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# Energy diffusion in weakly interacting chains with fermionic dissipation-assisted operator evolution

En-Jui Kuo,<sup>1,2,3</sup> Brayden Ware,<sup>3</sup> Peter Lunts,<sup>4,2</sup> Mohammad Hafezi,<sup>1,2,3</sup> and Christopher David White<sup>3</sup>

<sup>1</sup>Department of Physics, University of Maryland, College Park, MD 20742, USA

<sup>2</sup> Joint Quantum Institute, NIST/University of Maryland, College Park, MD 20742, USA

University of Maryland, College Park, Maryland 20742, USA

<sup>4</sup>Department of Physics, Harvard University, Cambridge MA 02138, USA

Interacting lattice Hamiltonians at high temperature generically give rise to energy transport governed by the classical diffusion equation; however, predicting the rate of diffusion requires numerical simulation of the microscopic quantum dynamics. For the purpose of predicting such transport properties, computational time evolution methods must be paired with schemes to control the growth of entanglement to tractably simulate for sufficiently long times. One such truncation scheme—dissipation-assisted operator evolution (DAOE)— controls entanglement by damping out components of operators with large Pauli weight. In this paper, we generalize DAOE to treat fermionic systems. Our method instead damps out components of operators with large fermionic DAOE (FDAOE), and another simulation method, density matrix truncation (DMT), in simulating energy transport in an interacting one-dimensional Majorana chain. The chain is found to have a diffusion coefficient scaling like interaction strength to the fourth power, contrary to naive expectations based on Fermi's Golden rule—but consistent with recent predictions based on the theory of *weak integrability breaking*. In the weak interaction regime where the fermionic nature of the system is most relevant, FDAOE is found to simulate the system more efficiently than DAOE.

# I. INTRODUCTION

Simulating transport in strongly interacting systems is a core challenge in quantum many-body physics, with implications from strange metal physics in cuprates and iron pnictides<sup>1-7</sup> to heavy-ion collisions.<sup>8-12</sup> Because complete numerical solution of a particular Hamiltonian is generally feasible only for small systems, transport simulations rely on approximate numerical methods. But transport is understood in terms of two largely separate languages, depending on the degree of interaction: nearly free fermion<sup>13</sup> (and nearly Bethe ansatz integrable<sup>14-20</sup>) systems can be understood in terms of Boltzmann theory while strongly interacting systems are understood in terms of an increasingly detailed theoretical understanding of how thermalization and hydrodynamics emerge from unitary microscopic dynamics.<sup>21-25</sup> Cold atom experiments highlight this gap: they can tune from free-fermion to strongly interacting by tuning a Feschbach resonance<sup>26,27</sup> or changing the geometry of a quasi-1D ladder geometry.<sup>28</sup> At the same time, progress in analytical and numerical treatment of systems showing Bethe ansatz integrability,<sup>29</sup> weakly broken Bethe ansatz integrability,<sup>14-20</sup> and strong integrability-breaking interactions<sup>22-25,30,31</sup> suggest that quantum simulation may not be necessary, at least for one-dimensional systems. But classical methods have not been shown to work in the crossover regime between weak interaction, tractable with Boltzmann methods, and strong interaction, tractable with recent methods. We present a matrix product operator method for simulating transport in one dimensional high-temperature quantum systems that is suitable for that regime; it can treat both nearly-free-fermion and strongly interacting Hamiltonians.

Existing methods for strongly interacting systems become impractical at weak interaction, lack a perturbatively small simulation parameter controlling deviation from the exact dy-



FIG. 1. **Top**: dissipation-assisted operator evolution (DAOE) compared with fermionic dissipation-assisted operator evolution (FDAOE). Where DAOE reduces widely-separated quadratic fermion operators almost to zero, FDAOE leaves them untouched; FDAOE depolarizes operators with fermion weight greater than some cutoff  $w_*$ . **Bottom left:** energy density as a function of position x and time t in the nearly-free Majorana model (2) at U = 0.3, simulated in FDAOE. **Bottom right:** finite-time estimates of the diffusion coefficient D. At small U, these estimates are consistent with  $D \propto U^{-4}$ , but not  $D \propto U^{-2}$ ; the power is due to weak integrability breaking.

namics, or both. Density matrix truncation (DMT)<sup>30</sup> works in all ranges of integrability,<sup>32–35</sup> but it is nontrivial to implement and difficult to analyze. It is also uncontrolled: like many matrix product operator methods, one checks the accuracy of DMT simulations by looking for convergence in bond dimension, but for large systems, practical bond dimensions cannot approach the bond dimensions required to exactly simulate the state. Indeed the premise of DMT, applied to systems that thermalize, is that most of the operator can be discarded, be-

<sup>&</sup>lt;sup>3</sup>Joint Center for Quantum Information and Computer Science,

cause it consists of physically-irrelevant correlations.

Dissipation-assisted operator evolution (DAOE)<sup>31</sup> offers a controllable approximation to a system's dynamics with a straightforward matrix product operator implementation-but it is not suitable for systems near free-fermion integrability. DAOE modifies the Heisenberg dynamics to include an artificial dissipation-like superoperator with a parametrically small rate  $\gamma$ . Just as depolarizing noise with rate  $\gamma$  reduces the amplitude of operators with Pauli weight (number of nontrivial Pauli strings) l at a rate  $\gamma l$ , the artificial dissipation reduces the amplitude of operators with Pauli weight  $l > l_*$  at a rate  $\gamma(l-l_*)$ . Fig. 1 top shows a cartoon of this process. It therefore reduces the state's complexity by decreasing the amplitude of long operators, without changing local operators. Because the long operators on which DAOE acts most strongly are-for chaotic, strongly interacting systems-unimportant to the finite-time dynamics<sup>23</sup>, one can think of the DAOE dissipation superoperator as perturbatively modifying the local dynamics. DAOE results at small but finite  $\gamma$  can therefore be extrapolated to the unitary  $\gamma = 0$  dynamics of interest, in a manner similar to zero-noise extrapolation.<sup>36,37</sup>

But when the system is not strongly interacting, the highweight operators affected by DAOE can be important to local dynamics, and the dissipation is not a small perturbation. In such a system momentum occupation numbers like  $c_k^{\dagger}c_k$ (where  $c_k$  is a fermion momentum mode annihilation operator) are nearly conserved quantities, so modifying them renders any description of the system's hydrodynamics unfaithful. But simple long-range fermion operators like  $c_k^{\dagger}c_k$  have large weight when written in Pauli matrices, due to Jordan-Wigner strings, so the artificial dissipation causes them to decay rapidly; this artificial decay will dominate the system's apparent transport properties.

We modify DAOE to respect the fermionic structure underlying weakly interacting 1D systems; we call the resulting method *fermionic DAOE* (FDAOE). FDAOE preserves quadratic fermion operators like  $c_k^{\dagger}c_k$  while dissipating operator components consisting of products of large numbers of fermion operators. Like DAOE it is efficient and easy to implement due to its compact matrix product operator representation. This allows us to study both strongly and weakly nonintegrable fermionic models using the same controlled and intuitive method.

We test FDAOE and a prior method, DMT, on a model displaying *weak integrability breaking*.<sup>38</sup> In such models an integrability-breaking perturbation is added to an integrable (in our case free fermion) model. At leading order, the perturbation dresses the integrable system's conserved quantities, giving ballistic transport; beyond leading order it scatters those quantities, giving diffusive transport. Ref. 38 predicts relaxation times  $\sim U^{2+2\nu}$ , where  $\nu$  is a positive integer for perturbations that exhibit weak integrability breaking and 0 for perturbations that do not.

We find that both FDAOE and DMT capture infinitetemperature dynamical correlation functions of energy density in such a system on short and intermediate timescales. Both methods are limited by rapid growth of the patch of the system they must simulate: on timescales short compared with Both methods give finite-time energy density diffusion coefficients consistent with  $D\sim U^{-4}$  but not the simple Fermi golden rule  $D\sim U^{-2}$  expected from ordinary integrability breaking. This  $U^4$  scaling confirms that weak integrability breaking governs the system's dynamics not only at times short compared to interaction and hopping, where 38 worked, but on long times as well.

The paper is organized as follows. In Sec. II we discuss the model used for benchmarking, give a brief overview of weak integrability breaking, and discuss the quantities of interest. In Sec. III we review DAOE, and present our new method FDAOE and describe simulations and simulation costs. In Sec. IV we present the results and discuss the performance of FDAOE compared to DAOE, and in Sec. V we conclude.

# II. MODEL AND QUANTITIES OF INTEREST

# A. Model

We study the infinite-temperature energy transport of an interacting Majorana chain

$$H = \sum_{n} i\eta_{n}\eta_{n+1} - U\sum_{n} \eta_{n-1}\eta_{n}\eta_{n+1}\eta_{n+2} .$$
 (1)

We work in the units where the quadratic "hopping" term has been set to one. We chose this model by starting with the simplest example of a 1D free-fermion model with energy conservation but without particle number conservation and adding the most natural fermion parity-conserving interaction. (The low-energy properties of this Hamiltonian were previously studied in Ref. 39.)

