U = 0\), the localization behavior and dynamics of charge and spin are identical. We have also checked \(U = 8\) (data not shown) with similar results to \(U = 1\).

Many measures of many-body localization have been proposed and implemented, including level statistics, logarithmic time dependence and area law scaling of entanglement entropy, memory of initial conditions, etc. Fully many-body localized systems can be described in terms of a macroscopic number of local conserved quantities: local integrals of motion. An advantage of building a measure around integrals of motion (IOMs) is that they are conserved, avoiding complications associated with determining how long a time scale is sufficient in a dynamical calculation. Meanwhile an advantage of building a measure around dynamical properties is the closer connection with experiments. Here we examine measures of both types.

A. Charge and spin-specific integrals of motion

A number of methods have been developed for identifying approximate local IOMs in large systems for which a full set of eigenstates is not known. However, when all eigenstates are known, there is a very simple approach. Let \(Q\) be the operator which generates the unitary transformation between the basis of local product states (the Fock basis), \(\{|n\}\), and the basis of energy eigenstates, \(\{|E_n\}\). If \(O\) is an operator that is diagonal in the Fock basis, then \(Q O Q^\dagger\) is diagonal in the energy basis and hence commutes with the Hamiltonian, making it a conserved quantity, i.e. an integral of motion. Specifically, if one chooses a local operator such as the number operator \(n_{i\sigma}\), and if \(Q\) also acts in a local way, then the resulting integral of motion \(Qn_{i\sigma}Q^\dagger\) can be argued to be local.

Our interest is in examining the localization of the charge and spin degrees of freedom separately, and we therefore start with operators which are not only local but also charge and spin specific. \(\tilde{d}_i \equiv \frac{1}{\sqrt{2}}(\tilde{n}_{i\uparrow} - \tilde{n}_{i\downarrow})\) and \(\tilde{m}_i \equiv \frac{1}{\sqrt{2}}(\tilde{n}_{i\uparrow} + \tilde{n}_{i\downarrow})\) are orthonormalized versions of the local charge density and magnetization operators, respectively, where \(\tilde{n}_{i\sigma} = 2c_{i\sigma}^\dagger c_{i\sigma} - 1\). Thus \((\tilde{d}_i, \tilde{d}_j) = (\tilde{m}_i, \tilde{m}_j) = \delta_{ij}\) and \((\tilde{d}_i, \tilde{m}_j) = 0\), where \((A, B) \equiv \frac{1}{N} \text{Tr}(A^\dagger B)\) is the Frobenius inner product, and \(N\) is the number of states being traced over. From these we construct conserved (and orthonormal) operators \(\tilde{a}_i\) and \(\tilde{m}_i\):

\[
\tilde{a}_i \equiv Q \tilde{d}_i Q^\dagger \quad \text{and} \quad \tilde{m}_i \equiv Q \tilde{m}_i Q^\dagger.
\]

The unitary operator \(Q\) is not unique, since any of the \(N!\) one-to-one matchings \(|n\rangle \leftrightarrow |E_n\rangle\) will also diagonalize the Hamiltonian. Which match is optimal? A search through all relevant matchings to find the one that minimizes a chosen localization length is only possible in exceedingly small systems. Here we choose the matching that maximizes the weight of \(Q\) on the identity, and therefore maximizes \(\text{Tr}(Q)\), similar to the approach taken by Ref. 37. Computationally, this is identical to the well-known combinatorial optimization task known as the Assignment Problem, and we implement the Hungarian algorithm which has a polynomial time-complexity \(O(N^3)\). A key feature of this method for our purposes is that it is unbiased towards the charge or spin sectors.

B. Measures of localization

To measure localization, we consider properties of both our IOMs and the dynamics of the system. From the IOMs, we calculate three quantities: the on-site overlap, the overlap as a function of distance, and the overlap localization length. The on-site overlap is defined as the overlap as a function of distance, and the overlap localization length. From the IOMs and the dynamics of the system. From the IOMs, we calculate three quantities: the on-site overlap, the overlap as a function of distance, and the overlap localization length. The on-site overlap is defined as

\[
O_c \equiv \frac{1}{N_{dc}} \sum_{\text{config}} \frac{1}{L} \sum_i \frac{1}{N} \text{Tr}(\tilde{d}_i \tilde{a}_i)
\]

and

\[
O_s \equiv \frac{1}{N_{dc}} \sum_{\text{config}} \frac{1}{L} \sum_i \frac{1}{N} \text{Tr}(\tilde{m}_i \tilde{m}_i)
\]

where the trace is performed over the half-filled, zero-net-spin subspace, and \(N\) is the dimension of this subspace.
Using a subspace with a fixed density of spin up and down fermions allows a clear investigation of system-size dependence, and omits single-particle states which naturally have the same charge and spin localization. In a system with localized charge degrees of freedom, $O_c$ should tend to a nonzero value in the thermodynamic limit. In contrast, if the charge degrees of freedom are delocalized, $O_c$ vanish in the thermodynamic limit. Similarly for $O_s$.

