

Finite-temperature charge transport in the one-dimensional Hubbard model

F. Jin,¹ R. Steinigeweg,^{2,3,*} F. Heidrich-Meisner,⁴ K. Michielsen,^{1,5} and H. De Raedt⁶

¹*Institute for Advanced Simulation, Jülich Supercomputing Centre, Forschungszentrum Jülich, D-52425 Jülich, Germany*

²*Department of Physics, University of Osnabrück, D-49069 Osnabrück, Germany*

³*Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany*

⁴*Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany*

⁵*RWTH Aachen University, D-52056 Aachen, Germany*

⁶*Department of Applied Physics, Zernike Institute for Advanced Materials, University of Groningen, NL-9747AG Groningen, The Netherlands*
(Received 10 August 2015; published 2 November 2015)

We study the charge conductivity of the one-dimensional repulsive Hubbard model at finite temperature using the method of dynamical quantum typicality, focusing at half filling. This numerical approach allows us to obtain current autocorrelation functions from systems with as many as 18 sites, way beyond the range of standard exact diagonalization. Our data clearly suggest that the charge Drude weight vanishes with a power law as a function of system size. The low-frequency dependence of the conductivity is consistent with a finite dc value and thus with diffusion, despite large finite-size effects. Furthermore, we consider the mass-imbalanced Hubbard model for which the charge Drude weight decays exponentially with system size, as expected for a nonintegrable model. We analyze the conductivity and diffusion constant as a function of the mass imbalance and we observe that the conductivity of the lighter component decreases exponentially fast with the mass-imbalance ratio. While in the extreme limit of immobile heavy particles, the Falicov-Kimball model, there is an effective Anderson-localization mechanism leading to a vanishing conductivity of the lighter species, we resolve finite conductivities for an inverse mass ratio of $\eta \gtrsim 0.25$.

DOI: [10.1103/PhysRevB.92.205103](https://doi.org/10.1103/PhysRevB.92.205103)

PACS number(s): 71.27.+a, 05.60.Gg, 05.70.Ln, 72.10.-d

I. INTRODUCTION

The Hubbard model is a paradigmatic model in the theory of strongly correlated electrons, capturing some of the essential many-body effects due to short-range electronic correlations in condensed matter physics: Mott-insulating behavior and the resulting localization of magnetic moments with antiferromagnetic spin correlations. Moreover, the Hubbard model is the parent Hamiltonian for the Heisenberg and t-J model, which describe its low-energy physics in the strongly interacting regime [1–3].

The interest in the one-dimensional (1D) version of the model arises because of the existence of an exact solution based on the Bethe ansatz [4] and its relevance for quasi-1D materials [5–9], nanostructures [10–12], and realizations with ultracold atomic gases in optical lattices [3,13]. A recent optical-lattice experiment has investigated the *nonequilibrium* charge transport in the two-dimensional Hubbard model [14].

The Hamiltonian of the 1D repulsive Hubbard model is given by $H = \sum_{l=1}^L h_l$ with local terms,

$$h_l = -t_h \sum_{\sigma} (c_{l,\sigma}^{\dagger} c_{l+1,\sigma} + \text{H.c.}) + U \left(n_{l,\uparrow} - \frac{1}{2} \right) \times \left(n_{l,\downarrow} - \frac{1}{2} \right), \quad (1)$$

with $c_{L+1,\sigma} = c_{1,\sigma}$, where $c_{l,\sigma}$ ($c_{l,\sigma}^{\dagger}$) annihilates (creates) a fermion with spin $\sigma = \uparrow, \downarrow$ on site l , and $n_{l,\sigma} = c_{l,\sigma}^{\dagger} c_{l,\sigma}$ is the local density. L is the number of sites, t_h is the hopping matrix element, and U denotes the on-site Coulomb repulsion.

Despite the success of the theory of such integrable systems in computing many equilibrium properties, the quantitative and qualitative understanding of transport within the linear response theory has proven to be a hard problem [15,16]. While the zero-temperature transport properties are completely understood (see, e.g., [17]), the main open questions concern transport of charge, spin, or energy at finite temperatures $T > 0$. The theory of the algebraic structure of the Bethe ansatz provides knowledge of local conservation laws, which can give rise to ballistic transport [18].

This ballistic transport is usually described via the Drude weight D , the zero-frequency contribution in the real part of the conductivity $\sigma(\omega)$,

$$\text{Re } \sigma(\omega) = 2\pi D \delta(\omega) + \sigma_{\text{reg}}(\omega). \quad (2)$$

As was argued by Zotos, Naef, and Prelovšek [18], a finite Drude weight exists if a lower bound is obtained from the Mazur inequality,

$$D \geq \frac{1}{2TL} \sum_i \frac{\langle Q_i j \rangle^2}{\langle Q_i^2 \rangle}, \quad (3)$$

where $\langle \bullet \rangle$ is the thermodynamic average at temperature T . Such a bound exists if at least one conserved charge Q_i has a finite overlap with the current operator j . The $Q_i = \sum_l q_{l,i}$ are commonly ordered by their range, $i = 1$ corresponding to particle number $Q_1 = N$ and $i = 2$ corresponding to the Hamiltonian $Q_2 = H$. Q_3 has range three (i.e., $q_{l,3}$ involves operators acting on three neighboring sites) and has the same structure as the energy-current operator, yet the two differ in the prefactor of one term [18]. As a consequence, thermal transport in the one-dimensional Hubbard model is ballistic at any finite temperature $T > 0$ [18,19]. Recently, it has been shown that