This Hamiltonian is equivalent to the spin-1/2 Hamiltonian

$$H = \sum_{n} \sigma_n^x \sigma_{n+1}^x + \sigma_n^z + U \left( \sigma_n^x \sigma_{n+2}^x + \sigma_n^z \sigma_{n+1}^z \right).$$
(2)

by Jordan-Wigner transformation. We work with the spinlanguage Hamiltonian (2).

We choose a model (1) with only a single conserved quantity, the energy density, so we can study transport in the simplest possible setting. We analyze our simulations through the lens of a single-component diffusion equation.<sup>22,24,31,35,40,41</sup>

We do not expect our simulation methods to break down in systems with multiple conserved quantities. But when a system has multiple conserved quantities, non-linear interactions between the conserved quantities can contribute significantly to transport properties, so going beyond the linear diffusion equation is necessary to analyze such systems<sup>42</sup>. Nonlinear effects can also appear in systems with a single conserved quantity,<sup>42–44</sup> but previous numerical simulations in spin chains with only energy conservation have not detected significant non-linear contributions to energy transport.<sup>35</sup> In this work we also do not detect significant non-linear contributions.

We have chosen an interaction that is not integrable using the Bethe ansatz. Bethe ansatz integrable systems have an infinite hierarchy of additional conserved quantities beyond energy density. The methods we use throughout this paper are designed to truncate irrelevant information while preserving the behavior of densities of conserved quantities, which are short-range or few-fermion operators like the energy density. So we would not expect them to be appropriate for Betheansatz integrable systems which have conserved quantities with arbitrarily large operator size: see Ref. 31 App. B and Ref. 45 for more discussion of this point.

While the Hamiltonian we study in this paper has no additional conserved quantities for non-zero U, we wish to study transport in a regime of small U, in the neighborhood of the free-fermion point. At this free point, the model has many additional conserved quantities that are quadratic in the fermion operators. Such quantities are almost conserved when U is small but non-zero, and thus may contribute significantly to long-time dynamics. Prior studies using tensor network algorithms have not attempted to predict transport properties in the nearly free-fermion regime of 1D chains, and it is not clear whether such methods would succeed for this purpose. On the other hand, FDAOE is designed specifically to preserve information about the low-fermion weight quantities that are almost conserved in the small U regime.

# B. Weak integrability breaking

In the regime of weak interactions, transport can sometimes be studied using simpler means, with the transport coefficients computed perturbatively in linear response using the Kubo formula, avoiding the need for simulations of operator dynamics.

However, we expect that the model studied in this paper evades a

simple perturbative analysis, as it exhibits *weak integrability breaking*.<sup>46</sup> The core prediction of weak integrability breaking for this model is that scattering times do not scale as predicted by Fermi's golden rule, with the square of the perturbation strength U, but with a different power-law scaling. This is due to a hidden non-local map that approximately transforms the Hamiltonian into a free fermion Hamiltonian, which we describe below. This implies that the in the perturbative calculation current-current correlators need to be computed to a higher order than expected to obtain a finite result (in this case fourth order rather than second order in U). The simulation methods in this paper are able to recover the unusual scaling with U without any explicit knowledge of the weak integrability breaking.

Weak integrability breaking starts from the elementary observation that if  $n_{\alpha}^{(0)}$  is a conserved quantity of some Hamiltonian  $H_0$ , then

$$n'_{\alpha} = e^{i\lambda X} n^{(0)}_{\alpha} e^{-i\lambda X} , \qquad (3)$$

where X is an Hermitian operator, is a conserved quantity of

$$H' = e^{i\lambda X} H_0 e^{-i\lambda X} . ag{4}$$

But for small  $\lambda$ , this H' is not so far from

$$H = H_0 + i\lambda[X, H_0] = H' + O(\lambda^2) .$$
 (5)

When the initial Hamiltonian  $H_0$  is chosen to be an integrable Hamiltonian with conserved quantities  $\{n_{\alpha}^{(0)}\}$ , the perturbed quantities

$$n_{\alpha} = n_{\alpha}^{(0)} + i\lambda[X, n_{\alpha}^{(0)}] = n_{\alpha}' + O(\lambda^2)$$
(6)

are nearly conserved. That is,

$$[H, n_{\alpha}] \propto \lambda^2 , \qquad (7)$$

in contrast to a generic perturbation which leads to matrix elements  $[H_0 + V, n_\alpha^{(0)}] \propto \lambda$ . Indeed by keeping higher commutators in (5), (6), one can engineer nearly conserved quantities with arbitrarily slow decays  $[H, n_\alpha] \propto \lambda^{2k}$ .

The challenge is to find generators X which produce a local perturbation V of interest via  $V = i[X, H_0]$ , which is only possible for select perturbations V. Ref. 46 systematically constructs a family of non-local generators X that produce local perturbations when the unperturbed Hamiltonian  $H_0$  is free-fermion or Bethe ansatz integrable. Specifically, the examples of generators X that they construct are bi-local combinations of conserved densities  $n_{\alpha}^{(0)}$  of  $H_0$  and their corresponding current operators.

For our purposes, we only need to consider one such generator X for a free Majorana chain that produces the interaction term of Eq. (1). The appropriate generator is constructed from a non-local combination of the energy density and energy current density operators of the unperturbed Hamiltonian:

$$X = \sum_{m < n} \{ \varepsilon_m^{(0)}, j_n^{(0)} \} + \frac{1}{2} \sum_n \{ \varepsilon_n^{(0)}, j_n^{(0)} \}$$
  

$$\varepsilon_n^{(0)} = \sigma_n^x \sigma_{n+1}^x + \frac{1}{2} (\sigma_n^z + \sigma_{n+1}^z)$$
  

$$j_n^{(0)} = \sigma_n^x \sigma_{n+1}^y - \sigma_n^y \sigma_{n+1}^x .$$
(8)

One can check (with some purely mechanical effort) that the interacting Hamiltonian in Eq. (1) satisfies

$$H = H_0 + i\lambda[X, H_0] \tag{9}$$

with

$$H_0 = \sum_j i\eta_j \eta_{j+1} \tag{10a}$$

and  $\lambda = U/4$ .

# C. Quantities of interest

If a system thermalizes, it approaches local thermal equilibrium: after a short time, it can be described by a density matrix

$$\rho(t) \propto \exp\left[-\sum_{x} \beta_x(t)\varepsilon_x\right],$$
(11)

where  $\beta_x(t)$  is a smoothly varying space- and time-dependent inverse temperature and  $\varepsilon_x$  is the energy density. (We consider systems with only one conserved quantity, the energy density; a discussion of systems with more than one conserved quantity would proceed analogously.) This state is specified entirely by the energy expectation values  $\mathrm{tr}\rho(t)\varepsilon_x$ . For times longer than the initial thermalization time the energy density correlation function

$$C(x,t) = \langle \varepsilon_x(t)\varepsilon_0(t) \rangle \tag{12}$$

therefore captures the whole dynamics in this long-time regime, and the extent to which it deviates from a gradientexpansion prediction from (11) diagnoses the local thermalization process.

On timescales long compared with the local thermalization time, the system's dynamics are given by the continuity equation and a gradient expansion of the state (11); the result is

$$\begin{aligned} \partial_t \varepsilon &= \partial_x j \\ \partial_t j &= D \partial_x \varepsilon + \dots \end{aligned}$$
 (13)

To the extent that the system is described by the leading-order term in the gradient expansion (13), the energy density correlation function is the Gaussian  $C(x, t) \propto \exp \left[-\frac{x^2}{4Dt}\right]$ .

But real systems are only described by (13) on timescales long compared to the microscopic thermalization timescale. To characterize the correlation function C(x, t) at short or intermediate timescales, we can measure the degree to which it spreads away from the initial point x = 0 to introduce a timedependent diffusion coefficient. The degree of spread is the mean squared displacement

$$V(t) = \frac{1}{\nu} \left[ \sum_{x} x^2 C(x,t) - \left( \sum_{x} x C(x,t) \right)^2 \right]$$
(14)

where  $\nu$  is a (time-independent) normalization

$$\nu = \sum_{x} C(x,t) = \sum_{x} C(x,0) = \left\langle \varepsilon_{L/2}^{2} \right\rangle .$$
 (15)

The time-dependent diffusion coefficient is

$$D(t) = \frac{1}{2} \frac{d}{dt} V(t).$$
(16)

If the system is diffusive, then in the long-time limit its dynamics approach the diffusion equation (13) with

$$D = \lim_{t \to \infty} D(t) . \tag{17}$$

We estimate D(t) by a numerical derivative of the mean squared displacement V(t).

