Entanglement and thermalization in open fermion systems

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Abstract

We numerically study two non-interacting fermion models, a quantum wire model and a Chern insulator model, governed by open system Liouville dynamics. The physical setup consists of a unitarily evolving “bulk” coupled via its boundaries to two dissipative “leads”. The open system dynamics is chosen to drive the leads to thermal equilibrium, and by choosing different temperatures and chemical potentials for the two leads we may drive the bulk into a non-equilibrium current carrying steady state. We report two main results in this context. First, we show that for an appropriate choice of dynamics of the leads, the bulk state is also driven to thermal equilibrium even though the open system dynamics does not act directly on it. Second, we show that the steady state which emerges at late time, even in the presence of currents, is lightly entangled in the sense of having small mutual information and conditional mutual information for appropriate regions. We also report some results for the rate of approach to the steady state. These results have bearing on recent attempts to formulate a numerically tractable method to compute currents in strongly interacting models; specifically, they are relevant for the problem of designing simple leads that can drive a target system into thermal equilibrium at low temperature.

1 Introduction

One of the most challenging problems in quantum many-body physics is the calculation of electrical and thermal currents in strongly interacting systems [1–5]. The formalism of linear response provides a general method to compute currents in the limit of weak bias, but the needed correlation functions involve real time computations at finite temperature. When the coupling is strong these computations are typically intractable or rely on uncontrolled approximations. A variety of other methods can be brought to bear upon the problem, ranging from numerical approaches to the use of AdS/CFT duality [6–16], but calculating transport properties of strongly interacting systems generally remains challenging. Given the wealth of experimental data on electrical and thermal currents in quantum many-body systems, it is important to address this ongoing challenge. We are particularly interested in low temperature dynamics, where collective modes can dominate the physics, e.g. at quantum critical points.

While a general approach to the problem of transport is difficult to imagine, recent ideas from the theory of quantum entanglement have offered some new hope in this direction. The starting point of this approach is to directly consider the physical properties of the state \( \rho_{\text{NESS}} \) corresponding to the non-equilibrium steady state (NESS) of the system of interest (this is a starting point of many approaches, e.g. [1, 2, 11, 17–24]). The steady state is imagined to carry a current at some finite temperature. Then while a general density matrix \( \rho_{\text{NESS}} \) can be exponentially complex, i.e. is a \( 2^n \times 2^n \) matrix for \( n \) spin-1/2s, it might be that the NESS steady state has relatively little entanglement, similar to a thermal state [25, 26], and can be effectively compressed to a much smaller set of physically meaningful data. Working in the context of one-dimensional
spin chains, it was indeed suggested that such NESS would have relatively little entanglement \cite{27}, e.g. that the mutual information between a region and its complement would obey an area law \cite{28,29}. This insight led to an efficient procedure to compute currents in chaotic spin chains using matrix product state technology \cite{26,27,30–35}.

There is evidence, from numerics \cite{36–42} and from integrable systems \cite{27,43–51}, that matrix product states can give a good description of NESS in one dimension. However, we also know that not every NESS has low entanglement \cite{52}. Recently, the framework of approximate conditional independence \cite{53–58} was used to argue that NESS of thermalizing systems would have an efficient tensor network representation in any dimension \cite{59}. The key idea is that in a thermalizing system, something like local thermal equilibrium is obtained in the NESS, at least if the system is driven only weakly away from equilibrium. If the entropic structure of such a local thermal equilibrium state follows reasonable expectations \cite{60}, then approximate conditional independence follows. Ref. \cite{59} gave a preliminary discussion of this physics within a free fermion open system model and using tools of AdS/CFT duality \cite{16,61,62}.

Although we are ultimately interested in physics of transport in interacting systems, the necessary algorithmic challenges have not yet been fully met. To help meet these challenges, non-interacting fermion models provide a useful testbed for some aspects of the physics. To set the stage, note that even if we grant that NESS have efficient tensor network representations, the non-trivial task of finding the right tensor network still remains. We cannot, for example, simply minimize the energy or the free energy of the system within a variational class of tensor network states since we are interested in an out-of-equilibrium state. One possible method for finding the steady state is a generalized variational principle adapted to out-of-equilibrium states \cite{36}. Another method is to design an open system dynamics \( \mathcal{L} \) such that \( \rho_{\text{NESS}} \) is equal to the time-independent steady state of \( \mathcal{L} \), \( \mathcal{L}(\rho_{\text{NESS}}) = 0 \). The parameters defining the NESS, e.g. the temperature gradient, would be built into the dynamics \( \mathcal{L} \). One could then find the NESS by simulating the time evolution \( \partial_t \rho = \mathcal{L}(\rho) \) until it converges to the steady state. Of course, simulating the dynamics of \( \mathcal{L} \) may be challenging in general, but simulating the dynamics within a suitable class of low entanglement tensor network states could be feasible \cite{27,30,63–65}.

Ref. \cite{27} found that a small bath consisting of just a few sites was sufficient to obtain interesting physics at high temperatures (compared to microscopic scales). It was also verified that the details of the bath did not strongly effect the results, again at high temperature. However, since we are particularly interested in low temperature physics, the problem of designing an open system dynamics whose steady state is the desired NESS is potentially non-trivial. To form a useful component of any computational method, such an open system dynamics must have three properties: (1) it must be able to drive the system to thermal equilibrium at low temperatures, (2) it must drive the system into the steady state in a reasonable (non-exponential) amount of time, and (3) it must not be excessively complex, e.g. it should not use the detailed properties of many-body energy eigenstates. In this work we investigate the problem of designing a suitable dynamics \( \mathcal{L} \) using a non-interacting fermion model.