The overlap versus distance is defined in a similar manner, comparing the integral of motion at site $i$ with the local density at a site a distance $\ell$ away. We average them over $N_{dc}$ disorder configurations.

$$O^c_i(\ell) = \frac{1}{N_{dc}} \sum_{\text{config}} \frac{1}{N} \text{Tr} (\hat{d}_i \hat{d}_i)$$

$$O^s_i(\ell) = \frac{1}{N_{dc}} \sum_{\text{config}} \frac{1}{N} \text{Tr} (\hat{m}_i \hat{m}_i)$$

In this case, the trace is over the full Hilbert space in order to ensure the orthonormality $(\hat{d}_i, \hat{d}_j) = (\hat{m}_i, \hat{m}_j) = \delta_{ij}$ indicating maximal overlap when $i = j$, or no overlap when $i \neq j$. The terms $O^c_i(\ell)$ (for $\ell > 0$) are then fit to an exponential $e^{-\ell/\xi_{ch}}$ to extract a charge localization length $\xi_{ch}$, and similarly for spin.

These overlap measures allow us to distinguish between charge and spin localization and also share a common foundation with many other measures used elsewhere, in the expectation values of local operators.

As for dynamical quantities, we quantify the memory of the initial charge and spin configurations using the local charge and spin correlations.

$$D(t) = D_0 \sum_{i} \langle \psi | (\hat{d}_i(t) - \bar{d})(\hat{d}_i(0) - \bar{d}) | \psi \rangle$$

$$M(t) = M_0 \sum_{i} \langle \psi | m_i(t)m_i(0) | \psi \rangle$$

where $D_0$ and $M_0$ are chosen such that $D(0) = M(0) = 1$. We average over many disorder configurations and initial product states $| \psi \rangle$ in the half-filled ($\bar{d} = 1$), zero-net-spin subspace. Also plotted are the saturation values of the local charge and spin correlations $D(\infty)$ and $M(\infty)$.

\section*{III. RESULTS}

Fig. 1 shows the dependence on distance of the charge and spin overlap. Results are shown for the IOMs built from the local charge and magnetization on sites $i = 1$, 2, and 3. The behavior is the same for all $i$. With charge disorder alone, the charge overlap decays exponentially with distance, indicating that the charge IOMs are spatially localized, but the spin overlap plateaus, Fig. 1(a). However, even a very small amount of disorder in the spin results in nearly the same localization in both charge and spin, Fig. 1(b).

To explore the evolution of this behavior with the strength of the charge disorder, Fig. 1(c) shows the decay of the charge and spin overlaps with distance for a fixed weak value of spin disorder and a range of values of charge disorder. When the disorder in both charge and spin is small, there is no localization in either channel. However, when the charge disorder is above a threshold, both charge and spin become localized, despite the spin disorder remaining very small. Fig. 1(d) emphasizes this point by showing the localization lengths for charge and spin extracted from the overlap data at more values of the charge disorder strength. Both charge and spin respond similarly to changes in the charge disorder alone. The difference between the charge and spin response may become even smaller for larger systems, as discussed further below.

Thus far we have focused on situations in which the disorder in the charge dominates. In prior work, the case of charge disorder alone has received the most attention, but spin disorder alone has also been studied. In both of these limits, the channel which is disordered is generally seen to be localized while the other is not. We have explored the full spectrum between these two limits, Fig. 2. The localization of charge grows smoothly with the charge disorder strength largely independent of the spin disorder for $W_{sp} < W_{ch}$. Meanwhile, spin, which is delocalized without spin disorder, shows a very sharp increase in localization, reaching localization comparable to that of the charge at spin disorder strengths an order of magnitude less than that of the
FIG. 2: Charge (a) and spin (b) single-site overlaps and $\delta$ (c), defined below, versus charge and spin disorder. Charge and spin overlap versus distance (d) comparing results for disorder strong for charge and weak for spin and vice versa. $L = 6$, $U = 1$, $10^4$ disorder configurations.

The symmetry between charge and spin is striking. When Fig. 2(a) is reflected across the diagonal, it is the same as Fig. 2(b). To emphasize this Fig. 2(c) shows the relative difference

$$\delta(W_{\text{ch}}, W_{\text{sp}}) = \frac{|O_c(W_{\text{ch}}, W_{\text{sp}}) - O_s(W_{\text{sp}}, W_{\text{ch}})|}{\frac{1}{2}(O_c(W_{\text{ch}}, W_{\text{sp}}) + O_s(W_{\text{sp}}, W_{\text{ch}}))} \ll 1$$

The relative error in the original data is of order 0.5%, which is of order the relative differences shown. While a few parameter values show larger differences, most are much smaller and there does not appear to be a systematic variation. Also shown, Fig. 2(d), is the overlap as a function of distance for two parameter sets on opposite sides of the diagonal, one with disorder large in charge and small in spin and the second the reverse.