*rsteinig@uos.de

there are also quasilocal conserved quantities in Bethe-ansatz integrable systems which can be crucial for some transport channels [20–22]. Using the Mazur inequality, one obtains a nonzero Drude weight for charge transport for any filling $n = N/L$ (N is the number of fermions) *other* than $n = 1/2$, from considering only the leading nontrivial local conserved charge Q_3 of range three. The case of half filling has been discussed controversially, with some studies arguing in favor of a finite charge Drude weight $D > 0$ [17,23] while others provided evidence for a vanishing $D = 0$ [24–26] or at best a very small D [26] in the thermodynamic limit (tDMRG gives a small upper bound to the Drude weight). The situation thus appears to be similar to spin transport in the spin-1/2 XXZ chain at zero magnetization, where also no local conservation law yields a nonzero bound to the spin Drude weight [18], while numerical results [27–33] and Bethe-ansatz-based calculations [34,35] strongly indicate a nonzero spin Drude weight at least in its gapless phase, with the possible exception of the point of full SU(2) symmetric exchange, i.e., the Heisenberg chain. For that model, though, quasilocal conservation laws have ultimately been identified as being at the heart of the ballistic spin transport [20,21] at zero magnetization and in its gapless phase.

The connection between (quasi-)local conservation laws and ballistic transport is closely related to how such conservation laws affect thermalization in integrable systems [36]. Consider a quantum quench in which the force driving the current is turned off. If this initial condition leads to a finite value of $\langle j Q_i \rangle$, then the current will never completely decay back to zero. A simple example is the quench of a flux piercing a ring, which has been studied in this context [37].

Besides the question of the (divergent) zero-frequency contribution, the actual frequency dependence of the optical conductivity $\sigma_{\text{reg}}(\omega)$ constitutes an equally interesting problem [26,38–40]. Some insight can be gained from effective low-energy theories such as bosonization [41–43], which is, however, limited to very low temperatures and may not correctly capture effects due to integrability without fine-tuning of parameters. An exact diagonalization study observed strong anomalous finite-size effects in $\sigma_{\text{reg}}(\omega)$ of integrable Mott insulators [38], while many studies conclude that the dc conductivity,

$$\sigma_{\text{dc}} = \lim_{\omega \rightarrow 0} \sigma_{\text{reg}}(\omega), \quad (4)$$

is nonzero in such systems [26,38]. A recent density matrix renormalization group study suggests a generic divergence of $\sigma_{\text{dc}}(T)$ at low temperatures with $\sigma_{\text{dc}} \propto 1/T$ [26], different from the Fermi-liquid behavior $\sigma_{\text{dc}} \propto 1/T^2$ that emerges in sufficiently high dimensions [44]. For the high-temperature regime, a lower bound for the diffusion constant \mathcal{D} has been derived [45], reading

$$\mathcal{D} \geq \text{const.} \times \frac{t_{\text{h}}^3}{U^2}. \quad (5)$$

(Note that $\mathcal{D} \neq D$.) While our primary interest is in the behavior in the linear response regime, we mention that numerical simulations of boundary-driven transport through open Hubbard chains also indicate diffusive high-temperature transport [46].

In our work, we revisit the problem of charge transport in the Hubbard chain at half filling by employing the method of dynamical quantum typicality (DQT). Basically, this approach uses single pure states that are constructed to yield *typical* thermal behavior at finite temperature to compute the time dependence of correlation functions. In the current context of transport, this method has recently been applied to the calculation of the spin Drude weight in XXZ chains [33] and to transport in various nonintegrable models [47–49]. Since only a pure state needs to be propagated in the DQT method, any means of propagating the wave function such as a forward integration or Krylov-space-based approaches can be used, giving access to system sizes as large as $L = 18$, which is comparable to what can be reached for the ground state via Lanczos methods.

We extract the Drude weight from the long-time behavior of current autocorrelation functions and study its finite-size dependence. We observe a power-law decay with system size to zero, which we interpret in the framework of the eigenstate thermalization hypothesis applied to integrable systems [50]. Thus, our results confirm the predictions of Ref. [24,25], i.e., a vanishing Drude weight $D = 0$ at finite temperatures. We further analyze the optical conductivity, for which our data suggest a finite σ_{dc} . Depending on how the time-dependent data are converted to frequency, one either recovers the anomalous, system-size dependent fluctuations discussed in [38] or one obtains a smooth, diffusivelike low-frequency dependence.

The Hubbard model can equivalently be formulated as a spin-1/2 model defined on a two-leg ladder: Spin-up and spin-down fermions live on the two separate legs, where the exchange is of the XY type along the legs, while on the rungs the Hubbard interaction translates into an Ising interaction. This reformulation is, on the one hand, useful for numerical implementations, and on the other hand, there are several natural ways of breaking the integrability that emerge in this picture. Transport in various spin Hamiltonians defined on spin ladders has in fact been intensely investigated [29,47,49,51–55].