The dynamical system has two components, illustrated in Figure 1: one is the system of interest (the “target”) and the other one is the designer leads which thermalize the target (or more generally drive it out of equilibrium). In this work both the target and the lead are non-interacting fermion systems. We propose that when studying an interacting system, the target should include the interactions of the system of interest, but the lead can still be taken to be non-interacting. Based on the general expectation that interacting systems which thermalize do so independent of the details of the bath, a non-interacting lead should be adequate to induce thermalization so long as it has the correct gross features. Taking the lead to be non-interacting immediately answers point (3) above, since such a lead, as we review below, is relatively simple. In the remainder of this work, we study points (1) and (2) in both one- and two-dimensional non-interacting fermion models. The basic parameter of our lead model is the size of the lead; such a lead with many sites we call an extended lead.

Our results are as follows. First, thermal equilibrium at relatively low temperatures can be reached using such an extended lead, but the required lead size typically grows with decreasing temperature. This addresses point (1) above. Second, the time to reach the steady state in a metallic state is an inverse polynomial in the system-plus-lead size. This addresses point (2) above. Third, the above two conclusions are modified when the system is insulating, either due to an energy gap or due to disorder. In these cases we find that the time to reach the steady state is significantly longer, scaling exponentially with the system size. Fourth, the steady states in our extended lead model are low entanglement states and exhibit approximate conditional
independence for appropriate regions. To the best of our knowledge, we study lower temperatures and larger systems than previously considered in the literature. Compared to the results of Ref. [59], we study in more detail the structure of the steady state, both in the unbiased and biased case, and we study a two-dimensional model to investigate the validity of our conclusions in more than one dimension.

In the remainder of this introductory section we introduce our models, define our observables, and discuss our methods. We then present two sets of results, one set for the one-dimensional quantum wire model and one set for the two-dimensional Chern insulator model [66]. We conclude with a brief discussion of future work and open questions.

1.1 Models

We study the transport and entanglement properties of two models. The setup for each model consists of three disjoint regions: the left lead (L), the middle part representing the wire (W) whose transport properties we investigate, and the right lead (R) (see Figure 1). The three parts consist of $N_L$, $N_W$, and $N_R$ fermion sites respectively. The leads are held at inverse temperatures $\beta_L = 1/T_L$, $\beta_R = 1/T_R$ and chemical potential $\mu_L$, $\mu_R$. This is accomplished using open system dynamics which drives the decoupled leads to thermal equilibrium with the indicated parameters. We first describe the Hamiltonian dynamics and then discuss the implementation of dissipation.

1.1.1 Hamiltonian dynamics

Quantum wire model: The first model is a one-dimensional quantum wire of fermions. Each of the segments described above is characterized by a hopping Hamiltonian which is quadratic in fermion creation and annihilation operators

$$H_a = -w \sum_{x=1}^{N_a-1} (c_{x}^\dagger c_{x+1} + c_{x+1}^\dagger c_{x}),$$

(1.1)

where $a = L, W, R,$ and $c_x$ is the annihilation operator at site $x$. The creation and annihilation operators obey the standard anti-commutation relation $\{c_x, c_y^\dagger\} = \delta_{x,y}$. The leads couple to the middle part of the wire through similar hopping terms: $-w'(c_{N_L}^\dagger c_{N_L+1} + c_{N_L+1}^\dagger c_{N_L} + h.c.)$ and $-w'(c_{N_L+N_W}^\dagger c_{N_L+N_W+1} + h.c.)$. One can also add an on-site potential term $V_x c_x^\dagger c_x$ for every fermion in the middle region $W$.

Chern insulator model: The second model is a two-band tight-binding Hamiltonian in two dimensions which exhibits the physics of the quantum anomalous Hall effect. This model is called the Chern insulator model and was first studied in [66]. We consider two states of fermions at each lattice site, which can be interpreted as $s$ and $p$ orbitals. The Hamiltonian in momentum space $\mathbf{k} = (k_x, k_y)$ is given by

$$H_W = \sum_{\mathbf{k}} [\epsilon(\mathbf{k}) + V h(\mathbf{k})],$$

(1.2)
We describe the interaction of our leads with an environment using Markovian open system dynamics. The time evolution of the density matrix is given by Lindblad’s equation

\[
\frac{d\rho}{dt} = \mathcal{L}(\rho) = -i[H, \rho] + \sum_j L_j \rho L_j^\dagger - \frac{1}{2} \sum_j \{L_j \dagger L_j, \rho\},
\]

where \( H \) is the full system Hamiltonian and \( L_j \) are jump operators describing the coupling to the environment. The operator \( \mathcal{L} \) is called the Liouvillian operator. The jump operators are taken to be linear in \( c_\alpha \) and \( c_\alpha^\dagger \) and therefore can be written as

\[ L_j = u_j \dagger c, \quad \text{or} \]
\[ L_j = c_j^\dagger v_j, \]

1.1.2 Dissipative dynamics

We can perform a Fourier transform and write the Hamiltonian in position space

\[
H_W = \sum_{x=1}^{N_{W,x}} \sum_{y=1}^{N_{W,y}} \epsilon_{x,y} c_{x,y}^\dagger c_{x,y} + \text{h.c.}
\]

where \( N_{W,x} \), \( N_{W,y} \) are the dimensions of the lattice, \( c_{x,y} = [c_{x,y,1}, c_{x,y,2}]^T \) is a two-component column vector containing the annihilation operators of the two fermion states at lattice position \((x,y)\). We treat \( \alpha = (x,y,i) \) as a composite index labeling the fermions, which obey the anticommutation relation \( \{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha,\beta} = \delta_{x,x'} \delta_{y,y'} \delta_{i,i'} \). Note that the Hamiltonian contains only nearest-neighbor couplings and there are no periodic boundary conditions imposed.

An important feature of the above Hamiltonian is the existence of edge states. If we rewrite \( H_W \) in the \((x,k_y)\) space, with periodic boundary conditions in \( y \)-direction and open boundary conditions in \( x \)-direction, we obtain a two-band energy spectrum with two edge states.