# III. METHOD: FERMION DISSIPATION-ASSISTED OPERATOR EVOLUTION

# A. Intuition and superoperator

Dissipation-assisted operator evolution<sup>31</sup> intersperses unitary time evolution with a dissipation superoperator that reduces the amplitude on high-weight Pauli strings. That dissipation superoperator is

$$\mathcal{D}_{l_*,\gamma}[\mathcal{S}] = \left\{ \begin{array}{ll} \mathcal{S} & \text{if } l_{\mathcal{S}} \leq l_* \\ e^{-\gamma(l_{\mathcal{S}} - l_*)} \mathcal{S} & l_{\mathcal{S}} > l_* \end{array} \right\} , \qquad (18)$$

where S is a Pauli string and  $l_S$  is the *Pauli weight* of S, or the number of nontrivial Pauli operators in S. In the  $l_* = 0$ limit, this reduces to a depolarizing channel, hence the name "dissipation superoperator"; from the point of view of DMT<sup>30</sup> or operator size truncated dynamics,<sup>24,35</sup> it is a soft truncation on long operators. When the dynamics of long operators is chaotic, the details of the dynamics of long operators does not affect local dynamical correlation functions<sup>23,24</sup>, and for  $l_* \gg 1$  the superoperator (18) modifies the local dynamics only by modifying the rate at which amplitude escapes from short operators to long operators. Heuristically, the DAOE superoperator projects out operators with weight  $l_S \gtrsim l_* + \gamma^{-1}$ .

But for many models of interest the dynamics of long operators is not chaotic, and the DAOE dissipation superoperator (18) dramatically changes operators of interest. In a system of weakly interacting fermions like (1), a momentum mode such as

$$n_k^{(0)} = \frac{1}{L} \sum_{m < n} \eta_m \eta_n \sin(n - m)k$$
(19)

is a conserved quantity of the non-interacting part, and the system's evolution is governed by the dynamics of these momentum modes, together with scattering between them. After Jordan-Wigner transformation the term  $\eta_m \eta_n$  picks up a Jordan-Wigner string between m and n, so it has Pauli weight  $l_{\eta_m\eta_n} = m - n + 1$ . The DAOE superoperator projects out operators with Pauli weight  $l_S \gtrsim l_* + \gamma^{-1}$ , so it truncates the momentum occupation number to range  $l_* + \gamma^{-1}$ . Because it changes the conserved quantities of the free model, one expects it to drastically change the transport properties of the interacting model.

In fermonic dissipation assisted operator evolution (FDAOE) we replace the Pauli weight  $l_S$  in the DAOE dissipation superoperator (18) by a fermion weight superoperator. To write the fermion weight superoperator, first represent each Pauli matrix by two Majorana fermion operators

$$\sigma_n^x = \eta_{2n+1} \left[ \prod_{m \ge n+1} i\eta_{2m} \eta_{2m+1} \right]$$

$$\sigma_n^y = \eta_{2n} \left[ \prod_{m \ge n+1} i\eta_{2m} \eta_{2m+1} \right]$$

$$\sigma_n^z = -i\eta_{2n} \eta_{2n+1} .$$
(20)

These Majorana operators form a Hermitian, orthogonal basis for the space of operators, so we can define our Majorana dissipation superoperator by its action on them: if  $\eta_J$  is a product of Majorana operators on the sites J

$$\eta_J = \prod_{j \in J} \eta_j , \qquad (21)$$

then

$$\mathcal{M}_{w_{*},\gamma}[\eta_{J}] = \begin{cases} \eta_{J} & w_{\eta_{J}} \le w_{*} \\ e^{-\gamma(w_{\eta_{J}} - w_{*})}\eta_{J} & w_{\eta_{J}} > w_{*} \end{cases}$$
(22)

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with

$$w_{\eta_J} = |J| . \tag{23}$$

All of the terms in the momentum mode  $n_k^{(0)}$  of (19) have Majorana weight 2, so for  $w_* \ge 2$  and any  $\gamma$ 

$$\mathcal{M}_{w_*,\gamma}(n_k^{(0)}) = n_k^{(0)}$$
 . (24)

Unlike DAOE, then, FDAOE preserves the conserved quantities of the non-interacting Hamiltonian.

The FDAOE superoperator (22) has an MPO representation with bond dimension  $w_* + 2$  when represented by its action on the Pauli basis related to the Majorana operators by the Jordan-Wigner transformation, Eq. (20). We give the MPO explicitly in Appendix A, but outline the construction here. As in the case of the DAOE superoperator described in Ref. 31, the MPO representation utilizes a constant rank-4 tensor which we denote as  $W^{nn'}_{ab}$ , with the upper indices n, n'taking values in the local Pauli operator basis  $\{I, X, Y, Z\}$ . As the FDAOE superoperator is diagonal in the basis of operators that consist of products of Majorana operators, it is also diagonal in the basis of Pauli strings; thus, the only non-zero matrix elements occur in the form  $W_{ab}^{II}$ ,  $W_{ab}^{XX}$ ,  $W_{ab}^{YY}$ , or  $W_{ab}^{ZZ}$ . The virtual indices a, b take values in the set  $\{0, 1, \ldots, w^* - 1\} \cup \{(w^*, +), (w^*, -)\}$ , which track the total fermionic operator weight as measured from the left end of the chain to the bond in question until it reaches  $w^*$ , and the fermion parity afterwards. Within each Pauli string, the additional fermionic weight represented by the presence of an Xor Y is always 1 and always flips the fermion parity, which is tracked by the virtual index. Consequently,  $W_{ab}^{XX}$  and  $W_{ab}^{YY}$  are zero unless  $a < w^*$  and b = a + 1 or  $a = (w^*, \pm)$  and  $b = (w^*, \mp)$ . The weight associated with I and Z however are context dependent; alone, they correspond to weights 0 and 2 respectively but within a Jordan-Wigner string they correspond to weights 2 and 0, swapping roles. The presence of a Jordan-Wigner string is locally accessible as the parity of the MPO virtual index a. In addition to tracking the fermion weight, the MPO tensor applies a decay factor of  $e^{-\gamma}$  for each unit of additional fermion weight beyond  $w^*$ . Finally, the tensors are contracted on the left and right ends with the vectors  $v_L = (1, 0, \dots, 0)$  and  $v_R = (1, 1, \dots, 1)$ ; this ensures the virtual index starts tracking the fermion weight from weight 0 on the left end of the chain and allows all values of fermion weight on the right end. Explicit expressions for the MPO tensors that meet these conditions are given in Appendix A.

## B. Computing dynamical correlation functions

We seek to measure dynamical correlation functions

$$\langle \varepsilon_x(t)\varepsilon_0(0)\rangle = \operatorname{tr}\left(\varepsilon_x e^{-i\mathcal{L}t}[\varepsilon_0]\right) ,$$
 (25)

where  $\mathcal{L}$  is the Liouvillian generated by  $\mathcal{L}[\cdot] = -i[H, \cdot]$  and where  $\varepsilon_x$  is the energy density, chosen as a parity symmetric operator that produces H when summed over sites. Explicitly, we represent  $\varepsilon_x$  as

$$\varepsilon_{x} = \frac{1}{3} \left( \sigma_{x}^{z} + \sigma_{x+1}^{z} + \sigma_{x+2}^{z} \right) + \frac{1}{2} \left( \sigma_{x}^{x} \sigma_{x+1}^{x} + \sigma_{x+1}^{x} \sigma_{x+2}^{x} \right) + \frac{U}{2} \left( \sigma_{x}^{z} \sigma_{x+1}^{z} + \sigma_{x+1}^{z} \sigma_{x+2}^{z} \right) + U \left( \sigma_{x}^{x} \sigma_{x+2}^{x} \right) .$$
(26)

To measure  $\langle \varepsilon_x(t)\varepsilon_0(0) \rangle$ , we time-evolve the initial operator  $\varepsilon_0$  by the Trotterization of that Liouvillian, interspersed with applications of the FDAOE MPO.

