Time Dependence, Disorder, and Many Body Localization

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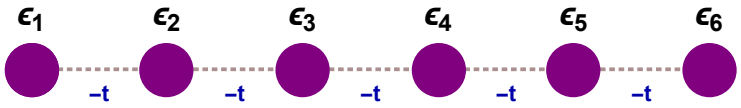
Abstract

We explore localization due to randomness in both single particle and many-body systems. Our results show that different forms of time-dependence of the system cause the system to behave in qualitatively different ways. We confirm the known result that random time dependence causes a disordered system to delocalize completely. However, we find that periodic time dependence causes an increase in localization length, but not a complete delocalization.

Introduction

In this paper, the fundamental question we ask is: When considering an isolated system, where is the use of statistical mechanics justified? In other words, under what conditions is it possible to calculate properties of a whole system by averaging over individual states of the system, weighted by the Boltzmann factor? The Eigenstate Thermalization Hypothesis provides a partial answer to this question by providing a connection between quantum mechanics and the predictions of statistical mechanics. The ETH states that after a sufficiently long time, a system will thermalize, so that the expectation value of any observable will be equal to the value predicted by statistical mechanics. However, the ETH is, in the end, only a hypothesis and sometimes breaks down. When the ETH breaks down, the system becomes localized, meaning that properties may vary from one region to the other and, furthermore, that information may not be exchanged between these regions. One



well-known way to cause the ETH to break down is to introduce randomness to the system [Ref. 1].

We consider an N-site, one-dimensional lattice with random onsite energies as shown above. [1] We add both random ("white noise") time dependence and periodic time dependence to onsite energies to explore where delocalization occurs. This model considers hardcore bosons, so that each orbital contains either 0 or 1 particles. (Although much research in solid state physics concerns fermions, boson models apply to cold atom systems and translate to systems of magnetic spins.) Our "white noise" model serves as an extension of the results of Ref. 2.

Methods

We examine both single particle (non-interacting) and many-body (interacting) systems. In each case, we begin with a lattice with N sites. Each site has an associated energy ("onsite energy") ϵ_i. Tunneling parameter t is the energy associated with tunneling between two sites. As in the tight binding model, particles are allowed to tunnel only between neighboring sites. Thus, the Hamiltonian of the single particle system is given by

$$H = -t \sum_{i=1}^{N} (c_i^+ c_{i+1} + c_{i+1}^+ c_i) + \sum_{i=1}^{N} \epsilon_i n_i \tag{1}$$

where c and c^+ are the annihilation and creation operators, respectively, and $n_i = c_i^+ c_i$ is the number operator. In the many-body system, we must allow for the possibility of interactions between particles, and so the Hamiltonian takes on an additional term:

[1] Note that N must be large enough for statistical mechanics to apply in the first place. An N-site system with periodic time dependence approximates an infinite system when the average inverse participation ratio of its eigenstates, defined later, is constant with respect to N.

$$H = -t \sum_{i=1}^{N} (c_i^+ c_{i+1} + c_{i+1}^+ c_i) + \sum_{i=1}^{N} \epsilon_i n_i - V \sum_{i=1}^{N} n_i n_{i+1} \tag{2}$$

We explore systems with random "white noise" time dependence (onsite energies given by $d_i + c\phi_i, \phi_i \in [-1, 1]$) and periodic time dependence (onsite energies given by $d_i + c\ Cos(\frac{2\pi m}{M} + \phi_i), \phi_i \in [0, 2\pi]$). d_i is a random number in $[-w, w]$. In our computations, all random numbers are obtained from random number generators in Python.

To quantify localization or delocalization for a given eigenstate ψ of the system, we calculate the participation ratio defined for the single particle system as

$$IPR = \frac{1}{\sum_i |\psi_i|^4} \tag{3}$$

where ψ_i is the i^{th} entry of the eigenstate. A larger IPR indicates that more sites in the lattice are "participating," and the system is more delocalized. An IPR of 1 indicates that the particle is completely localized to one site. True delocalization occurs when IPR increases linearly with system size N. We compare the participation ratios of a given system to that of a corresponding time independent system, whose onsite energies have $c = 0$.