The lead Hamiltonians are also given by Eq. (1.2), where we set \( V = 0 \) and \( t = \omega \). The resulting lead Hamiltonian is similar to the 1D lead Hamiltonian because it involves only simple nearest-neighbor hopping. The coupling between the left lead and the Chern insulator is given by

\[
H_{LW} = \sum_{y=1}^{N_{L,y}} c_{N_{L,x},y}^\dagger \begin{bmatrix} -w' & -w' \\ -w' & -w' \end{bmatrix} c_{N_{L,x}+1,y} + \text{h.c.}
\]

An analogous term \( H_{WR} \) can be written for the coupling between the Chern insulator and the right lead.
where \( u_j, v_j, c = [c_1, \ldots, c_n]^T \) are column vectors. In the case of a non-interacting fermion system with bath operators linear in the fermion modes, the Lindblad equation reduces to a single particle equation for the Green’s function \([67]\), as reviewed in Appendix A of \([59]\).

We construct the jump operators so that, absent a coupling to the wire, each lead would be driven to the thermal equilibrium state appropriate to its decoupled lead Hamiltonian. The precise construction is discussed in Appendix B of \([59]\); we review it here. The right and left jump operators are computed in the same way, so in what follows we focus only on the jump operators for the left bath. Let \( H_L \) be the single particle Hamiltonian of the left bath, and let \( \epsilon_j \) and \( \psi_j \) be its eigenvalues and eigenvectors. The eigenvectors are written in the \( \{c_{\alpha}\} \) basis and can be viewed as a function of lattice site. Then we will have \( N_L \) in rates

\[
\gamma_{\text{in},j} e^{\beta_L (\epsilon_j - \mu_L)} = \gamma_{\text{out},j}. \tag{1.10}
\]

Since only the ratio of the two matters, we can set \( \gamma_{\text{in},j} = \gamma \) for all \( j = 1, 2, \ldots, N_L \). Therefore we get the jump operators

\[
I_{L,j}^\text{in} = \sqrt{\gamma_c} \psi_j^\dagger c_j, \tag{1.11}
\]

\[
I_{L,j}^\text{out} = \sqrt{\gamma} e^{\beta_L (\epsilon_j - \mu_L)} \psi_j^\dagger c_j, \tag{1.12}
\]

Similar formulas are obtained for the right bath.

1.2 Observables

For each of the two models defined above, we compute several observables that reveal the transport and entanglement properties of non-equilibrium steady states. We study electrical currents to probe out-of-equilibrium physics, energy occupation numbers to probe thermalization, decay rates of the open system dynamics to probe timescales, and mutual information and conditional mutual information to probe the entanglement structure of the state.

**Currents:** For the one-dimensional wire, the current operator through the link \((j, j+1)\) is

\[
I = -i (c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j). \tag{1.13}
\]

For the two-dimensional lattice, we define the current flowing in the \(x\)-direction across the link \(((x, y), (x+1, y))\)

\[
I_x = i c_{x,y}^\dagger \begin{bmatrix}
-\frac{V}{2} + t & -\frac{V}{2} \\
\frac{V}{2} & \frac{V}{2} - t
\end{bmatrix}
c_{x+1,y} + \text{h.c.} \tag{1.14}
\]

and the current flowing in the \(y\)-direction across the link \(((x, y), (x, y+1))\)

\[
I_y = i c_{x,y}^\dagger \begin{bmatrix}
-\frac{V}{2} + t & i \frac{V}{2} \\
-i \frac{V}{2} & \frac{V}{2} - t
\end{bmatrix}
c_{x,y+1} + \text{h.c.} \tag{1.15}
\]

**Occupation Numbers:** Next we are interested in computing the occupation numbers of the energy eigenstates of the bulk in NESS and comparing them to the thermal equilibrium distribution. Write the bulk Hamiltonian \( H_W \) as a \( N_W \times N_W \) matrix in \( \{c_{\alpha}\} \) basis. Let \( \epsilon_k \) and \( \psi_k \) be the eigenvalues (single-particle energies) and eigenvectors of \( H_W \). Then, for each energy mode \( k \), we can define an annihilation operator

\[
c_{\epsilon_k} = \sum_{j=1}^{N_W} \psi_k^\dagger(j) c_j, \tag{1.16}
\]
where the sum is over all the fermion modes in the bulk wire. The number operator for energy mode $k$ is given by

$$
\langle c^\dagger_k c_k \rangle = \sum_{i=1}^{N_W} \sum_{j=1}^{N_W} \psi_k(i) \psi_k^*(j) \langle c^\dagger_i c_j \rangle.
$$

(1.17)

We will compare these expectation values in two different states, one is the exact thermal state and the other one is the steady state of the open system dynamics.

**Decay Rates:** We will also compute the rate of relaxation $\Delta$ to the steady state. This is obtained from the spectrum of the Liouvillean operator $\mathcal{L}$ as discussed in Section 1.3 and Appendix A. The inverse of this rate determines the time needed to come exponentially close to the steady state. The rate typically decreases with increasing system size $n$, either as an inverse polynomial $\Delta \sim 1/n^a$ or exponentially $\Delta \sim e^{-bn}$.

**Entanglement:** Finally, to study the entanglement structure of the current-carrying states we compute the mutual information and conditional mutual information. If we consider two regions, A and B, of our system, then the mutual information is defined as

$$
MI(A : B) = S(A) + S(B) - S(AB),
$$

(1.18)

where $S(X)$ denotes the von Neumann entropy of region $X$. The conditional mutual information between three regions, A, B, and C (see Figure 2), of a system is given by

$$
CMI(A : C | B) = S(AB) + S(BC) - S(B) - S(ABC).
$$

(1.19)

Notice that the quantities defined above are expressed in terms of von Neumann entropy only. To compute the entropy of a region $X$, we first define the correlation matrix

$$
G_{\alpha\beta}^X = \langle c^\dagger_\alpha c_\beta \rangle,
$$

(1.20)

where $\alpha$ and $\beta$ denote orbitals within $X$. It is worth mentioning that $G^X$ has eigenvalues between 0 and 1. We can then define the entropy as

$$
S(X) = -\text{Tr}(G^X \ln G^X + (1 - G^X) \ln(1 - G^X)).
$$

(1.21)

The interpretation of vanishing mutual information is simple. If $MI(A : C) = 0$ then $\rho_{AC} = \rho_A \otimes \rho_C$ and the AC is uncorrelated. The interpretation of vanishing conditional mutual information is more subtle. If $CMI(A : C | B) = 0$ then $A \rightarrow B \rightarrow C$ forms a “quantum Markov chain” [54] meaning that $C$ is independent of $A$ given the state of $B$. As discussed at length in Refs. [53–60], a quantum Markov chain generalizes the classical notion of a Markov chain in the sense that the total state $\rho_{ABC}$ can be recovered from the marginals $\rho_{AB}$ and $\rho_{BC}$. This does not imply that $A$ is uncorrelated with $C$, but it does imply that they are unentangled. Hence vanishing conditional mutual information indicates a certain kind of short-range

![Figure 2: The partition of the system into three disjoint regions A, B, and C to compute the mutual information $MI(A : C)$ and the conditional mutual information $CMI(A : C | B)$.