Because much of the work to date has focused on time-dependent quantities, we note that the parameter dependence of our IOM-based measures is consistent with that of the dynamics. Fig. 3 compares the variation with charge disorder strength of the charge and spin single-site overlap (a) to that of the saturation value of the local charge and spin correlations (b). The two figures are qualitatively the same and even very similar quantitatively. In our small systems, only a broad crossover is visible, but the variation between $L = 4$ and 6 is suggestive of the expected evolution at larger system sizes to an abrupt transition. Specifically, at high disorder the single-site spin overlap moves to larger values as the system size is increased, while at low disorder the overlap decreases as the system size is increased. Indeed it is possible that the difference between the charge and spin values may be smaller for larger systems.

FIG. 3: Average charge and spin single-site overlap (a) and saturation value of the local charge and spin correlations (b) versus charge disorder for fixed weak spin disorder. $U = 1$; $W_{\text{sp}} = 0.1$; $10^6$, $10^7$, and $10^8$ disorder configurations for $L = 2$, 4, and 6, respectively.

FIG. 4: Local charge and spin correlations versus time for fixed charge disorder $W_{\text{ch}} = 16$ and five different values of spin disorder. $L = 8$, $U = 1$, $10^5$ disorder configurations. Inset shows the same spin correlation data versus $W_{\text{sp}}t$.

A key issue in characterizing the system through its dynamics is the time scale at which localization will be visible. Fig. 4 shows the local charge and spin correlations versus time on a log scale for a fixed large value of charge disorder and a range of different spin disorder values. The turnover to the saturation value occurs at later times for smaller values of the spin disorder. The inset shows the same results with time measured in units of the inverse of the spin disorder, demonstrating that the localization is reflected in the dynamics at a time of $\sim 1/W_{\text{sp}}$.

IV. DISCUSSION

We have explored localization in the Hubbard model with a wide range of independent values of charge and spin disorder, using measures of localization which pro-
vide independent information on charge and spin. We have focused on measures based on charge and spin-specific integrals of motion which are optimized for maximum locality. Results for these measures are consistent with those based on dynamics, with the advantage that they avoid the question which arises in the case of time-dependent measures of whether sufficiently long times have been included.

Our results show a symmetry between the response of the charge to spin disorder and vice versa. We find that for sufficient disorder in one degree of freedom, only a small amount of disorder in the other degree of freedom localizes both degrees of freedom. Indeed, the responses of charge and spin are clearly coupled in the sense that the level of localization in one sector is not simply dependent on the disorder in that sector. These observations suggest that the reason for the delocalized behavior observed in the case of charge disorder only, and spin disorder only is likely due to the presence of perfect symmetry in local spin and local charge respectively, as opposed to the absence of strong disorder in the second channel. Consistent with this, we note that Ref. [18], which concluded that sufficient charge disorder did result in full localization, included a magnetic field at a single site in their system, breaking the local SU(2) symmetry. Indeed, we have repeated this result, showing that a local field at a single site is sufficient to allow localization to occur – at sufficiently long times – in both charge and spin. Interestingly Ref. [18] noted in the supplementary material that the effect of this single-site symmetry-breaking term increased with system size.

We note that the time scale needed to observe localization in the dynamics of the less-disordered degree of freedom is proportional to the inverse of the disorder strength in that sector. Thus, we suggest that in an experiment with a nearly uniform magnetic field it would take an exceedingly long time to observe localization in the spin degrees of freedom. Indeed, it will be interesting in future work to explore further the time scale(s) associated with the coupling between the charge and spin degrees of freedom. Ref. [22] noted that even with charge disorder alone there was a crossover at long times to a slower decay of spin correlations, perhaps marking a time scale associated with coupling of the spin to the charge. The charge and spin-specific integrals of motion introduced here provide a convenient tool for this work.

In this work we have focused on half filling and $S_{\text{tot}}^z = 0$, but varying these represents another avenue for future exploration. Ref. [25] considers disorder in the interaction term of the Hubbard model, resulting in different localization of singly and doubly occupied sites and hence significant filling dependence of the dynamics. Ref. [21] also explores away from half filling, finding similarly distinct behavior at different fillings in the entanglement entropy. In the absence of spin disorder, when $S_{\text{tot}}^z = 0$, the local magnetization expectation values $\langle E_n | m_i | E_n \rangle$ are confined to zero by symmetry [20] in subspaces where $S_{\text{tot}}^z \neq 0$, this is no longer the case. Our preliminary results for the variation with charge disorder of the distribution of these expectation values, in the absence of spin disorder, are suggestive of localization behavior [22].

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41. Note that this construction of the conserved operator is distinct from a unitary transformation as the operation is not applied to all states and operators.