In the limit of large bond dimension, the dominant cost is truncation after MPO application. Since the FDAOE MPO has bond dimension  $w_* + 2$ , an exact truncation has cost

$$\sim \left[d^2\chi \cdot (w_* + 2)\right]^3 \tag{27}$$

per bond, where d = 2 is the physical on-site Hilbert space dimension. This cost comes about because the exact truncation requires two sweeps, the first to put  $\mathcal{M}_{w_*,\gamma} \circ e^{-i\mathcal{L}t}[\varepsilon_0]$  in canonical form and the second to do the truncation. Switching to a so-called "zip-up" truncation, in which one truncates at each site immediately after applying the MPO tensor, reduces the cost to

$$\sim (w_* + 2) \left[ d^2 \chi \right]^3 \tag{28}$$

per bond at the cost of some imprecision.<sup>47,48</sup>

The cost of the whole calculation can further be reduced by noting that  $e^{-i\mathcal{L}t}[\varepsilon_0]$  acts as the identity outside a lightcone of diameter ~ 2vt for some speed v. Both the unitary dynamics and the FDAOE MPO  $\mathcal{M}_{w_*}$  act trivially outside that lightcone. So the cost of an MPO application at simulation time t generically grows with t: it is

$$\sim (w_* + 2) d^6 \sum_x \chi(x, t)^3 \sim d^6 (w_* + 2) \chi(t)^3 \cdot 2vt$$
, (29)

where we write  $\chi(x,t)$  for the bond dimension at site x and some site t, and  $\chi(t)$  for a typical magnitude at time t. The memory requirements are

$$\sim (2vt) \cdot d^6 \chi(t)^2 . \tag{30}$$

# C. Simulation parameters

We use a fourth-order Trotter decomposition; specifically, we use the three term formula recommended by Ref. 49, that



FIG. 2. Diffusion coefficient D(t) as a function of time for the nearly free Majorana model of Sec. II at interaction U = 0.3. D(t) is estimated via Eq. 16 using FDAOE at  $w_* = 5$  and a range of artificial dissipations  $\gamma$  (colored lines), and DMT at bond dimension 256 and Trotter step 0.125 (black line). (See App. D for DMT convergence data.) The noise in the FDAOE D(t) is due to an SVD cutoff  $\epsilon = 10^{-8}$  (see App. C). For plots of other U, see Fig. 7.)

consists of 21 layers of three site gates for each time step. The size of the time steps is of size dt = 0.1 throughout the paper. The FDAOE MPO is applied after each time step.

After each Trotter gate and during zip-up MPO application we discard the smallest singular values  $s_{\alpha}$  such that<sup>50</sup>

$$\sum_{\alpha \text{ discarded}} s_{\alpha}^2 < \epsilon \left[ \sum_{\beta} s_{\beta}^2 \right] , \qquad (31)$$

where  $\epsilon$  is the SVD truncation error.

In App. C we discuss convergence in the cutoff  $\epsilon$  and the magnitude of the noise in the numerical derivative D(t) (cf Fig. 2). We empirically find that truncating singular values causes noise in D(t) of magnitude

$$\Delta t_{\rm pred} \sim \sqrt{\epsilon} V(t) , \qquad (32)$$

and give a heuristic argument for why the noise should have that form. We also empirically find that the magnitude of the noise gives a reasonable estimate of the convergence error in  $\epsilon$ .

The DMT simulations are run at Trotter step dt = 0.125and a fixed bond dimension cap  $\chi = 256$ ; we discuss convergence in bond dimension (and other details of the DMT simulations) in App. D.

### **IV. RESULTS**

Fig. 2 shows D(t) in the nearly free Majorana model of Sec. II at interaction U = 0.3, estimated by taking the numerical derivative of FDAOE simulations of  $\langle \varepsilon_x(t)\varepsilon_0(0)\rangle$ . The simulations are limited to times  $t \leq 200$  by the computational cost, which grows with time as the lightcone of  $\varepsilon_x(t)$ grows. Each D(t) shows high-frequency noise; this is noise



FIG. 3. Diffusion coefficients extracted from D(t) via fit to exponential form (33) in FDAOE (blue lines, labeled "F" in legend) and DAOE (yellow-red lines, labeled "D" in legend). DAOE does not give consistent results across  $l_*$ , even when extrapolated to  $\gamma = 0$ , indicating that it cannot capture the crossover from free-fermion to diffusive dynamics. FDAOE gives consistent results across  $w_*$ ; the diffusion coefficients extrapolated to  $\gamma = 0$  are  $D_{w_*=4} = 95$ ,  $D_{w_*=5} = 89$ , against a DMT value  $D_{\text{DMT}} = 102$ . Error bars indicate uncertainty resulting from choice of fit window; they do not include uncertainty due to Trotter or truncation error.

is controlled by the SVD truncation cutoff, here  $\epsilon = 10^{-8}$  (cf App. C.)

After an initial transient behavior, D(t) is described by exponential decay to a long-time limit

$$D(t) = D - Ae^{-t/\tau}$$
 (33)

Fig. 2 inset shows |D(t) - D| in FDAOE simulations, where D is extracted by fitting FDAOE D(t) to the form (33). The result appears exponential over the range of our simulations, although that range is small (covering only a factor of about 3 in decay of |D(t) - D| for U = 0.3). Fig. 4 shows the current-current correlator

$$\frac{1}{L} \langle J(t)J(0) \rangle \propto \frac{d}{dt} D(t)$$
(34)

in DMT simulations for U = 0.3, 0.4, 0.5. (See App. D for details of the DMT simulations, including convergence testing, Trotterization, and the definition of the current operator. Note that that current operator corresponds to a different definition of energy density, for reasons of convenience in analytical calculations; this explains the difference in transient early-time behavior.) For each U the current-current correlator displays an early-time transient decay followed by a long-time exponential decay. For U = 0.5 this decay covers approximately two orders of magnitude, but for U = 0.3 it covers less than a decade. As in Ref. 35 we cannot rule out that the system displays long-time tails, but we expect that if they exist their coefficients are small.

To characterize how the system's long but finite-time behavior depends on U we fit to the form (33) for U-dependent time windows and consider the "asymptotic" diffusion coefficient D; if the long-time tails are small or non-existent, this



FIG. 4. **Current-current correlator** in DMT simulations across interaction strengths U (solid lines), together with a single-exponential fit to the t > 25 data. In each case the correlator displays a long-time exponential decay, supporting our choice of fit form (33) for the diffusion coefficient. (We cannot rule out power-law behavior at longer times, especially for U = 0.3, which displays less than a decade of decay over the time simulated.

*D* will match the system's true diffusion coefficient. We fit on time windows  $15/U = t_{\min} \le t \le t_{\max} = 30/U$ ; this form is chosen by eye to avoid both the early-time non-exponential behavior and late-time noise. The window choice is fairly arbitrary. To characterize how the window choice affects the fit, we take end times  $t_{\max} = 30/U - 10, 30/U, 30/U + 10$ , fit for each window, compute the standard deviation of the three resulting diffusion coefficients, and plot the result as error bars.

Fig. 3 shows the resulting diffusion coefficients for U = 0.3as a function of the artificial decay  $\gamma$ . We show both FDAOE and DAOE at a variety of  $l_*, w_*$ . In each case we linearly extrapolate the smallest two points ( $\gamma = 0.05, \gamma = 0.1$ ) to  $\gamma =$ 0. We extrapolate each fit window separately; the point and error bar in the FDAOE extrapolation, like the point and error bar in each of the finite- $\gamma$  points, show the mean and standard deviation across the three fit windows. The DAOE diffusion coefficients are not converged in  $l_*$ , in the sense that different  $l_*$  give different extrapolations to  $\gamma = 0$ ; this indicates that DAOE is not in the perturbative small- $\gamma$  regime.

The FDAOE diffusion coefficients are converged in  $w_*$  in the sense that the error bars in the extrapolation to  $\gamma = 0$  overlap: the difference between  $w_* = 4$  and  $w_* = 5$  is less than the fit uncertainty. In judging convergence it is important to note that in simulations of  $\varepsilon_x(t)$ , FDAOE with these two  $w_*$ in fact leave the same operator Hilbert space untouched. Because the Hamiltonian and the energy density are both fermion parity even,  $\varepsilon_x(t)$  is also fermion parity even, and the lowestweight operators that suffer dissipation have weight w = 6, regardless of whether  $w_* = 4$  or  $w_* = 5$ . ( $w_* = 6$  simulations were prohibitively time consuming.)

The FDAOE diffusion coefficients also broadly agree with the DMT simulations (black dots in Fig. 3) and in Fig. 1.) The error bars do not all overlap, meaning the difference between DMT, FDAOE at  $w_* = 4$ , and FDAOE at  $w_* = 5$  is not within fit uncertainty. But the fit is not the only source of uncertainty; DMT also has some error due to bond dimension



FIG. 5. Bond dimension saturation plot with  $w_* = 5$  and U = 0.4 for various  $\gamma$ . We can see the bond dimension hits the peak and falls down. Here we pick the truncation error to be  $10^{-8}$ .

convergence, FDAOE has some error due to SVD cutoff, and both methods have uncertainty due to (different) Trotter decompositions. (See App. B for other interaction strengths and some convergence data, and App. C and D for discussions of convergence.) The fit to D(t) seems to be more more sensitive to convergence error than D(t) itself.

Fig. 3 shows that the diffusion coefficient is approximately linear in  $\gamma$  for  $\gamma \leq 0.15$ . This, together with (broad) agreement between the different  $w_*$  and agreement between FDAOE and DMT, suggest that we can treat the FDAOE superoperator perturbatively, although a rigorous justification for such a perturbative treatment is lacking.