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entanglement in the state. It is this physics of approximate conditional independence which was used in Refs. [59, 60] to show that certain NESS have tensor network representations.

1.3 Methods

In order to compute our observables, we use a technique developed by Prosen [68], which allows us to solve the Lindblad master equation using a canonical quantization in the Fock space of operators. The method is applicable under the condition that the Hamiltonian is quadratic and the jump operators $L_k$ are linear in fermionic operators. The key idea is to write the Liouvillian (see Appendix A) in terms of adjoint Majorana maps and diagonalize it in terms of normal master modes (anti-commuting operators acting on the Fock space of density operators). Then the physical NESS is given by the zero-mode eigenvector. Below we review the main results of Ref. [68]. A more detailed discussion of the method is included in Appendix A.

First, rewrite the canonical fermion operators in terms of Majorana operators

$$w_{2j-1} = c_j + c_j^\dagger, \quad w_{2j} = i(c_j - c_j^\dagger)$$  \hspace{1cm} (1.22)

satisfying the anti-commutation relation $\left\{ w_j, w_k \right\} = 2\delta_{jk}$. Throughout this section the labels $i, j, ...$ run over all fermion modes in the problem, spatial and otherwise. Then the Hamiltonians of our systems can be written as quadratic forms in Majorana fermions

$$H = \sum_{j,k=1}^{2n} w_j H_{jk} w_k$$  \hspace{1cm} (1.23)

while the Lindblad operators can be written as linear combinations of $w_j$

$$L_k = \sum_{j=1}^{2n} l_{k,j} w_j.$$  \hspace{1cm} (1.24)

Ref. [69] shows that the properties of the NESS can be derived from the Liouvillian shape matrix $A$, which is an antisymmetric $4n \times 4n$ matrix incorporating the parameters of the bath operators and Hamiltonian

$$A_{2j-1,2k-1} = -2iH_{jk} - M_{kj} + M_{jk}$$
$$A_{2j-1,2k} = 2iM_{kj}$$
$$A_{2j,2k-1} = -2iM_{kj}$$
$$A_{2j,2k} = -2iH_{jk} - M_{jk} + M_{kj}$$  \hspace{1cm} (1.25)

where $M$ is a Hermitian matrix with entries

$$M_{jk} = \frac{1}{2} \sum_i l_{i,j} l_{i,k}^\dagger.$$  \hspace{1cm} (1.26)

It is worth mentioning that our formula for $A$ is different from the one in Ref. [68] in that we swap the indices of $M^1$. We believe this merely reflects a typo in Ref. [68].

Recall that the eigenvalues of a complex antisymmetric matrix of even dimension always come in pairs $\pm \beta$. Therefore we can order the eigenvalues of $A$ as $\beta_1, -\beta_1, \beta_2, -\beta_2, \ldots, \beta_{2n}, -\beta_{2n}$, with $\text{Re}(\beta_1) \geq \text{Re}(\beta_2) \geq \ldots \geq \text{Re}(\beta_{2n}) \geq 0$. Let $v_1, v_2, \ldots, v_{4n}$ be the corresponding eigenvectors, written as column vectors.

Ref. [69] proves three key results that we use to compute our observables. If the eigenvalues of $A$ have strictly positive real parts, $\text{Re}(\beta_j) > 0$, then

1. The non-equilibrium steady state is unique.

2. The rate of exponential relaxation to NESS is given by $\Delta = 2 \text{Re}(\beta_{2n})$.

\footnote{There is also an extra factor of $\frac{1}{2}$ in the definition of $M$ which comes from a rescaling of Lindblad operators $L_k \to \frac{L_k}{\sqrt{2}}$, relative to their definition in Ref. [68].}
3. The expectation value of any quadratic observable \( w_jw_k \) in NESS is given by

\[
\langle w_jw_k \rangle = 2 \sum_{m=1}^{2n} v_{2m,2j-1}v_{2m-1,2k-1}.
\] (1.27)

These results may be understood intuitively by noting that, roughly speaking, the \( \beta_j \) represent the “energies of excitations”. Hence the NESS is unique when all \( \beta_j \) have non-zero real part because all other states decay. Similarly, the rate of relaxation is determined by the slowest decaying excitation, corresponding to \( \beta_{2n} \) in the ordering we have chosen.

Notice that the results above provide all the necessary information to compute our observables, since they are all expressed in terms of the two-point correlation functions \( \langle c_j^\dagger c_k \rangle \), which of course is quadratic in Majorana operators. One can further use Wick’s theorem to compute expectation values of any higher order observable with an even number of fermion operators.

The implementation of these techniques involves computing the eigenvalue decomposition of very large matrices. We used the Multiprecision Computing Toolbox for MATLAB [70] to solve for the eigenstates and eigenvalues of \( A \) with high precision (32 digits). The extra precision was required to ensure that we can correctly group the eigenvalues into \((\beta,-\beta)\) pairs and that the eigenvectors are orthonormal.