In addition to IPR, we calculate thermodynamic quantities (such as entropy and specific heat), the time-evolution of a given initial state, and properties of the time evolution operator. For the many-body system, we also calculate density-density correlation functions, structure factor, and entanglement entropy of the system employing an approximation scheme called the Numerical Link Cluster Method.

Because the Hamiltonian itself has time dependence, the calculation of these quantities becomes more complicated. Any quantum mechanics textbook describes the time-evolution of eigenstates of a time-independent Hamiltonian, but to describe the states of a time-dependent Hamiltonian, we must employ different methods. For a time-independent Hamiltonian, an eigenstate at time 0 $|\psi_0\rangle$ evolves as

$$|\psi(t)\rangle = e^{iHt} |\psi_0\rangle \tag{4}$$

(We use units where $\hbar = 1$.) Feynman generalized this result to find the eigenstates of a time-dependent Hamiltonian by introducing the time-evolution operator U:

$$U(t,0) = \mathcal{T} e^{-i \int_0^t H(t')dt'} \tag{5}$$

where $\mathcal{T}$ is the time-ordering operator. Then, each eigenstate evolves as

$$|\psi(t)\rangle = U(t,0)\,|\psi(0)\rangle\,. \tag{6}$$

In our case, we consider a piecewise constant Hamiltonian. We break the total time period T into M time intervals so that equation (5) becomes

$$U_{tot} = T e^{-i[H_1+H_2+...H_{M-1}+H_M]\Delta t} = U_M U_{M-1} ... U_2 U_1. \tag{7}$$

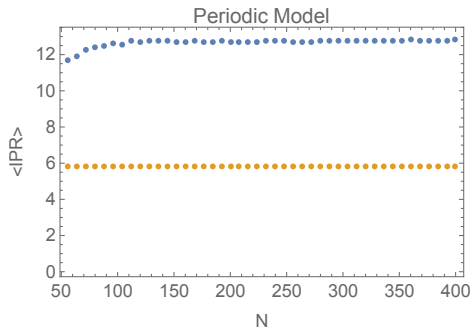
Thus, our calculations require us to find the time evolution operator for each time segment and then multiply them together to describe the evolution of the system over the whole time interval.

Results

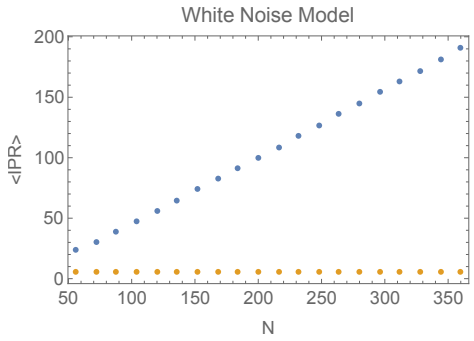
Varying N

For time-independent systems, inverse participation ratios increase only for small N and then remain roughly constant, with variation due only to disorder and vanishing with averaging over a sufficient number of disorder realizations. The inverse participation ratios of the periodic time-dependent system increase with increasing N but level off for sufficiently large system sizes. This behavior indicates that periodic time dependence causes the localization length to increase, but not for the system to become truly delocalized. In contrast, the $\langle IPR \rangle$ white noise system increases linearly with increasing system size, which indicates that the system is truly delocalized. Also note that, because the $\langle IPR \rangle$ of the periodic system becomes virtually constant at sufficiently large N, our calculations at these lattice sizes approximate the behavior of an infinitely long system.

In addition to average IPR, we consider the highest IPR of the system. For the periodic system we find that even the highest IPR does not show complete delocalization and behaves qualitatively like the average IPR of the system.



(a) Periodic system with $w = 2$, $T = 6$, $M = 40$, averaged over 10 disorder realizations



(b) White noise system also with $w = 2$, $T = 6$, $M = 40$, averaged over 10 disorder realizations

Varying w

For both forms of time dependence, larger w has a stronger localizing effect. IPR decreases for increasing w for both the time-dependent and time-independent systems. This behavior makes intuitive sense because larger w means that some orbitals will have stronger potentials, and so the particle will be more tightly bound or strongly repulsed. For small w, the time-dependent system has a smaller participation ratio than the corresponding time-independent system because time dependence adds a nonzero onsite energy.