The premise of FDAOE is that a weak projection on manyfermion operators will reduce simulation complexity, while changing transport properties in a controlled way, which can safely be extrapolated to the limit of zero projection. Fig. 3 establishes that the change in transport properties is controlled, but not that simulation complexity is decreased.

Simulation complexity is controlled by bond dimension; Fig. 5 shows the maximum bond dimension as a function of time for U = 0.4,  $w_* = 5$ . The bond dimension displays a fast initial rise followed by a slow decay, as occurs in other examples of dissipative operator evolution.<sup>31,51</sup> The initial rise occurs as the operator  $\varepsilon_x(t)$  spreads ballistically. The long-time decay results from a split into conserved and non-conserved operators; the non-conserved operators are destroyed by the FDAOE projection.<sup>21</sup> Concretely, FDAOE turns the Heisenberg dynamics into an effective Liouvillian  $\mathcal{L}_{\text{FDAOE}}$ . This effective Liouvillian has slow eigenoperators given by the Fourier transform of the energy density and the energy current:

$$\mathcal{L}_{\text{FDAOE}}[\tilde{\varepsilon}_k] = -iDk^2\tilde{\varepsilon}_k , \qquad (35)$$

with

$$\tilde{\varepsilon}_{k} = \varepsilon_{k} + ikDaj_{k} + \dots$$

$$\varepsilon_{k} = \sum_{x} e^{ikx} \varepsilon_{x}$$

$$j_{k} = \sum_{x} e^{ikx} j_{x} .$$
(36)

Here a is a constant related to the normalization of  $\varepsilon_k$  and  $j_k$ . At long times, then,  $\varepsilon_x(t)$  becomes a sum of these Fourier modes; performing an inverse Fourier transform it becomes

$$\varepsilon_0(t) = \sum_x \left[ \beta(x,t)\varepsilon_x + \eta(x,t)j_x + \dots \right],$$
 (37)

with in fact  $\eta(x,t) \propto D\partial_x\beta(x,t)$ . (This  $\beta(x,t)$  is not identical to the inverse temperature of (11), but it plays a similar role.) At finite times this has small, decaying bond dimension; in the long time limit  $\lim_{t\to\infty} \partial_x\beta(x,t) = 0$ , so the bond dimension will decay to that of the Hamiltonian.

We can rephrase the argument in the picture of 21. In that picture the initial energy density  $\varepsilon_0$  develops weight on other energy densities  $\varepsilon_x$  as it evolves, but it also emits non-conserved, ballistically spreading operators. In the exact unitary dynamics, these non-conserved operators would give large bond dimension. But these operators not only spread spatially but also develop large fermion weight, so FDAOE destroys them, leaving the energy density and its current.

To measure performance in a hardware- and algorithmagnostic way, we use the time complexity of SVD truncation after application of the superoperator MPO; we call this time complexity the *SVD cost*. Truncation dominates the time complexity of both DAOE and FDAOE, so the SVD cost crudely estimates the number of floating point operations needed for the simulation. Asymptotically, the time complexity of the SVD<sup>52</sup> at bond *i* is  $\sim D\chi_i^3$ , where *D* is the bond dimension of the superoperator MPO:  $D = l_* + 1$  for DAOE, and  $D = w_* + 2$  for FDAOE. For each method we sum over bonds at each time, and maximize over times:

SVD cost = 
$$\max_{t} \sum_{i} D\chi_i(t)^3$$
. (38)

Fig. 6 shows the SVD cost for DAOE and FDAOE for U = 0.3and cutoff  $\epsilon = 0.3$ . Fig. 6 top plots SVD cost against the artificial dissipation rate  $\gamma$ ; it shows that—at any fixed  $\gamma$ — DAOE is one to two orders of magnitude cheaper.

But DAOE is not accurate: recall that DAOE gave inconsistent diffusion coefficients between lengths  $l_*$ , and that none of those diffusion coefficients agreed with DMT. FDAOE, by contrast, can be improved (at some cost in SVD time) by decreasing the artificial dissipation rate  $\gamma$ . Fig. 6 bottom shows the error in the diffusion coefficient, compared to extrapolated FDAOE simulations, as a function of SVD cost. Where DAOE plateaus at some large,  $l_*$ -dependent error, FDAOE error decreases as the SVD cost increases.



FIG. 6. (a) SVD cost with various  $\gamma$  for fixed U = 0.3 and truncation error  $10^{-8}$  (b) Relative error in the diffusion coefficient as a function of SVD cost. We can see that given a fixed cost, the FDAOE method has a faster convergence rate compared to DAOE.

### V. DISCUSSION

We have presented a new method, fermionic dissipation assisted operator evolution (FDAOE), for dynamics of interacting fermions in 1+1 dimensions at high temperature. FDAOE modifies a previous method, dissipation assisted operator evolution  $(DAOE)^{31}$ , to perform a soft truncation of operators with large fermionic weight. We tested FDAOE, DAOE, and another prior method, density matrix truncation (DMT), on an interacting Majorana model displaying weak integrability breaking. In weak integrability breaking, interactions dress the conserved quantities of the free model, leading to slow scattering and large diffusion coefficients. We find that FDAOE and DMT agree and give diffusion coefficients consistent with the  $D \ \sim \ U^4$  scaling (U is the interaction strength), as expected from scattering of dressed fermions. We further found that FDAOE decreases the bond dimension of the MPO representation of the Heisenberg picture energy density, when combined with SVD truncation with a small error cutoff, but we also found that that small error cutoff induces noise in the time-dependent diffusion coefficient D(t).

That SVD cutoff indirectly controlles the uncertainties in our diffusion coefficient estimates. These uncertainties were controlled by uncertainty in the fit to the exponential form  $D(t) = D - Ae^{-t/\tau}$ . This fit uncertainty was driven in turn by truncation error, because we stopped the fit where truncation error (estimated by noise in D(t)) became appreciable. With less truncation error, we could measure D(t) deeper into the exponential-decay regime, improving our estimates of the asymptotic  $D = \lim_{t\to\infty} D(t)$ . But most strategies for decreasing truncation error would impose substantial run-time and memory costs. Reducing the SVD cutoff, e.g. from  $10^{-8}$ to  $10^{-9}$ , would directly increase the bond dimension throughout the simulation, and replacing the SVD cutoff with a bond dimension cap would prevent the simulation from taking advantage of the decay of the bond dimension (Fig. 5).

But two strategies, measuring a current-current correlator and using a variable SVD cutoff—may reduce truncation error without imposing an appreciable runtime or memory cost. Estimating D(t) as we do, via the mean square displacement V(t), is costly because it requires measuring  $\varepsilon(x, t)$  precisely at large x. Indeed, the truncation error in D(t) is  $\propto \sqrt{\epsilon} V(t)$ . Measuring a current-current correlator would avoid this problem, because the requisite spatial integral has no  $x^2$  (unlike the integral giving V(t)). Alternatively, one could use a timevarying SVD cutoff  $\epsilon(t) = \epsilon_0/V(t)^2$ . This would allow coarse simulations at early times, e.g. around the bond dimension peak in Fig. 5, and fine simulations at later times. Because the runtime cost contains large contributions from the bond dimension peak, this might in fact decrease runtime cost on net.

While DMT is difficult to analyze, FDAOE can be understood as a perturbative modification to the system's dynamics. This is consistent with our observation that the FDAOE diffusion coefficient is linear in the artificial dissipation  $\gamma$ . And the intuition is clear: at small  $\gamma$  FDAOE acts weakly on fewfermion operators, and in systems that eventually thermalize, many-fermion operators are not important to transport. But establishing this formally will be nontrivial; to do so will require modifying arguments like those of 23 to work away from the strongly-interacting, chaotic limit.

In one-dimensional fermion chains, the Jordan-Wigner transformation produces an equivalent local Hamiltonian that takes the form of a spin chain; a fermionic description of the transport is unnecessary in the generic case. For this reason, we have focused on weakly-interacting systems, where transport receives important contributions from the nearly conserved quadratic fermion operators of all sizes. While the Hamiltonian can be written as a local operator in the spin language, these nearly conserved operators cannot. By contrast, in higher dimensional fermionic systems, the energy density has no local spin representation. The dynamics of such systems can be computed using MPS by picking a one-

dimensional ordering of the sites and using the Jordan-Wigner representation to convert to a spin Hamiltonian, with some terms involving non-local Jordan-Wigner strings. In this scenario, the DAOE superoperator will cause the energy density to decay rapidly, while the FDAOE superoperator will not. Thus, we expect that FDAOE is the appropriate choice for fermionic systems of all interaction strengths in higher dimensions.