2 Results

2.1 Quantum wire model

In this subsection we describe our analysis of the steady state physics of the quantum wire model. Throughout this discussion we set the nearest neighbor hopping \( w = 1 \), so that we effectively measure all energies in units of \( w \) and all times in units of \( 1/w \). We first study the physics of thermalization when the leads are unbiased. Then we consider the physics of NESS when the leads are biased. Next we discuss the structure of entanglement in the steady state. Finally, we discuss the effects of disorder.

2.1.1 Unbiased thermal equilibrium

We begin our analysis of the quantum wire model by investigating thermalization with unbiased leads. To this end we take \( \beta_L = \beta_R = \beta \) and \( \mu_L = \mu_R = 0 \). Recall that the open system dynamics is designed to drive each decoupled lead (L and R) into its decoupled thermal state. However, the leads are coupled to the middle wire which, except for the lead coupling at its boundaries, enjoys unitary dynamics. The Hamiltonian couplings are taken to be \( w = w' = 1 \). The question is how well the wire is thermalized by its boundary couplings to the leads.

We answer this question by comparing the exact thermal occupation numbers of the decoupled wire (with \( w' = 0 \)) with the expectation values of the corresponding number operators in the steady state. We expect agreement if (1) the leads are effectively thermalizing the wire and (2) the effects of the lead-wire coupling \( w' \) is small. To be clear, throughout the analysis we use the decoupled \( (w' = 0) \) wire energy eigenstates and we compare the expectation value of the number operator in thermal equilibrium and in the steady state of the open system dynamics. Data for \( \beta = .1, 1, 5 \) as a function of \( \gamma \) (the strength of the dissipative terms in \( L \)) is shown in Panels (a), (b), and (c) of Figure 3.

For \( \beta = .1, 1 \), we find that \( \gamma = .01 \) leads to a steady state distribution of occupation numbers that agrees well with the thermal result. Increasing the lead size does not dramatically effect the final steady state. For the the lowest temperatures reached, \( \beta = 5 \), a lead of size \( N_L = N_R = 40 \) is not sufficient to thermalize a wire of size \( N_W = 120 \). As demonstrated in Panel (d) of Figure 3, by taking larger leads we are able to achieve thermal equilibrium even for temperatures as low as \( \beta = 5 \).

What lead size is required to have approximate thermalization of the wire as a function of inverse temperature \( \beta \)? Figure 4 shows the minimal size \( N_L = N_R \) of the leads needed in order for the occupation numbers to be close (within a few percent) to the thermal distribution for different temperatures. Note again that the size of the contacts is only important at low temperatures. Similar results are also obtained when studying energy eigenstates of the entire coupled wire and lead system. We conclude that a sufficiently large lead is able to thermalize a wire even at low temperature via only boundary couplings.
Figure 3: Comparison of energy eigenstate occupation numbers between thermal equilibrium and the steady state of $\mathcal{L}$. (a) Occupation numbers for $\beta = 0.1$, $N_L = N_R = 40$ and $N_W = 120$, (b) Occupation numbers for $\beta = 1.0$, $N_L = N_R = 40$ and $N_W = 120$, (c) Occupation numbers for $\beta = 5.0$, $N_L = N_R = 40$ and $N_W = 120$, and (d) Occupations number for $\beta = 5.0$ and $N_L = N_R = N_W = 120$.

Figure 4: The minimal size of the leads required to approximately thermalize the wire as a function of $\beta$. Approximate thermalization is roughly defined as having energy occupation numbers within a few percent of the thermal result. Recall that we do not expect exact agreement with the decoupled ($w' = 0$) thermal result anyway since $w' \neq 0$ in the Liouvillean $\mathcal{L}$. 

9
Inverse temperature $\beta$

Linear response conductance $G$

Numerically computed

Ballistic transport

Figure 5: Landauer formula for ballistic conductance (red) compared to the numerically evaluated conductance in the steady state of $L$ (blue) as a function of $\beta$. System parameters are $N_L = N_W = N_R = 80$, $w = w' = 1$, and $\gamma = 0.05$.

2.1.2 Biased steady state

We continue our analysis by probing the extent to which biased leads define a steady state with the expected transport physics. To this end we take $\beta_L = \beta_R = \beta$ and $\mu_L = -\mu_R$. We compare the value of the current flowing through the wire in steady state with the corresponding Landauer formula for conductance [71]. Recall that this formula is obtained from an infinite wire model where the left and right moving particles are emitted from separate reservoirs with potentially different temperatures and chemical potentials.

The linear response conductance is defined as $G = I/(\mu_L - \mu_R)$ for small $\mu_L - \mu_R$. We study the conductance as a function of temperature $\beta_L = \beta_R = \beta$ by computing the current in the middle of the chain in the steady state with weakly biased leads. As reviewed in Appendix D of [59], the current predicted by the ballistic Landauer formula [71] is

$$I = \frac{1}{2\pi} \left[ \int_{\beta_L}^{\beta_R} \frac{d\epsilon_k}{2\pi} v_k f(\epsilon_k - \mu_L, \beta_L) + \int_{-\pi}^{0} \frac{d\epsilon_k}{2\pi} v_k f(\epsilon_k - \mu_R, \beta_R) \right], \quad (2.1)$$

where $\epsilon_k = -2w \cos k$ is the energy, $v_k = \frac{\partial \epsilon_k}{\partial k} = 2w \sin k$ is the group velocity, and $f(\epsilon, \beta) = (e^{\beta \epsilon} + 1)^{-1}$ is the Fermi distribution. This can be explicitly integrated to give

$$I = \frac{1}{2\pi} \left[ \frac{1}{\beta_L} \ln \left( \frac{e^{\beta_L(\mu_L+2w)} + 1}{e^{\beta_L(\mu_L-2w)} + 1} \right) + \frac{1}{\beta_R} \ln \left( \frac{e^{\beta_R(\mu_R-2w)} + 1}{e^{\beta_R(\mu_R+2w)} + 1} \right) \right]. \quad (2.2)$$

Next, in Figure 5 we plot the ballistic transport conductance and the numerically computed conductance in the steady state as a function of $\beta = \beta_L = \beta_R$, for a system with 240 sites ($N_L = N_W = N_R = 80$) with $w = w' = 1$ and $\gamma = 0.05$. Although there is an interesting feature near $\beta = 2$, the steady state current generally matches the Landauer formula quite well. We also obtained numerical evidence that the low temperature Landauer result is well approximated by the steady state value in the limit of large leads. Together we take these data as evidence that, just as the unbiased steady state captures well the physics of thermal equilibrium, the biased steady state captures well the physics of current carrying states in the non-interacting fermion wire.