Here, we consider the *mass-imbalanced* Hubbard model as an example of a nonintegrable system. The local Hamiltonian now takes the form,

$$h_l = - \sum_{\sigma=\uparrow,\downarrow} [t_{\sigma}(c_{l,\sigma}^{\dagger} c_{l+1,\sigma} + \text{H.c.})] + U \left(n_{l,\uparrow} - \frac{1}{2} \right) \times \left(n_{l,\downarrow} - \frac{1}{2} \right), \quad (6)$$

i.e., we introduce different hopping matrix elements t_{σ} , $\sigma = \uparrow, \downarrow$, for the two fermionic species. We define the inverse mass ratio as

$$\eta = \frac{t_{\downarrow}}{t_{\uparrow}}. \quad (7)$$

In the limit of $\eta = 0$, also known as the Falicov-Kimball model, one naturally obtains perfectly insulating behavior at any temperature due to an effective Anderson-localization mechanism. In this case, all the local density operators $n_{l,\downarrow}$ of the heavy species become conserved quantities, i.e., $[H, n_{l,\downarrow}] = 0$. Thus, for a given random distribution of immobile spin-down fermions, via the interaction term $U n_{l,\uparrow} n_{l,\downarrow}$, one effectively

obtains a diagonal disorder potential for the light fermions with local potentials $\epsilon_l = U n_{l,\downarrow}$ drawn from a binary distribution $\epsilon_l = 0, U$. The translational invariance of the original model at a given density of $n_\downarrow = N_\downarrow/L$ is restored by averaging over many random distributions of the heavy fermions.

We are interested in the dependence of the conductivities $\sigma_\uparrow(\omega)$ and $\sigma_\downarrow(\omega)$ of the heavy and light species, respectively, as a function of the inverse mass ratio η . First, we compute the associated Drude weights, which vanish approximately exponentially fast with system size, as expected for a nonintegrable model [50,56,57]. For intermediate values of η , we observe a regular form of $\sigma_\uparrow(\omega)$ and $\sigma_\downarrow(\omega)$. The dc conductivity of the heavy component appears to simply vanish quadratically with t_\downarrow , while the presence of the heavy fermions leads to an approximately exponential decay of the dc conductivity of the light fermions as a function of decreasing η , which we are able to resolve for $\eta \gtrsim 0.25$.

The mass-imbalanced Hubbard model has recently attracted renewed interest in the context of many-body localization [58,59] since several authors have considered the possibility of many-body localization in translationally invariant systems [60–62]. In our model, interactions could thus potentially lead to a nontrivial effect in the strongly mass-imbalanced regime. Recent work has suggested, though, that there likely is no mass-imbalance driven localization-delocalization transition in our model at a nonzero η , but a quasi-many-body localized behavior with anomalous diffusion at small values of η [63]. These results are based on exact diagonalization with $L \leq 10$. Our results suggest a finite, albeit exponentially small dc conductivity at least for $\eta \gtrsim 0.25$.

The plan of the paper is the following. Section II summarizes the definitions and expressions of the conductivity, the Drude weight, and current autocorrelation functions. In Sec. III, we provide a brief introduction to the DQT method and its application to the calculation of finite-temperature current autocorrelation functions. Section IV contains our results for the integrable Hubbard chain at half filling, while we present our data and the discussion of the mass-imbalanced model in Sec. V. We conclude with a summary and an outlook in Sec. VI.

II. DEFINITIONS

Using the Jordan-Wigner transformation, the mass-imbalanced Fermi-Hubbard model can equivalently be formulated as a spin-1/2 model defined on a two-leg ladder,

$$h_l = \sum_{\sigma=\uparrow,\downarrow} -2t_\sigma (S_{l,\sigma}^x S_{l+1,\sigma}^x + S_{l,\sigma}^y S_{l+1,\sigma}^y) + U S_{l,\uparrow}^z S_{l,\downarrow}^z, \quad (8)$$

where spin-up and spin-down fermions live on the two separate legs and the Hubbard interaction translates into an Ising interaction. Our numerical implementation is formulated in the spin language.

We derive the charge current from the continuity equation [18], leading to $j = j_\uparrow + j_\downarrow$ and $j_\sigma = i \sum_l [n_{l,\sigma}, h_l]$ in the Hubbard notation. In the spin notation,

$$j_\sigma = -2t_\sigma \sum_l (S_{l,\sigma}^x S_{l+1,\sigma}^y - S_{l,\sigma}^y S_{l+1,\sigma}^x), \quad (9)$$

is the spin current in the first ($\sigma = \uparrow$) or second ($\sigma = \downarrow$) leg. We correspondingly study the two current autocorrelation functions at inverse temperature $\beta = 1/T$,

$$C_\sigma(t) = \frac{\text{Re} \langle j_\sigma(t) j_\sigma \rangle}{LZ} = \frac{\text{Re} \text{Tr} \{ e^{-\beta H} j_\sigma(t) j_\sigma \}}{L \text{Tr} \{ e^{-\beta H} \}}, \quad (10)$$

where the time argument of $j_\sigma(t)$ refers to the Heisenberg picture, $j_\sigma(0) = j_\sigma$, and $C_\sigma(0) = t_\sigma^2/2$ in the high-temperature limit $\beta \rightarrow 0$.