Varying c

For both random and periodic time dependence, IPR increases with increasing c up to a point, reaches a peak (called the relocalization point), and then decreases. For very large c, inverse participation ratios fall below those of the time independent system.

Relocalization point

We define the relocalization point of a given system as the value of c at which the IPR begins to decrease. Below, the relocalization point is plotted as a function of w. We find that the relocalization point increases for increasing w. The IPR of the relocalization point (also shown below) decreases with

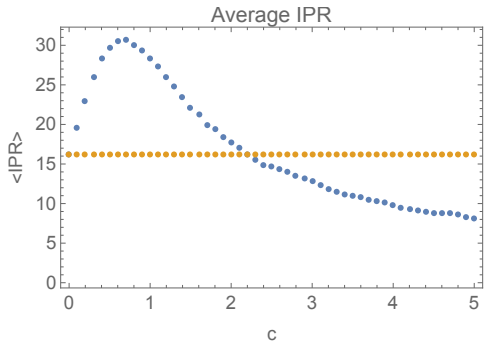


Figure 2: Periodic system with N = 128, w=1., T = 6, M = 100 averaged over 10 disorder configurations.

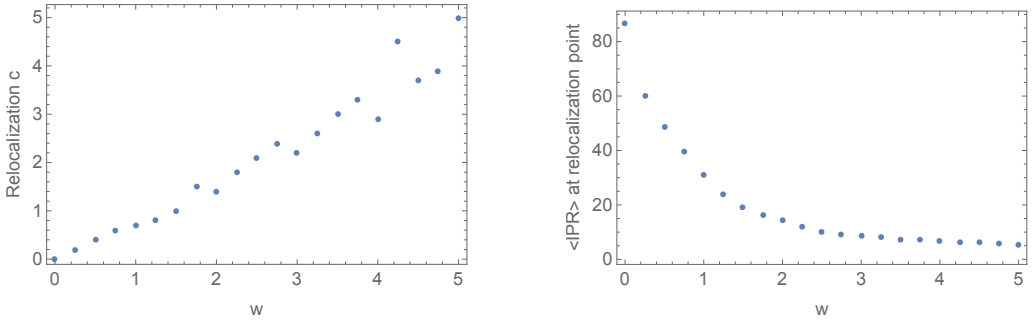


Figure 3: Relocalization point (a) and $\langle IPR \rangle$ at relocalization point (b) for a periodic system with $N = 128$, $T = 6$, $M = 40$ averaged over 10 disorder realizations.

increasing w.

Varying T and M

For periodic time dependence, increasing T causes greater delocalization (IPR increases). Increasing M causes IPR to decrease up to a point. However, because cosine is a continuous function, once we consider large enough M, we are essentially approximating the cosine function. Thus, the IPR and other properties remain the same as M is increased further.

For the white noise system, IPR decreases with increasing M, eventually falling below the IPR of the corresponding time-independent system. IPR

increases with increasing T and eventually levels off.

$\langle x \rangle$ and $\langle x^2 \rangle$

Consider a particle placed on the first site at t=0 (state $|\psi_0\rangle$). We can describe the motion of the particle through the lattice by calculating the quantities $\langle x \rangle$ and $\langle x^2 \rangle$, where x is the displacement of the particle from its starting point. With the piecewise constant Hamiltonian defined above, the state of a particle in time sector m is given by

$$|\psi\rangle = U_m |\psi_0\rangle . \tag{8}$$

$|\psi\rangle$ can be written in the basis of real state positions as

$$|\psi\rangle = \sum_i c_i |i\rangle . \tag{9}$$

We define

$$\langle x \rangle = \sum_i |c_i|^2 f_i$$

$$\langle x^2 \rangle = \sum_i |c_i|^2 f_i^2 \tag{10}$$

where

$$f_i = \begin{cases} i-1 & \text{for } 1 \leq i \leq \frac{N}{2} \\ -N+i-1 & \text{for } \frac{N}{2}+1 \leq i \leq N. \end{cases}$$

Because x measures displacement, $\langle x \rangle$ remains nearly zero over the entire period (once several disorder realizations are averaged). During the first time segments, the particle's motion is ballistic: it moves randomly in one direction or the other away from its starting point at a near-constant velocity. As shown in Fig. 4 the particle's squared displacement is roughly parabolic in the beginning. After a number of time segments, the displacement squared curve becomes linear. The $\langle x^2 \rangle$ versus m curve flattens after some time (larger lattices require more time).