We can also show that relaxation to the steady state takes place in a reasonable time frame, inverse polynomial in the system size. Recall that the relaxation rate is determined from the real part of the spectrum of the Liouvillian as described in Section 1.3. Figure 6 shows the relaxation rate $\Delta$ as a function of total system size $n$ for different inverse temperatures $\beta$. Other parameters are $w = w' = 1$, $\gamma = 0.01$, and $\mu_R = -\mu_L = 0.1$.

\[\text{It doesn’t matter where in the wire we measure the current because in a stationary state the current is conserved.}\]
2.1.3 Entanglement structure of the steady state

We continue our analysis of the wire model by studying the entanglement structure of the steady state. The region configurations we study were defined in Ref. [59] and are motivated by the physics of approximate condition independence [60], [53–58]. Consider a system with \( w = w' = 1, \mu_R = -\mu_L = 0.1, \) sufficiently large leads \( N_L = N_R = N_W = 120, \) and sufficiently small \( \gamma = 0.05 \) (these choices are based on the parameters that give the best thermalization results). The mutual information \( MI(A : C) \) and conditional mutual information \( CMI(A : C|B) \) for the partition in Figure 2, as a function of the size of the middle region \( B \) are presented in Figure 7. Different curves correspond to different values of \( \beta = \beta_L = \beta_R. \) Notice that the mutual information is basically equal to the conditional mutual information, and both decrease exponentially fast. When the logarithm of the MI/CMI is less than \(-30, \) this should be interpreted as the system having 0 MI/CMI. The reason those quantities are not exactly 0 is due to the numerical precision of the computation.

We may also study the slope \( s \) of the linear regions as a function of temperature. A plot of \( 1/s \) vs \( \beta \) is shown in Figure 8 where we find an approximately linear scaling of \( 1/s \) with \( \beta. \)

2.1.4 Effects of disorder

As we briefly mentioned in Section 1.3 we can add a disorder term \( V_x c_x^\dagger c_x \) at every site \( x \) in the region \( W \) of the wire. We choose \( V_x \) from a continuous uniform distribution over the interval \([-V_0, V_0]\). We look at small disorder values, where \( V_0 = 0.1w, \) although the results of this section hold true for larger \( V_0. \) For a system with \( w = w' = 1, \mu_R = -\mu_L = 0.1, N_L = N_R = N_W = 120, \) and \( \gamma = 0.05, \) we plot the mutual information and conditional mutual information (averaged over 500 disorder realizations) in Figure 9. We see that the two quantities decay roughly the same way as in the absence of disorder.

Similarly, we study the effect of disorder on relaxation rates. Consider the 1D system with \( w = w' = 1, \)
Figure 8: The inverse of the slope of the linear region of CMI as a function of $\beta$. The linear dependence on $\beta$ is expected, at least at large $\beta$, from the low temperature thermal physics in which there is a thermal correlation length proportional to $\beta$.

Figure 9: (a) Log of $MI(A : C)$ as a function of separation between regions $A$ and $C$ for different inverse temperatures $\beta$ in the presence of disorder $V_0 = 0.1w$. (b) Log of $CMI(A : C|B)$ as a function of size of region $B$ for different inverse temperatures $\beta$ in the presence of disorder $V_0 = 0.1w$. Averaging is performed over 500 disorder realizations.
2.2 Chern insulator model

In this subsection we describe our analysis of the steady state physics of the Chern insulator model. Throughout this discussion we set the nearest neighbor hopping $w = 1$, so that we effectively measure all energies in units of $w$ and all times in units of $1/w$. We first study the physics of thermalization when the leads are unbiased. Then we consider the physics of the NESS when the leads are biased. Finally we discuss the structure of entanglement in the steady state. A related study of a bosonic symmetry protected state subject to open system dynamics may be found in Ref. [72]

2.2.1 Unbiased thermal equilibrium

Here we follow closely our analysis of the one-dimensional quantum wire in the case of the two-dimensional Chern insulator. In what follows, the parameters of the model are set to $V = 3$, $c = 1$, $e_s = 0.5$, $t = 1$, $w = 1$, $w' = 0.1$, so that the system has an energy gap with two edge states. Consider the unbiased case where $\beta_L = \beta_R = \beta$ and the chemical potential is inside the gap $\mu_L = \mu_R = -3.6$. We find that the leads are able to drive the system to thermal equilibrium in the high temperature limit. The energy occupation numbers for a system with $N_{L,x} = N_{L,y} = N_{W,x} = N_{W,y} = N_{R,x} = N_{R,y} = 10$ and $\beta = 0.1$ are shown in Panel (a) of Figure 11.

In the limit $V \to 0$, the energy gap closes, and the system behaves like an ordinary metal. In this regime, we find that sufficiently large leads can thermalize the system even at low temperatures. The energy occupation numbers for $\beta = 1.0$ are shown in Panel (b) of Figure 11. However, we have not been able to find a parameter regime which thermalizes the Chern insulator with $V \neq 0$ at the lowest temperatures. As we show below, the rate of decay to the steady state is also slow for the Chern insulator, and these observations may be related.

2.2.2 Biased steady state

The structure of the current carrying state is generally more complex in the Chern insulator model relative to the quantum wire model because there exist many more current carrying modes in the two-dimensional model. However, when the chemical potential is chosen to sit within the bulk energy gap, then the edge
Figure 11: (a) Occupation numbers for $\beta = 0.1$ and $V = 3$, (b) Occupation numbers for $\beta = 1.0$ in the limit $V \to 0$.