From the time dependence of $C_\sigma(t)$ we determine the quantities,

$$\bar{C}_\sigma(t_1, t_2) = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} dt C_\sigma(t), \quad (11)$$

in a time interval $[t_1, t_2]$ where $C_\sigma(t)$ has decayed to its long-time value $C(t_1 < t < t_2) \approx C(t \rightarrow \infty)$ and is practically constant. Thus, the quantities $\bar{C}_\sigma(t_1, t_2)$ approximate the finite-size Drude weights of the two legs given by

$$D_\sigma = \frac{1}{2\pi} \lim_{t_2 \rightarrow \infty} \bar{C}_\sigma(0, t_2). \quad (12)$$

We determine the frequency-dependent optical conductivity $\text{Re} \sigma_{\sigma, t_{\max}}(\omega)$ via the finite-time Fourier transformation,

$$\text{Re} \sigma_{\sigma, t_{\max}}(\omega) = \frac{1 - e^{-\beta\omega}}{\omega} \int_0^{t_{\max}} dt e^{i\omega t} C_\sigma(t). \quad (13)$$

Here, the choice of a particular t_{\max} implies a frequency resolution $\delta\omega \approx \pi/t_{\max}$. In the thermodynamic limit $L \rightarrow \infty$, $\text{Re} \sigma_{\sigma, t_{\max}}(\omega)$ is a smooth function on an arbitrarily small scale $\delta\omega \rightarrow 0$ and does not depend on the actual value of t_{\max} chosen, as long as it is large compared to the current relaxation time [48]. For any finite L , however, it is important to find a reasonable t_{\max} where finite-size effects are well controlled. In particular, for integrable systems, finding such a t_{\max} can be a subtle issue, as discussed later in detail. Note that, to leading order in β , $\text{Re} \sigma_\sigma(\omega) \propto \beta$ and that $\text{Re} \sigma_\sigma(\omega) = \sigma_\sigma(\omega)$ in the high-temperature limit.

If we find a (t_{\max}, L) region with no significant dependence on t_{\max} and L , we extract the dc conductivity $\sigma_{\sigma, \text{dc}}$ as the low-frequency limit,

$$\sigma_{\sigma, \text{dc}} = \lim_{\omega \rightarrow 0} \sigma_{\sigma, t_{\max}}(\omega). \quad (14)$$

In case of vanishing Drude weights, $\sigma_{\sigma, \text{dc}}/\chi$ is identical to the time-dependent diffusion constant,

$$\mathcal{D}_\sigma(t_{\max}) = \frac{\beta}{\chi} \int_0^{t_{\max}} dt C_\sigma(t), \quad (15)$$

with χ being the static susceptibility and reading, at $\beta \rightarrow 0$,

$$\frac{\chi}{\beta} = \frac{\text{Tr} \{ (\sum_l S_{l,\sigma}^z)^2 \} - (\text{Tr} \{ \sum_l S_{l,\sigma}^z \})^2}{L} = \frac{1}{4}. \quad (16)$$

In the case of significant finite-size Drude weights, however, $\mathcal{D}_\sigma(t_{\max})$ may not depend on t_{\max} and L , while $\sigma_{\sigma, \text{dc}}$ clearly does. Therefore, in such cases, the time-dependent diffusion constant provides a useful alternative for extracting transport coefficients on the basis of finite systems. Beyond technical aspects, $\mathcal{D}(t)$ also has a clear physical interpretation: It directly yields information on how spatial variances of density profiles evolve in time [64–67] for any finite L .

III. DYNAMICAL QUANTUM TYPICALITY

A. Concept

In this section we first introduce a very accurate approximation of current autocorrelation functions. This approximation then provides the basis for the numerical technique used throughout our work. The central idea is to replace the trace operation $\text{Tr}\{\bullet\} = \sum_i \langle i | \bullet | i \rangle$ in Eq. (10) by a single scalar product $\langle \psi | \bullet | \psi \rangle$, where $|\psi\rangle$ is a single pure state drawn at random. Since we aim at describing the current dynamics in the full Hilbert space, $|\psi\rangle$ is drawn at random in the full basis. Conveniently, $|\psi\rangle$ is randomly chosen in the eigenbasis of the particle number,

$$|\psi\rangle = \sum_N |\psi_N\rangle, \quad |\psi_N\rangle = \sum_s^{d_N} (a_s + i b_s) |s\rangle, \quad (17)$$

where $s = s(N)$ is a label for the eigenstates with particle number N . The coefficients a_s and b_s are random real numbers. To be precise, these coefficients are chosen according to a Gaussian distribution with zero mean. Thus, the pure state $|\psi\rangle$ is chosen according to the unitary invariant Haar measure [68,69] and, according to typicality [70–75], a representative of the statistical ensemble.

The pure state $|\psi\rangle$, and each $|\psi_N\rangle$, correspond to the limit of high temperatures $\beta \rightarrow 0$. We incorporate finite temperatures $\beta \neq 0$ by introducing $|\psi_N(\beta)\rangle = \exp(-\beta H/2) |\psi_N\rangle$ and rewriting the current autocorrelation function in Eq. (10) in the form [33,47,68,69,76,77] (skipping the index σ for clarity),

$$C(t) = \frac{\text{Re} \sum_N \langle \psi_N(\beta) | j(t) j | \psi_N(\beta) \rangle}{L \sum_N \langle \psi_N(\beta) | \psi_N(\beta) \rangle} + \epsilon(|\psi\rangle), \quad (18)$$

where $\epsilon(|\psi\rangle)$ is a statistical error resulting from the random choice of $|\psi\rangle$. This error vanishes when sampling over several $|\psi\rangle$ is performed, i.e., $\bar{\epsilon} = 0$.