While we focused in this paper on infinite-temperature transport, extending the methods to allow for finite-temperature calculations is needed for many physical scenarios of interest. In scenarios where the equilibrium state is dominated by quadratic fermionic operators — particularly at high temperatures with weak interactions — the FDAOE operator will only weakly perturb the equilibrium. Thus, it may still be possible in these cases to recover the correct dynamics using FDAOE with the extrapolation to zero dissipation rate. We leave this question to future studies.

*Note added.* – We would like to bring the reader's attention to a related independent work 53.

# VI. ACKNOWLEDGEMENTS

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# Appendix A: Matrix product operator representation of fermionic DAOE

In this appendix, we give more details on the construction of the MPO representation of the fermionic DAOE superoperator  $\mathcal{M}_{w_*,\gamma}$ . As explained in Sec. III A, this construction relies on the Jordan-Wigner embedding of fermionic operators into the space of operators of qubits. This mapping maps each Pauli string – a single product of Pauli operators or the identity operator on each site – to a corresponding product of Majorana operators with 0, 1, or 2 Majorana factors at each site, up to a phase factor. Similarly, every product of Majorana operators maps to a Pauli string. As the MPO representation of the superoperator is by construction a linear superoperator, and because the Pauli string operators form a basis for the full space of operators, it is sufficient to confirm that the MPO representation has the correct action on each Pauli string.

The MPO is constructed with a constant rank-4 tensor  $W_{ab}^{nn'}$ , where  $n, n' \in \{I, X, Y, Z\}$ . To use a convenient notation, we will allow the virtual indices to take values of the form  $a_s \in \{0_+, 0_-, 1_+, 1_-, \dots, w_+^*, w_-^*\}$ , where the integer part of the label a is used to track a fermion weight and the subscript s is used to track a fermion parity. There are  $2(w^* + 1)$  such labels — however, we will find that we only use the labels  $0_+, 1_-, 2_+, 3_-, \dots$  and  $w_+^*, w_-^*$ , where for  $a < w^*$  the parity label s matches the parity of a as an integer. This results in a set of  $w^* + 2$  total labels, and thus the bond dimension of our MPO representation is  $w^* + 2$ .

The non-zero matrix elements of our MPO tensor  $W_{ab}^{nn'}$  are as follows:

$$W_{a_{+},b_{+}}^{II} = W_{a_{-},b_{-}}^{ZZ} = \delta_{a,b}$$

$$W_{a_{+},b_{-}}^{XX} = W_{a_{+},b_{-}}^{YY} = \delta_{a+1,b} + e^{-\gamma}\delta_{a,w^{*}}\delta_{b,w^{*}}$$

$$W_{a_{-},b_{+}}^{XX} = W_{a_{-},b_{+}}^{YY} = \delta_{a+1,b} + e^{-\gamma}\delta_{a,w^{*}}\delta_{b,w^{*}}$$

$$W_{a_{-},b_{-}}^{II} = W_{a_{+},b_{+}}^{ZZ} = \delta_{a+2,b} + e^{-2\gamma}\delta_{a,w^{*}}\delta_{b,w^{*}}$$

$$+ e^{-\gamma}\delta_{a,w^{*}-1}\delta_{b,w^{*}}$$
(A1)

The left and right most tensor in the MPO representation are to be contracted with vectors  $v_a^L = \delta_{a,0_+}$  and  $v_b^R = 1$  on the left and right virtual bond, respectively.

To understand this implementation of the MPO, we first note that the non-zero elements listed guarantee a consistent tracking of fermion parity. In more exact terms, the only contributions to  $M_{w^*,\gamma}[O]$  for a Pauli string  $O = \prod_i O_i$  occur when the parity index of the bond between site j and j + 1matches the fermion parity of  $\prod_{i \leq j} O_i$  for all j. This is convenient, as matching the fermion parity allow us to determine whether the basis operator O has an even or odd number of Jordan-Wigner string factors from Eq. (20) that cross the bond  $j \rightarrow j + 1$ .

Similarly, we can see that at all bonds the fermion weight of the virtual index must match either the fermion weight of  $\prod_{i \leq j} O_i$  or  $w^*$ , whichever is smaller. When there are an even number of Jordan-Wigner string factors, the presence of an I in a Pauli string corresponds to a Majorana product with 0 Majorana operators on that site; if instead there are an odd number, the presence of Z does instead. This gives the first



FIG. 7. Analogues of 2 and 3 for U = 0.4 and U = 0.5. The left panel is U = 0.5 and the right one is U = 0.4. All data comes from Trotter step dt = 0.1, and cutoff  $\epsilon = 10^{-8}$ .

line of Eq. (C1). The second line corresponds to fermion weight 1 operators, which either increases the fermion weight counter by 1 or keeps it constant if it has reached the maximum  $w^*$ . The  $e^{-\gamma}$  factor dissipates Pauli strings for each additional unit of fermion weight beyond  $w^*$ . Finally, in the last line of Eq. (C1), we have Pauli string factors that correspond to fermion weight 2 operators, which requires increasing the fermion weight counter twice or increasing it to  $w^*$  and dissipating the operator by a factor of  $e^{-\gamma}$  or  $e^{-2\gamma}$ , depending on whether the fermion weight goes 1 or 2 units beyond  $w^*$ .

# Appendix B: D(t) and extrapolation for other interaction strengths

Fig. 7 shows analogues of Fig's 2 and 3 for U = 0.4 and U = 0.5. Fig. 7 top shows D(t), together with fits and (in the inset) a logarithmic difference from the  $D = \lim_{t\to\infty} D(t)$  resulting from the fit, across  $\gamma$ . Fig. 7 bottom shows D from fit as a function of  $\gamma$ , together with the extrapolation from the last two points. Table

U	$\delta t$	$\chi_{\rm max}$	D (mean)	D (std)
0.3	0.0625	128	96.8	5.7
0.3	0.125	128	106.238	14.6
0.3	0.125	256	102.367	2.38278
0.4	0.0625	128	39.4765	2.01023
0.4	0.0625	256	38.2516	0.703325
0.4	0.125	128	36.3361	0.853394
0.4	0.125	256	37.9766	0.126748
0.5	0.0625	128	21.1115	1.213
0.5	0.0625	256	21.3559	0.333348
0.5	0.125	128	20.1833	0.896041
0.5	0.125	256	20.6832	0.359822

TABLE I. Diffusion coefficients from fit to DMT D(t). Mean and standard deviation are across three different fit-window end times.



FIG. 8. We compared D(t) with two truncation errors  $10^{-8}$  and  $10^{-9}$  with U = 0.55,  $w_* = 4$ ,  $\gamma = 0.2$ . We also do the exponential extrapolation and see that D only differs less than 5 percent.

U	$w_*$	D (mean)	D (std)
0.3	4.0	94.9121	4.37422
0.3	5.0	89.4662	2.67036
0.35	4.0	59.2131	3.09694
0.35	5.0	51.6491	1.63505
0.4	4.0	36.2878	1.60103
0.4	5.0	35.2506	4.91012
0.45	4.0	24.3317	1.3542
0.45	5.0	25.2716	1.03157
0.5	4.0	19.8595	2.73888
0.5	5.0	20.9656	0.495984
0.55	4.0	16.4897	0.502595
0.55	5.0	15.1526	0.807459
0.6	4.0	14.0067	0.270231
0.6	5.0	13.8689	0.562507

TABLE II. Diffusion coefficients from fit to FDAOE D(t). Mean and standard deviation are across three different fit-window end times.

### Appendix C: Convergence in SVD cutoff $\epsilon$

In simulating dynamics with FDAOE we apply Trotter gates and the FDAOE MPO; after each application we discard small singular values

$$\sum_{\alpha \text{ discarded}} s_{\alpha}^2 < \epsilon \left[ \sum_{\beta} s_{\beta}^2 \right] . \tag{C1}$$

Fig. 8 shows D(t) for  $\epsilon = 10^{-8}$ ,  $10^{-9}$  at U = 0.55,  $\gamma = 0.2$ . The noise in each D(t) worsens with time, and it is smaller for  $\epsilon = 10^{-9}$  than for  $\epsilon = 10^{-8}$ . Fig. 9 top shows the RMS noise as a function of time for U = 0.3,  $\gamma = 0.05$ ,  $\epsilon = 10^{-8}$ ; there we see that it is in fact roughly proportional to the mean square displacement V(t). (We describe how we calculate the noise in App. C2 below.) A heuristic a priori argument (App. C1)



Heuristically, the truncation applies a random perturbation of magnitude  $\sqrt{\epsilon}$  to the operator truncated. When the operator truncated is the Heisenberg operator  $\varepsilon_{L/2}(t)$ , truncation maps

$$\varepsilon_{L/2}(t) \mapsto (1 + \sqrt{\epsilon}W)[\varepsilon_{L/2}(t)],$$
 (C3)

where V is some (not necessarily unitary) superoperator; this changes the correlation function to

$$C^{\varepsilon\varepsilon}(x,t) = \operatorname{tr}\left(\varepsilon_x(1+\sqrt{\epsilon}W)[\varepsilon_{L/2}(t)]\right)$$
  
=  $C^{\varepsilon\varepsilon}(x,t) + \sqrt{\epsilon}\operatorname{tr}\left(\varepsilon_xW[\varepsilon_{L/2}(t)]\right).$  (C4)

The superoperator W acts locally. To understand this, recall that  $\varepsilon_{L/2}(t)$  is a low-bond dimension MPO, so it has a correlation length set by the leading nontrivial eigenvalue of the transfer matrix. Perturbations like truncation heal within that correlation length, so the superoperator W acts with a range given by that correlation length.