Figure 12: The magnitude of the current flowing through every link of the Chern insulator model. The physical parameters are $N_{L,y} = N_{W,y} = N_{R,y} = N_{W,x} = 20$, $N_{L,x} = N_{R,x} = 10$, $\mu_L = -3.7$, $\mu_R = -3.5$, and $\beta_L = \beta_R = 1$. As expected for this parameter regime, most of the current is carried by the edge states with very little bulk conduction.

Figure 13: (a) Log of relaxation rate $\Delta$ as a function of system size $n$ for the insulator state, (b) Log of relaxation rate $\Delta$ as a function of log of system size $n$ for the metallic state.
Figure 14: (a) Log of $MI(A : C)$ as a function of x-coordinate separation between regions A and C for different inverse temperatures $\beta$, (b) Log of $CMI(A : C|B)$ as a function of the width of region B for different inverse temperatures $\beta$.

states of the Chern insulator are the primary carriers of current at low temperature. The current for a system with $N_{L,y} = N_{W,y} = N_{R,y} = N_{W,x} = 20$ and $N_{L,x} = N_{R,x} = 10$ biased by $\mu_L = -3.7$ and $\mu_R = -3.5$ at temperatures $\beta_L = \beta_R = 1$ is shown in Figure 12. We see that, as expected, the current is carried primarily by the edge states. We conclude that in addition to driving the system to thermal equilibrium, the leads can also drive the system into a NESS with the expected properties.

We also study the time needed to reach the NESS in the Chern insulator model. Fix $N_{L,y} = N_{W,y} = N_{R,y} = 8$ and vary the length of the insulator and leads $N_{L,x} = N_{W,x} = N_{R,x}$. Also fix the chemical potential inside the gap $\mu_L = -3.7, \mu_R = -3.5$ and take $\gamma = 0.05$. Figure 13 shows the relaxation rate $\Delta$ as a function of total system size for different values of inverse temperature $\beta$. Panel (a) shows that the decay rate depends exponentially on system size in the Chern insulating phase. This indicates a rather slow approach to the NESS and is similar to the decay rate obtained for the one-dimensional disordered insulator. Panel (b) shows that the decay rate for the metallic phase depends approximately inverse polynomially on system size. This is the same qualitative structure as obtained from the one-dimensional clean metallic wire.

2.2.3 Entanglement structure of the steady state

Finally, we turn again to an analysis of the entanglement structure of the NESS. Consider a 2D system with $N_{L,x} = N_{R,x} = 10$, $N_{W,x} = 40$, and $N_{L,y} = N_{W,y} = N_{R,y} = 8$. We set $\gamma = 0.05$ and place the chemical potential in the energy gap $\mu_L = -3.6, \mu_R = -3.5$. The plots for MI and CMI with different values of $\beta$ are shown in Figure 14. Note that the discontinuity in the graphs occurs exactly when region B becomes the hole insulator, and regions A and C become the left and right lead respectively. As in all other cases, the MI and CMI decay exponentially with separation or with the size of B respectively. Hence the physics of approximate conditional independence survives in the NESS of a two-dimensional model.

3 Discussion

In this paper we have given detailed evidence that one can design a relatively simple lead that thermalizes target non-interacting fermion systems in one and two dimensions. By biasing the leads, the systems can also be driven out of equilibrium to give expected results. Furthermore, we found that not every lead is able to thermalize a given target, at least in the non-interacting limit considered here. In particular, low temperatures seem to require a larger lead. It is reasonable to conjecture that adding interactions to the target system will help render thermalization more universal, e.g. independent of the details of the bath, but much remains to be understood in this context. In particular, it would be desirable to have a better understanding of what parameters, e.g. lead size and $\gamma$, lead to the best thermalization. More generally, this is just one small step towards a general framework for constructing leads that are able to effectively thermalize a variety of models.

We also showed that the time to reach a steady state is reasonable and scales with an inverse power of the system-plus-lead size, at least for the one-dimensional quantum wire and two-dimensional Chern insulator.
in its metallic phase. We did find that the environment-lead interaction rate, $\gamma$, needed to be taken small to achieve thermalization. Such a small $\gamma$ further slows the rate of approach to the steady state, but we did not find evidence that $\gamma$ had to scale with system size. In the presence of disorder in one dimension or in the insulating phase in two dimensions, we found that the time to reach a steady state was longer, scaling exponentially with the system size. This presents a potential challenge to the open system dynamics method for finding NESS, although at least in one dimension we know this slowdown is physical and is due to the physics of localization \[73\]. Given that larger baths better approximate thermal equilibrium but have slower relaxation times, it would be interesting to investigate optimizing the bath size with respect to these two competing demands. It would also be desirable to investigate the effects of interactions on the relaxation times of the open system dynamics.

Finally, we showed that the systems we investigated have little entanglement in their steady states. Thus although we used free fermion technology in our calculations, the low degree of entanglement implies that the states in question could also have been represented in a tensor network form. Such a low entanglement structure has been argued to generalize beyond the non-interacting limit \[27, 59\]. It might be illuminating to go through the exercise of writing the non-interacting fermion steady states using tensor networks, particularly as a first step towards including the effects of interactions.

In summary, our results provide further support for the previously outlined entanglement-based approach to calculating electrical and thermal currents in strongly interacting systems. The main idea is to represent the state of the system using tensor network methods and then to dynamically evolve, using an appropriate open system dynamics, to a current carrying steady state. Here we have shown how to design a non-interacting fermion lead which has three key properties: (1) it effectively thermalizes the system down to low temperatures, (2) it does so in a reasonable time frame, and (3) it is not overly complex. Pioneering matrix product based computations have already been carried out in one dimension at high temperature \[27\], and while there are still algorithmic and conceptual barriers to implementing the general program outlined in the introduction, our results have shed light on the design of lead systems. We have also raised several issues in the physics of thermalization of open non-interacting fermion models. Our future work will be concerned with testing these ideas for interacting systems at low temperatures in a variety of dimensions.