However, the central advantage of Eq. (18) is not the vanishing mean error $\bar{\epsilon} = 0$ but the knowledge about the standard deviation of errors $\Sigma(\epsilon)$. This standard deviation is bounded from above by [33,68,69,77],

$$\Sigma(\epsilon) \leq \mathcal{O}\left(\frac{\sqrt{\text{Re} \langle j(t) j j(t) j \rangle}}{L \sqrt{d_{\text{eff}}}}\right), \quad (19)$$

where d_{eff} is the effective dimension of the Hilbert space. In the limit of high temperatures $\beta \rightarrow 0$, $d_{\text{eff}} = 4^L$ is the full Hilbert-space dimension. Consequently, if the length L is increased, $\Sigma(\epsilon)$ decreases exponentially fast with L . At arbitrary β , $d_{\text{eff}} = \text{Tr}\{\exp[-\beta(H - E_0)]\}$ is the partition function with ground-state energy E_0 , reflecting the number of thermally occupied states, and also scales exponentially fast with L [33]. Therefore, while the error is exactly zero in the thermodynamic limit $L \rightarrow \infty$, this error can be already very small at finite but large L and sampling is unnecessary, as is the case for all examples considered in our work.

B. Numerical implementation

Most importantly, the approximation in Eq. (18) can be calculated without knowing the eigenstates and eigenvalues of the Hamiltonian. This calculation is based on the two auxiliary

pure states,

$$|\Phi_N(\beta, t)\rangle = e^{-iHt - \beta H/2} |\psi_N\rangle, \quad (20)$$

$$|\varphi_N(\beta, t)\rangle = e^{-iHt} j e^{-\beta H/2} |\psi_N\rangle. \quad (21)$$

Both states are time- and temperature-dependent and the only difference between the two states is the additional current operator j in the right-hand side of Eq. (21). Using these states, the approximation in Eq. (18) reads

$$C(t) = \frac{\text{Re} \sum_N \langle \Phi_N(\beta, t) | j | \varphi_N(\beta, t) \rangle}{L \sum_N \langle \Phi_N(\beta, 0) | \Phi_N(\beta, 0) \rangle}. \quad (22)$$

Apparently, the full time and temperature dependence in Eq. (22) results from the evolution of the pure states only, i.e., there the current operator j is simply applied to the initial or time-evolved states.

For, e.g., $|\Phi_N(\beta, t)\rangle$, the β dependence is generated by an imaginary-time Schrödinger equation,

$$i \frac{\partial}{\partial(\beta)} |\Phi_N(\beta, 0)\rangle = \frac{H}{2} |\Phi_N(\beta, 0)\rangle, \quad (23)$$

and the t dependence by the usual real-time Schrödinger equation,

$$i \frac{\partial}{\partial t} |\Phi_N(\beta, t)\rangle = H |\Phi_N(\beta, t)\rangle. \quad (24)$$

These differential equations can be solved by the use of straightforward iterative methods such as, e.g., Runge-Kutta [33,47,77]. We use a massively parallel implementation of a Suzuki-Trotter product formula or Chebyshev polynomial algorithm [78,79], allowing us to study quantum systems with as many as $2L = 36$ lattice sites ($L = 18$ in the fermionic language), where the Hilbert-space dimension is $d = \mathcal{O}(10^{11})$. As compared to exact diagonalization, this dimension is larger by orders of magnitude. Yet, we do not exploit translation invariance of Hamiltonian and current. This symmetry adds momentum as a good quantum number and an additional layer of parallelization [47].

In practice, we use the Chebyshev polynomial algorithm to compute $e^{-\beta H/2} |\psi_N\rangle$. The results of this algorithm are exact to at least ten digits. For the propagation in real time, we mostly use a unitary, second-order product formula algorithm with a time step $\delta t t_h = 0.02$, which is sufficiently small to guarantee that the total energy is conserved up to at least six digits. Occasionally, we have used the Chebyshev polynomial algorithm to compute the real-time evolution: No significant differences between these and the product-formula results were found. Most of the simulations were carried out on JUQUEEN, the IBM Blue Gene/Q located at the Jülich Supercomputer Centre. A simulation of the largest system studied in the present paper (36 spins) required 3 TB of memory, the computation was distributed over 131 072 (MPI) processes, and the total elapsed time to carry out 400 times steps was about 10 h (1.3 million core hours).

IV. RESULTS FOR THE HUBBARD MODEL

This section contains our results for the charge transport in the 1D Hubbard model, focusing at half filling. We consider infinite temperature $\beta = 1/T \rightarrow 0$ unless stated otherwise.

First, we discuss the overall time dependence of the current autocorrelation function for various values of U/t_h . Second, we extract the Drude weight D from the long-time behavior of $C(t)$. Finally, we discuss the frequency dependence of the regular part and its zero-frequency limit.