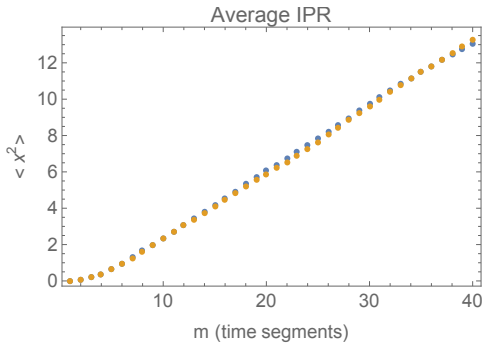


Figure 4: $\langle x^2 \rangle$ for $w = 1$, $T = 6$, $c = 2$, system sizes 111 (yellow) and 251 (blue) averaged over 100 disorder configurations.

Many particle system (Interacting system)

Instead of considering one particle free to move around the lattice, we allow for the possibility of multiple particles, anywhere between 0 and N. We work in the grand canonical ensemble, so that for a given calculation the number of particles in the system is allowed to vary. V is the energy of interactions between particles on neighboring sites. In our conventions, $V < 0$ gives a repulsive potential (since the energy required to sustain this configuration is increased) and $V > 0$ gives an attractive potential.

Calculation of IPR

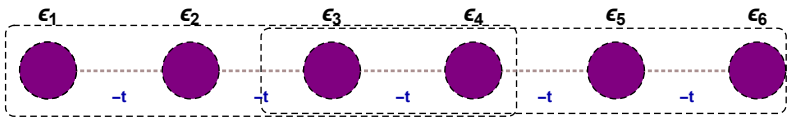
Because there may be more than one particle in the system, we need to redefine the IPR in order to quantify localization. We first define the single body density matrix M, whose entries are given by

$$M = \langle \psi | \, c_i^+ c_j \, | \psi \rangle \, . \tag{11}$$

Diagonalizing the single body density matrix gives eigenstates $|n\rangle$ and eigenvalues λ_n. Writing each eigenstate in its position state basis gives

$$|n\rangle = \sum_i c_i^n \, |i\rangle \, . \tag{12}$$

We then use these coefficients c_i^n to calculate IPR:



$$IPR = \frac{1}{N} \sum_n \lambda_n \sum_i |c_i^n|^4 \, |i\rangle \, . \tag{13}$$

We find that the IPR for the many-body system behaves in qualitatively similar ways to that of the single-body system when interactions are weak.

The Numerical Link Cluster Method

The presence of multiple particles presents the challenge that the size of the Hamiltonian increases as N^2, rather than N. (Intuitively, the dimension of the Hamiltonian is the same as the number of eigenstates of the system. Furthermore, the total number of eigenstates for our system, which may have any number of particles in the range $[0, N]$, is the sum of the number of eigenstates for a system with 0 particles, 1 particle, 2 particles,..., N particles.)

The Numerical Link Cluster method is a solution to this computational difficulty. The NLC is a series expansion method for calculating a given extensive property in a lattice. This method involves partitioning the lattice into clusters up to size $N - 1$, calculating the weight of each cluster, and calculating the property within each cluster. The property for the entire lattice is the sum of weights of the clusters. The NLC method is described further in Ref 3. Note, however, that the NLC method only converges in the many-body localized phase.

The NLC method is much more computationally efficient than direct diagonalization (which we employed for the single particle system) because it is only necessary to diagonalize a $(N-1)^2$-dimensional matrix rather than a N^2-dimensional matrix (or, in some cases, an $(\frac{N}{2}+1)^2$-dimensional matrix) and, more importantly, it is able to approximate the behavior of an infinite system at smaller lattice sizes than is possible with direct diagonalization. We employ this method to calculate correlation functions, structure factors, entanglement entropies, and other properties of our system.