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A Review of Prosen’s method

In this appendix we discuss in more detail the method for solving the Lindblad master equation for a system with Hamiltonian and bath operators given by Equations (1.23) and (1.24) respectively. Begin with the definition of Liouvillean as the operator acting on $\rho$ on the right hand side of Lindblad’s equation

$$ \frac{d\rho}{dt} = -i[H, \rho] + \sum_k L_k \rho L_k^\dagger - \frac{1}{2} \sum_k \{L_k^\dagger L_k, \rho\} \equiv \hat{L}\rho. \quad (A.1) $$

Consider a $4^n$ dimensional Liouville space of operators $\mathcal{K}$, with an inner product defined as follows

$$ \langle x | y \rangle = 2^{-n} \text{tr}(x^\dagger y), \quad x, y \in \mathcal{K}. \quad (A.2) $$

A complete orthonormal basis for this space is given by operator-products

$$ P_{\alpha_1, \alpha_2, \ldots, \alpha_{2n}} = w_1^{\alpha_1} w_2^{\alpha_2} \cdots w_{2n}^{\alpha_{2n}}, \quad \alpha_j \in \{0, 1\}. \quad (A.3) $$

It turns out that $|P_{\vec{\alpha}}\rangle$ is a fermionic Fock basis and we can define creation and annihilation linear maps over $\mathcal{K}$

$$ \hat{c}_j |P_{\vec{\alpha}}\rangle = \alpha_j |w_j P_{\vec{\alpha}}\rangle, \quad \hat{c}_j^\dagger |P_{\vec{\alpha}}\rangle = (1 - \alpha_j) |w_j P_{\vec{\alpha}}\rangle, \quad (A.4) $$

which satisfy the canonical anti-commutation relations.
The Liouvillean can be written as a quadratic form in terms of these maps

\[
\hat{\mathcal{L}} = -4i \sum_{j,k=1}^{2n} \hat{c}_j^\dagger H_{jk} \hat{c}_k + \frac{1}{2} \sum_i \sum_{j,k=1}^{2n} \ell_{i,j,k}^l \hat{\mathcal{L}}_{j,k},
\]

where

\[
\hat{\mathcal{L}}_{j,k} = (1 + \exp(i\pi\hat{N}))(2\hat{c}_j^\dagger \hat{c}_k^\dagger - \hat{c}_j \hat{c}_k) + (1 - \exp(i\pi\hat{N}))(2\hat{c}_j^\dagger \hat{c}_k^\dagger - \hat{c}_j \hat{c}_k^\dagger)
\]

and \(\hat{N} = \sum_j \hat{c}_j^\dagger \hat{c}_j\) is the number of adjoint fermions. Notice that the Liouvillean commutes with the parity operator \(\hat{P} = \exp(i\pi\hat{N})\) and hence the operator space can be decomposed into even and odd subspaces via an orthogonal projection \(\mathcal{K}^\pm = \frac{1}{2}(1 \pm \hat{P})\). Since we are interested in expectation values of observables quadratic in fermion operators, we restrict ourselves to the subspace \(\mathcal{K}^+\) where \(\hat{\mathcal{L}}_{j,k}\) has the form

\[
\hat{\mathcal{L}}_{j,k}|_{\mathcal{K}^+} = 4\hat{c}_j^\dagger \hat{c}_k^\dagger - 2\hat{c}_j^\dagger \hat{c}_k^\dagger - 2\hat{c}_j \hat{c}_k.
\]

Combining Equations (A.6) and (A.8) yields a compact representation of the Liouvillean on the even subspace

\[
\hat{\mathcal{L}}_+ = -2\hat{c}^\dagger (2iH + M + M^T)\hat{c} + 2\hat{c}^\dagger (M - M^T)\hat{c}^\dagger,
\]

where \(\hat{c} = [\hat{c}_1, \hat{c}_2, \ldots, \hat{c}_{2n}]^T\) is a column vector, \(M\) is the matrix containing information about the baths, defined in Equation (1.26), and \(H\) is the Hamiltonian matrix with entries \(H_{jk}\). We can further simplify this representation by introducing \(4n\) Hermitian Majorana maps \(\hat{\alpha}_k\)

\[
\hat{\alpha}_{2j-1} = \frac{1}{\sqrt{2}}(\hat{c}_j + \hat{c}_j^\dagger), \quad \hat{\alpha}_{2j} = \frac{i}{\sqrt{2}}(\hat{c}_j - \hat{c}_j^\dagger).
\]

In terms of these maps, Equation (A.9) becomes

\[
\hat{\mathcal{L}}_+ = \hat{\alpha} A \hat{\alpha} - A_0 \mathbb{1},
\]

where \(\hat{\alpha} = [\hat{\alpha}_1, \hat{\alpha}_2, \ldots, \hat{\alpha}_{4n}]^T\) is a column vector, \(A\) is the antisymmetric matrix introduced in 1.25, and \(A_0 = 2\text{tr}(M)\).

Assuming that \(A\) is diagonalizable with eigenvalues \(\beta_1, -\beta_1, \beta_2, -\beta_2, \ldots, \beta_{2n}, -\beta_{2n}\) and eigenvectors \(v_1, v_2, \ldots, v_{4n}\), the Liouvillean can be written in normal form

\[
\hat{\mathcal{L}}_+ = -2 \sum_{j=1}^{2n} \beta_j \hat{b}_j^\dagger \hat{b}_j,
\]

where \(\hat{b}_j\) and \(\hat{b}_j^\dagger\) are normal master mode maps defined by

\[
\hat{b}_j = v_{2j-1} \cdot \hat{\alpha}, \quad \hat{b}_j^\dagger = v_{2j} \cdot \hat{\alpha},
\]

and obeying the anti-commutation relations

\[
\{\hat{b}_j, \hat{b}_k\} = 0, \quad \{\hat{b}_j, \hat{b}_k^\dagger\} = \delta_{j,k}, \quad \{\hat{b}_j^\dagger, \hat{b}_k^\dagger\} = 0.
\]

This normal form representation of the Liouvillean leads to the results stated in Section 1.3. We encourage the reader to refer to [68] for a more detailed derivation.
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