A. Time dependence of autocorrelation functions

Figures 1(a)–1(c) show typical results for the real-time decay of the current autocorrelation function $C(t)$ for $U/t_h = 4, 8, 16$, respectively, and several system sizes $L \leq 18$. The figures show $C(t)$ for times up to $t/t_h \lesssim 8$, where the dominant decay of $C(t)$ from its initial value occurs. Typically, the data from these different L coincide for $t/t_h \lesssim 2.5$. Beyond $t/t_h = 2.5$, $C(t)$ is a monotonically decreasing function of system size as indicated by the arrow in Fig. 1(b). The figures further include real-time density matrix renormalization group (tDMRG) data from [26] for comparison. Our DQT results are in excellent agreement with the tDMRG data.

As U/t_h increases, $C(t)$ approaches small values increasingly faster as a function of time. On the other hand, the larger U/t_h , the more high-frequent and pronounced are the oscillations in $C(t)$. These are inherited from the large U/t_h limit, in which the spectrum consists of bands of eigenstates

separated by gaps of order U . These bands correspond to excitations with multiple doublons. Thus, the oscillatory dynamics in $C(t)$ at large U/t_h is quite similar to the behavior in the spin-1/2 XXZ chain in the strong Ising limit [67] and spin-1/2 XX ladders in the strong rung-coupling limit [47].

B. Drude weight

In order to extract the nondecaying portion of $C(t)$, which equals the Drude weight, much longer times than $t/t_h \sim 12$ need to be considered [33]. Therefore, we display $C(t)$ for $t/t_h \leq 25$ in Fig. 2(a) for the example of $U/t_h = 4, 8, 16$ and for $L = 15$. At times $t/t_h \geq 10$, the oscillations in $C(t)$ have decayed to a sufficiently small amplitude and hence we estimate the Drude weight by averaging $C(t)$ in the time window $t \in [t_1, t_2]$, yielding $\bar{C}(t_1, t_2)$. Note that $\bar{C}(t_1, t_2)$ does not depend on this specific choice of t_2 [see the inset of Fig. 2(b)].

The resulting, L -dependent $\bar{C}(t_1, t_2)$ are shown in Fig. 2(b) in a log-log plot. The system-size dependence of $\bar{C}(t_1, t_2)$ is consistent with a $1/L$ decay of the Drude weight to zero as system size increases. This scaling of D with system size is typical for integrable systems: It has been observed for the spin Drude weight of the spin-1/2 XXZ chain as well [29,30,32,33].

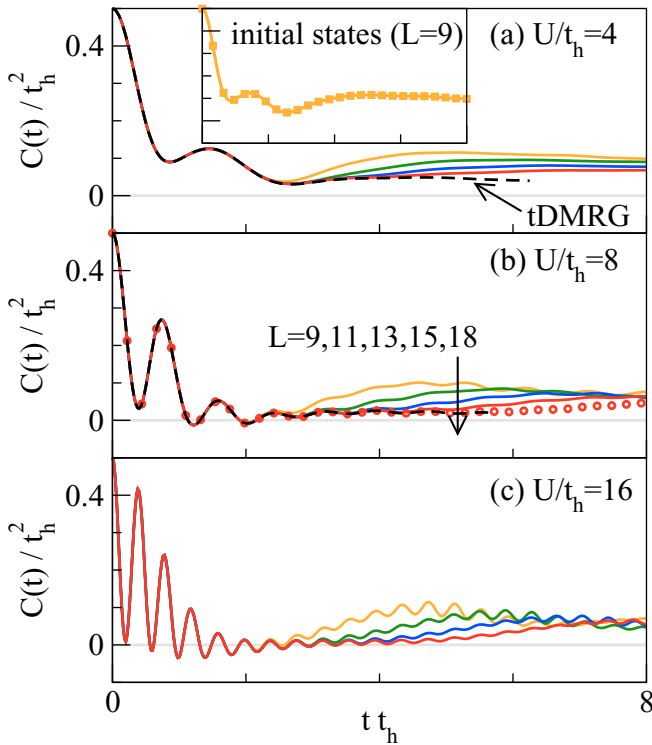


FIG. 1. (Color online) Real-time decay of the current autocorrelation function $C(t)$ for (a) $U/t_h = 4$, (b) $U/t_h = 8$, (c) $U/t_h = 16$ for various $L = 9, 11, 13, 15, 18$ and at infinite temperature $\beta t_h \rightarrow 0$ (solid curves and circles). For the largest $L = 15$ and 18, convergence to system-size independent values is reached at times $t/t_h \sim 5$. For comparison, tDMRG data from [26] are included in (a) and (b) (dashed curves). The inset in (a) shows the $L = 9$ result for two different initial random states (solid curve, first state; squares, second state), which demonstrates small statistical errors for this L already.