Density-density correlation function and structure factor

For the following calculations we consider the ground state of a lattice at half-filling ($\frac{N}{2}$ particles). The density-density correlation function and structure factor provide a means of determining, for a given set of parameters, how particles tend to configure themselves relative to one another. The correlation function for two lattice sites i and j is given by

$$C_{ij} = \langle\psi|\, n_i n_j \,|\psi\rangle - \langle\psi|\, n_i \,|\psi\rangle \langle\psi|\, n_j \,|\psi\rangle\,. \tag{14}$$

For a translationally invariant lattice, we reproduce an already known result: for sufficiently large-magnitude $V < 0$ (i.e. $|V| >> \epsilon$), we observe a charge density wave, where particles tend to fill every other orbital. The correlation function shows this by alternating between values of -0.5 and 0.5 for consecutive j values. Our results for a translationally invariant model and for a random, time-independent model are shown in the plot below. Further work is needed to confirm these results. For $V > 0$, we find a phase separation, wherein orbitals on one side of the lattice are occupied and orbitals on the other side of the lattice are unoccupied.

The structure factor is defined in terms of the density-density correlation function:

$$S = \frac{1}{N}\sum_{ij} C_{ij}, V > 0 \tag{15}$$

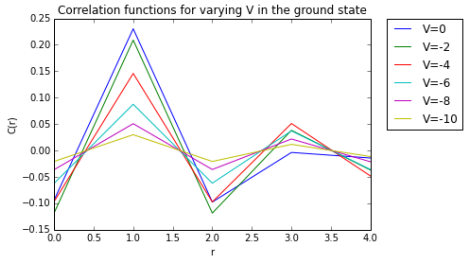
$$S = \frac{1}{N}\sum_{ij} (-1)^{i+j} C_{ij}, V < 0. \tag{16}$$

Again assuming a sufficiently large-magnitude V, a translationally invariant model has $S = 1$.

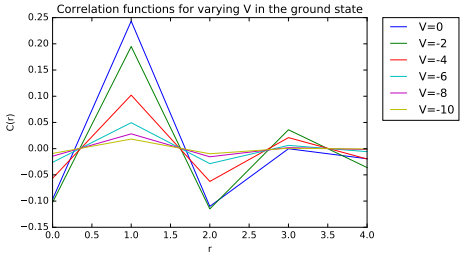
Future work: Entanglement entropies

The entanglement entropy of a system can be used to determine whether the system is in the many-body localized phase or the thermal phase. In the thermal phase, entanglement obeys a volume law and in the localized phase obeys an area law. To calculate entanglement entropy, one must first determine a "cut" in the system, and perform a Schmidt decomposition of the system's eigenstates:

$$|\psi\rangle = C_{i_L,j_R} \,|n_1 n_{d_L}; n_{d_L+1} n_{d_L+d_R)}\rangle \; = C_{i_L,j_R} \,|i_L; j_R\rangle \tag{17}$$



(a) Translationally invariant, time-independent system $V < 0$



(b) Random, time-independent system with $V < 0$

Then, it is possible to write the reduced density matrix as

$$\rho^L_{i_L,i'_L} = \sum_{j_R} C^*_{i_L,j_R} C_{i'_L,j_R}. \tag{18}$$

Using the reduced density matrix, we can calculate the entanglement entropy:

$$S = -Tr\,(\rho\, log_2 \rho) = -\sum p_i\, log\, p_i. \tag{19}$$

We have followed the conventions of Ref. 4 and chosen our cut to be the middle of a $2N-2$ orbital lattice. The next step is to reproduce the results of Ref. 3 and then possibly to explore other configurations.

Conclusion and further work

Our calculations of participation ratios and other quantities demonstrate the differing behaviors of the system in the localized phase and in the thermal phase. We find that the white noise model has a truly delocalized phase, while the period model does not. Future work includes calculation of the entanglement for the many-body system. We also hope to explore the time evolution of non-equilibrium states for this system.

Acknowledgments

This project was completed under the supervision of Prof. Rajiv Singh, and with the collaboration of Prof. Richard Scalettar and, for the single particle system, Natasha Proctor.

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