Since W acts locally, estimate

$$\operatorname{tr}[\varepsilon_{x}W\varepsilon_{L/2}(t)] = \xi(x,t)\operatorname{tr}[\varepsilon_{x}\varepsilon_{L/2}(t)] \\ \equiv \xi(x,t)C^{\varepsilon\varepsilon}(x,t)$$
(C5)

where  $\xi(x, t)$  is a random variable with

$$\langle \xi(x,t)\xi(x',t')\rangle = \alpha^2 \delta_{xx'}\delta(t-t') , \qquad (C6)$$

 $\alpha$  some constant. Truncation then takes

$$C^{\varepsilon\varepsilon} \mapsto [1 + \sqrt{\epsilon} \,\xi(x,t)] C^{\varepsilon\varepsilon}(x,t) \,.$$
 (C7)

and the mean squared displacement

$$V(t) \mapsto V'(t) = \sum_{x} x^2 [1 + \sqrt{\epsilon} \xi(x, t)] C^{\varepsilon \varepsilon}(x, t)$$
  
=  $V(t) + \Delta V_{trunc}(t)$ , (C8)

with

$$\Delta V_{trunc}(t) = \sqrt{\epsilon} \sum_{x} x^2 C^{\varepsilon \varepsilon}(x, t) \xi(x, t) .$$
 (C9)

This truncation appears as noise in the time-dependent diffusion coefficient: the numerical derivative leading to the diffusion coefficient is

$$D(t) = \frac{1}{2}\delta t^{-1} [V'(t+\delta t) - V(\delta t)]$$
 (C10)

$$= D_{phys} + \frac{1}{2}\delta t^{-1}\Delta V_{trunc}(t)$$
 (C11)

where  $D_{phys}$  is the "physical" contribution to the numerical derivative, coming from the pre-truncation timestep, and the second term  $\propto \Delta V_{trunc}(t)$  is the noise coming from the truncation. We can then estimate the magnitude of the noise by

FIG. 9. Top: Noise magnitude at U = 0.3,  $\gamma = 0.05$ ,  $\epsilon = 10^{-8}$  compared to the prediction  $\Delta D_{\text{pred}}(t) = \alpha \sqrt{\epsilon} V(t)$  (C2), with the fit parameter  $\alpha$  chosen by eye. **Bottom**: noise at a variety of  $U, \gamma$ , and  $\epsilon$  normalized by the prediction  $\Delta D_{\text{pred}}$  with  $\alpha = 1$ .

below) predicts a noise magnitude

$$\Delta D_{\rm pred}(t) = \alpha \sqrt{\epsilon} V(t) , \qquad (C2)$$

where  $\alpha$  is a fit parameter depending (in part) on the timestep  $\delta t$ .

Fig. 9 shows the ratio of the measured noise magnitude  $\Delta D_{\text{meas}}$  to the prediction  $\Delta D_{\text{pred}}$  of (C2) for a variety of  $U, \gamma$ , and  $\epsilon$ . For short times ( $t \leq 25$ ) the ratio is large. This is in part because the prediction  $\Delta D_{\text{meas}}$  is initially small, because the mean square displacement V(t) is small. Additionally the measured noise displays a small peak at t = 0, already visible in Fig. 9 top, resulting from the details of our noise measurement procedure. For  $t \geq 25$ , the noise magnitude is reasonably well-predicted by (C2).



treating  $\xi(x, t)$ , hence  $\Delta V_{trunc}$ , as random variables and estimating the variance:

$$\left\langle \Delta V_{trunc}(t)^2 \right\rangle = \epsilon \left\langle \left[ \sum_{x} x^2 C^{\varepsilon \varepsilon}(x, t) \xi(x, t) \right]^2 \right\rangle$$
  
=  $\epsilon \sum_{x} x^4 C^{\varepsilon \varepsilon}(x, t)$   
=  $\alpha \epsilon V(t)^2$  (C12)

using  $\langle \xi(x,t)\xi(x',t')\rangle = \alpha \delta_{xx'}\delta(t-t')$  and sweeping some dimensionless factors into  $\alpha$ . The standard deviation of the noise in D(t) is therefore

$$\alpha \sqrt{\delta t^{-1} \epsilon/2} V(t) . \tag{C13}$$

This expression includes a dependence on Trotter step  $\delta t$  coming from the numerical derivative. But the numerical derivative is not the only source of  $\delta t$  dependence. Consider, for example, the limit of small  $\delta t$ . In that limit a Trotter step introduces only small Schmidt values, which are all discarded by truncation: that is, the truncation can undo the effect of time evolution. We do not claim to consider all sources of  $\delta t$ dependence, so we sweep it into the constant  $\alpha$ . The predicted standard deviation of the noise is then

$$\Delta D_{\rm pred} = \alpha \sqrt{\epsilon/2} \, V(t) \,. \tag{C14}$$

Fig. 9 shows the noise compared to the prediction; we see reasonable agreement.

## 2. Estimating the noise magnitude

We seek to estimate the noise magnitude without reference to a global fit like the exponential fit of (IV), In brief, we estimate noise by binning in time, averaging D(t) in each bin, constructing a linear interpolant between averages, mand measuring the RMS deviation from the interpolant. In more detail, we

- 1. compute variances  $V_j$  at timesteps  $(j-1)\delta t$ ,  $j = 1 \dots$ (Throughout this section  $\delta t = 0.1$ .)
- 2. compute time-dependent diffusion coefficients

$$D_j = \delta t^{-1} [V_{j+1} - V_j] ; \qquad (C15)$$

assign them to times

$$t_j = (j - 1/2)\delta t$$
 . (C16)

3. Bin and average D(t) over bins of width n = 30, corresponding to a time window 3: that is, compute

$$\bar{D}_k = \frac{1}{n} \sum_{j=n(k-1)+1}^{nk} D_j$$

$$= (n\delta t)^{-1} [V_{nk+1} - V_{n(k-1)+1}].$$
(C17)

Assign  $\bar{D}_k$  to a time

$$\bar{t}_k = (nk - 1 - n/2)\delta t$$
. (C18)

- 4. Form a linear interpolant T(t) between the points  $(\bar{t}_k, \bar{D}_k)$ . (For  $t < \bar{t}_1$  we linearly extrapolate.)
- 5. Form errors

$$E_j = D_j - T(t_j) \tag{C19}$$

with  $D_j, t_j$  from step 2.

6. Take the RMS of  $E_j$  over windows of 30 points, corresponding to time windows of size 3, for  $\Delta D_{\text{meas}}$ 

# **Appendix D: DMT simulations**

### 1. DMT

In TEBD<sup>54–56</sup> one truncates an MPO with a single SVD, resulting in a local approximation that is optimal with respect to the Frobenius norm. But the Frobenius norm is blind to the fact that some operators—especially local operators like energy density—are more important than others.

Density matrix truncation<sup>30</sup> replaces the SVD truncation with a truncation that exactly preserves operators with support up to some preservation diameter  $l_{\text{pres}}$ , and truncates longer operators via SVD; it has been successfully applied to thermalizing and integrable systems.

We implement DMT as modified in 35 for Heisenberg dynamics; for simplicity of implementation, we take a preservation diameter  $L_{\text{pres}} = 3$ . We use a second-order boustrophedon (sweeping, DMRG-like) Trotter decomposition, rather than the usual brickwork Trotter decomposition; this seems to give better convergence in Trotter step.