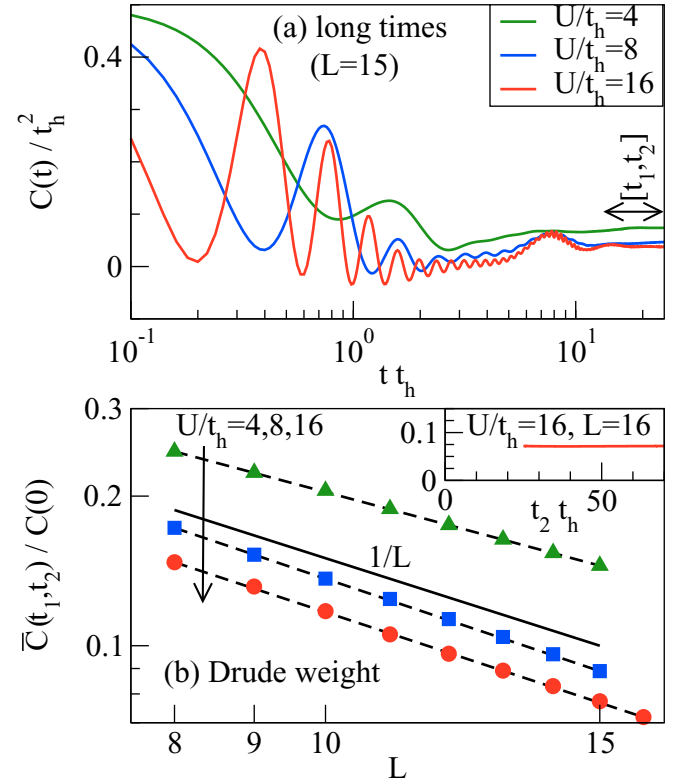


FIG. 2. (Color online) (a) Long-time limit of the current autocorrelation function $C(t)$ for different $U/t_h = 4, 8, 16$, fixed $L = 15$, and high temperatures $\beta t_h \rightarrow 0$. (b) Finite-size scaling of the Drude weight $\bar{C}(t_1, t_2)$, as extracted from the time interval $[t_1, t_2] = [12.5, 25]$, in a log-log plot. As a guide to the eyes, power laws (dashed lines) and a function $\propto 1/L$ (solid line) are indicated. The inset in (b) shows, for $U/t_h = 16$ and $L = 16$, that $\bar{C}(t_1, t_2)$ does not depend on the specific choice of t_2 .

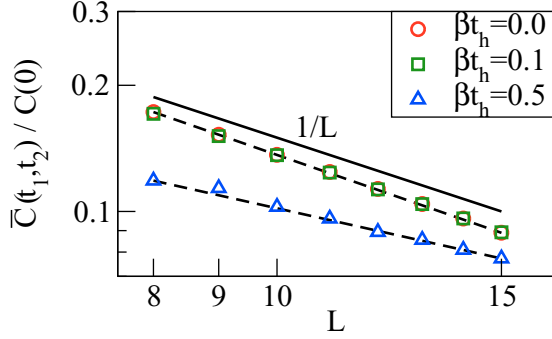


FIG. 3. (Color online) The same information as shown in Fig. 2(b) but for fixed $U/t_h = 8$ and different $\beta t_h = 0, 0.1, 0.5$. Data for $\beta t_h = 0.0$ and 0.1 almost coincide.

Moreover, the Drude weight approximately measures the fluctuations of diagonal matrix elements of the associated current operator [50]. Such system-size-dependent fluctuations are commonly investigated to access the validity of the eigenstate thermalization hypothesis [80–82]. For integrable systems, most numerical studies indicate a slow, power-law decay of these fluctuations [50, 57, 83]. Most notably, our data are consistent with a vanishing Drude weight $D = 0$ at infinite temperature, in agreement with [25].

In principle, if the infinite-temperature Drude weight vanishes, this does not necessarily imply that $D(T) = 0$ at any finite T . To see this, one can write the Drude weight in a high-temperature expansion,

$$D(T) = \frac{D_1}{T} + \frac{D_2}{T^2} + \dots, \quad (25)$$

where D_1 is the infinite-temperature Drude weight studied in Fig. 2(b). To substantiate that in the Hubbard model at half filling $D(T) = 0$ at any finite T , we have also computed $D(T)$ at $T/t_h = 2, 10$, where D also seems to vanish as L increases. This is illustrated in Fig. 3.

C. Optical conductivity

Since the Drude weight appears to vanish as $L \rightarrow \infty$, all weight in $\text{Re } \sigma(\omega)$ will ultimately be in the regular part $\sigma_{\text{reg}}(\omega)$. This optical conductivity has recently been studied using tDMRG [26], where a finite dc conductivity was observed that diverges as $\sigma_{\text{dc}} \sim 1/T$ as temperature decreases.

We first demonstrate that it is indeed possible to extract the dc conductivity from our time-dependent data for $C(t)$. At infinite temperature, the dc conductivity σ_{dc}/χ is simply equal to the integral $\mathcal{D}(t)$ over $C(t)$ as defined in Eq. (15), i.e., connected to the diffusion constant by an Einstein relation.

At large U/t_h , \mathcal{D} increases quickly and then settles into a plateau, as is evident from the example presented in Fig. 4(a). At large times, \mathcal{D} further increases, which is due to both the nonzero Drude weight on finite systems and other finite-size effects. Plotting data for \mathcal{D} for several system sizes clearly suggests that finite-size data gradually approach the plateau value at longer times as well; see Fig. 4(a).

The presence of such a plateau, following the reasoning of [64], suggests a finite dc conductivity and diffusion constant.