### 2. Current decay

## a. Diffusion coefficients and the current-current correlator

In the main text we extract the diffusion coefficient from the variance of the energy density correlator. That correlator is

$$C^{\varepsilon\varepsilon}(x,t) = \langle \varepsilon_x(t)\varepsilon_x(L/2) \rangle$$
 . (D1)

To extract a time-dependent diffusion coefficient we first compute the mean squared displacement

$$V(t) = \frac{1}{\nu} \sum_{x} x^2 C^{\varepsilon\varepsilon}(x,t) - \left(\sum_{x} x C(x,t)\right)^2$$
(D2)

where  $\nu$  is a normalization

$$\nu = \sum_{x} C(x,t) = \sum_{x} C(x,0) = \left\langle \varepsilon_{L/2}^{2} \right\rangle .$$
 (D3)

The time-dependent diffusion coefficient is

$$D(t) = \frac{1}{2} \frac{d}{dt} V(t) ; \qquad (D4)$$

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FIG. 10. Top row: current-current correlator  $\langle J(t)J(0)$  of Eq. D7 computed with DMT for U = 0.3 (left), U = 0.4 (center), U = 0.5 (right). After a fast initial oscillation, the correlator displays a slow decay well approximated by a two-exponential fit (blue line; Eq. D9). Bottom row: convergence in bond dimension. All curves are at Trotter step dt = 0.125

we estimate this via a numerical derivative. We then estimate the physical diffusion coefficient

$$D = \lim_{t \to \infty} D(t) \tag{D5}$$

by fitting D(t) to the functional form

$$D(t) = D - Be^{-t/\tau}, \quad t > t_0$$
 (D6)

after some initial time  $t_0$ .

It is useful to check the functional form (D6) by computing directly computing the derivative  $\frac{d}{dt}D(t)$ . We can write  $\frac{d}{dt}D(t)$  as a correlator by repeatedly applying the conservation law  $\partial_t \varepsilon_x = j_{x-1} - j_x$ , summation by parts, time translation invariance, and spatial translation invariance to the correlator C(x, t); the result is

$$\frac{d}{dt}D(t) = \frac{1}{\nu} \langle J(t)J(0)\rangle \tag{D7}$$

where

$$J(t) = \sum_{x} j_x(t) , \qquad (D8)$$

 $j_x(t)$  the local energy current operator, and  $\nu$  is the same normalization (D3).

### b. Results and convergence

Fig. 10 shows the current-current correlator  $\langle J(t)J(0)\rangle$  as a function of time for U = 0.3, 0.4, 0.5. In each case the correlator shows fast early oscillations, followed by a slow decay. The fast oscillations result from the definition of the current (see App. D 2 c). The slow decay is well-approximated by a phenomenological functional form

$$\langle J(t)J(0)\rangle = Ae^{-t/\tau_1} + Be^{-t/\tau_2}$$
. (D9)

We fit to the  $t \ge 5$  data to avoid the initial oscillations, and give the resulting time constants  $\tau$  in Table III.

Fig. 10 bottom row shows convergence of the DMT currentcurrent correlator in bond dimension for U = 0.3, 0.4, 0.5.



FIG. 11.

FIG. 12. Trotter step convergence of the current-current correlator in DMT simulations. Each curve is at bond dimension  $\chi = 256$ .

U	$ au_1$	$ au_2$
0.3	15.3	133
0.4	6.22	44.7
0.5	4.38	21.45

TABLE III. Time constants for the phenomenological twoexponential fit (Eq. D9) to the current-current correlation function (D7) plotted in Fig. 10

We plot

$$\frac{\langle J(t)J(0)\rangle [\chi]}{\langle J(t)J(0)\rangle [\chi = 256]} . \tag{D10}$$

In each case we find that  $C_{\chi=256}^{JJ}(t)$  is within 10% of  $C_{\chi=512}^{JJ}$ .

This 10% difference understates convergence error, because  $C_{\chi}^{JJ}(t)$  trends upward as the bond dimension  $\chi$  increases. (The trend is unambiguous for U = 0.3, 0.5; for U = 0.4 it is less clear, but arguably still present.) It appears that DMT systematically underestimates  $C_{\chi}^{JJ}(t)$ . We believe this underestimate results from our choice of preservation diameter We use DMT with preservation diameter 3, meaning it exactly preserves only those operators with support on up to 3 sites, but the energy current is a 4-site operator. We believe that simulations with preservation diameter  $\geq 4$  would converge more quickly.

Fig. 12 shows convergence of the DMT current-current correlator in Trotter step dt. We plot

$$\frac{\langle J(t)J(0)\rangle \left[dt = 0.125\right]}{\langle J(t)J(0)\rangle \left[dt = 0.0625\right]} \tag{D11}$$

for U = 0.3, 0.4, 0.5; in each case Trotter step dt = 0.125 is within 10% of Trotter step dt = 0.0625.

# c. Definitions of energy density and energy current

In this appendix we have used definitions of energy density and energy density current that are natural in fermion language, rather than in spin language, because the requisite analytical calculations (especially of the current itself) were more convenient in fermion language. In Majorana language the energy density is

$$\varepsilon_{\xi}^{(M)} = i\eta_{\xi}\eta_{\xi+1} - U\eta_{\xi-1}\eta_{\xi}\eta_{\xi+1}\eta_{\xi+2} .$$
 (D12)

 $\varepsilon_\xi^{(M)}$  is symmetric under reflection about the bond  $(\xi,\xi+1).$  The current of this energy density  $\varepsilon^{(M)}$  can be written

$$j_{\xi}^{(M)} = -2i \Big[ P_{\xi} - iU(A_{\xi-2} + A_{\xi-1} + B_{\xi-1} + B_{\xi}) \\ + U^2(D_{\xi-1} - C_{\xi-3} - C_{\xi-2} - C_{\xi-1}) \Big] \\ P_{\xi} = \eta_{\xi}\eta_{\xi+2} \\ A_{\xi} = \eta_{\xi}\eta_{\xi+1}\eta_{\xi+2}\eta_{\xi+4} \\ B_{\xi} = \eta_{\xi}\eta_{\xi+2}\eta_{\xi+3}\eta_{\xi+4} \\ C_{\xi} = \eta_{\xi}\eta_{\xi+1}\eta_{\xi+2}\eta_{\xi+4}\eta_{\xi+5}\eta_{\xi+6} \\ D_{\xi} = \eta_{\xi}\eta_{\xi+4} \end{aligned}$$
(D13)

where we label the Majorana sites  $\xi = 2, \ldots, 2L$ .

In preparation for Jordan-Wigner transformation it is helpful to group sites: one grouped site x corresponds to two Majorana sites (2x, 2x + 1). The energy density (D12) is then

$$\varepsilon_{x} = \varepsilon_{2x}^{(M)} + \varepsilon_{2x+1}^{(M)}$$

$$= i\eta_{2x}\eta_{2x+1} - U\eta_{2x-1}\eta_{2x}\eta_{2x+1}\eta_{2x+2}$$

$$+ i\eta_{2x+1}\eta_{2x+2} - U\eta_{2x}\eta_{2x+1}\eta_{2x+2}\eta_{2x+3};$$
(D14)

the current of this energy density can be written

$$j_x = j_{2x}^{(M)}$$
 . (D15)

Note that the total currents are not the same:

$$J := \sum_{x} j_x = \sum_{x} j_{2x}^{(M)}$$
(D16a)

$$J^{(M)} := \sum_{\xi} j_{\xi}^{(M)} = \sum_{x} [j_{2x}^{(M)} + j_{2x+1}^{(M)}]$$
(D16b)  
$$\neq J .$$

The difference between J and  $J^{(M)}$  explains the early-time oscillations of the energy current in Fig. 10. Take U = 0, for simplicity. In that case one can check

$$d_t J^{(M)} = 0$$
. (D17)

If we decompose

$$J^{(M)} = J + J' , (D18)$$



FIG. 13. Top row time-dependent diffusion coefficients D(t) extracted from DMT simulations of the mean square displacement V(t) for U = 0.3, 0.4, 0.5. Bottom row: bond dimension convergence of extracted D(t); in each case D(t) differs between bond dimension  $\chi = 64$  and bond dimension  $\chi = 256$  by less than 5%. DMT simulations use Trotter step dt = 0.125



FIG. 14. MSD Trotter

J the total current of (D16a) consisting only of even terms and

$$J' = \sum_{x} j_{2x+1}^{(M)}$$
(D19)

consisting of odd terms, then  $d_t J^{(M)} = 0$  implies

$$d_t J = -d_t J' \tag{D20}$$

leading to oscillations.

This is a lattice-scale phenomenon. If  $U \neq 0$ , for any but the shortest times  $\varepsilon_{2x}^{(M)} \approx \varepsilon_{2x+1}^{(M)}$  and  $j_{2x}^{(M)} \approx j_{2x+1}^{(M)}$ , so the decay of J broadly matches that of  $J^{(M)}$ .

# 3. Mean square displacement in DMT simulations

The DMT diffusion coefficients in the main text come from the mean square displacement V(t), analyzed in the same way asthe FDAOE data. Fig. 13 top shows the diffusion coefficient extracted from the mean square displacement for U = 0.3, 0.4, 0.5; Fig. 13 bottom shows convergence in bond dimension, and Fig. 14 shows convergence in Trotter step. Bond dimension convergence error is  $\lesssim 3\%$  for  $\chi = 128$ compared to  $\chi = 256$  (with better convergence for larger U). Trotter error is also  $\lesssim 3\%$  for times  $t \lesssim 90$ , but growing.