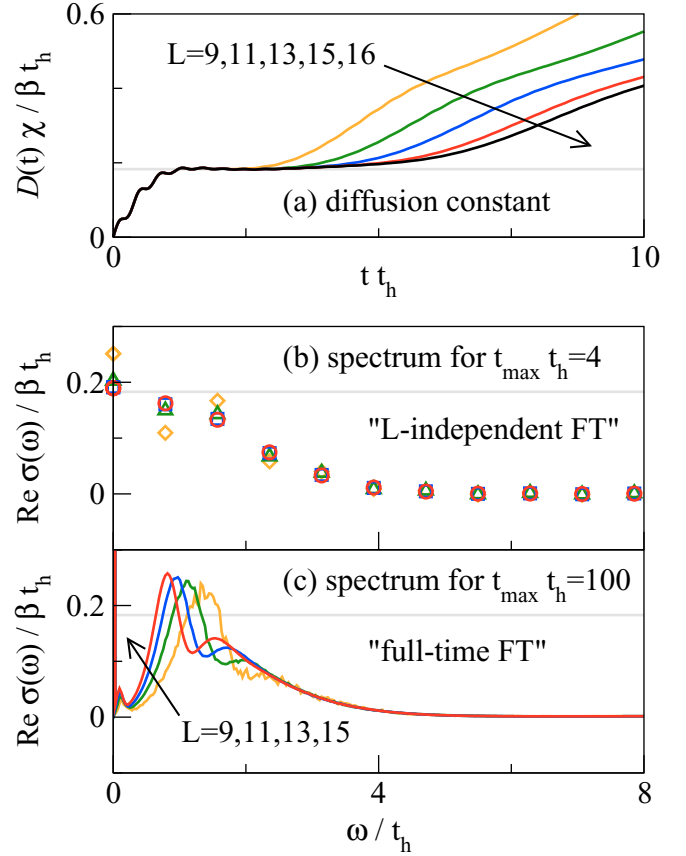


FIG. 4. (Color online) (a) Time-dependent diffusion constant $\mathcal{D}(t)$ for $U/t_h = 16$, various $L = 9, 11, 13, 15, 16$, and high temperatures $\beta t_h \rightarrow 0$. A plateau is clearly visible at intermediate times before the finite-size Drude weight yields a linear increase in the long-time limit. The plateau height is independent of L and the plateau width increases with L . (This behavior is almost identical to the XXZ chain at $\Delta > 1$.) (b) and (c) Frequency dependence of the optical conductivity $\text{Re } \sigma(\omega)$, as resulting from $t_{\text{max}} t_h = 4, 100$. (c) Does not respect the “better” limit of $L \rightarrow \infty$ first and $t_{\text{max}} t_h \rightarrow \infty$ afterward. Apparently, (c) shows strong finite-size effects at both $\omega = 0$ and $\omega \neq 0$. However, in the thermodynamic limit $L \rightarrow \infty$, (c) seems to approach (b).

As shown in Fig. 5, the diffusion constant exhibits a peculiar behavior at $T = \infty$: As U/t_h increases, it saturates at a U -independent value. This saturation results from the structure of the energy spectrum in the large- U/t_h limit: It consists of bands separated by U that have a band width given by t_h . Since we are taking the limit $U/t_h \rightarrow \infty$ after taking the limit $T \rightarrow \infty$, the dominant contribution to scattering comes from interband processes. This behavior appears to be generic for systems with an emergent ladderlike spectrum and has also been observed in the Ising regime of spin-1/2 XXZ chains [67] and in spin-1/2 XX ladders [47]. The independence of the diffusion constant on U observed in Fig. 5 also unveils that the lower bound of [45], as given in Eq. (5), is not exhaustive in the large- U/t_h regime.

For the purpose of computing $\text{Re } \sigma(\omega)$, the existence of the plateau implies that the asymptotic behavior has been reached. Moreover, the value of the plateau in $\mathcal{D}(t)$ is independent of

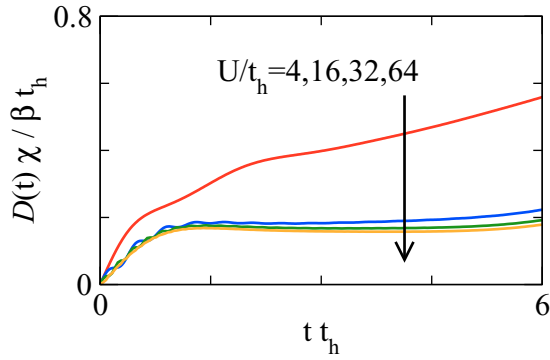


FIG. 5. (Color online) Time-dependent diffusion constant $\mathcal{D}(t)$ for various $U/t_h = 4, 16, 32, 64$, fixed $L = 15$, and high temperatures $\beta t_h \rightarrow 0$. Clearly, the plateau value of $\mathcal{D}(t)$ becomes independent of U in the limit of large U .

system size for the parameters of Fig. 4. Thus, we will compare two ways of computing $\text{Re } \sigma(\omega)$: (i) The first version uses the full-time dependence of $C(t)$, up to and including times where we clearly observe finite-size effects (later dubbed full-time FT); (ii) in the second, we restrict the time window for the Fourier transformation to times at which we have system-size independent data for $C(t)$ (later referred to as L -independent FT).

The results of both approaches are presented in Figs. 4(b) and 4(c), respectively. The full-time FT resolves the strong finite-size dependent structures that were known to exist from Ref. [38]. The positions of these sharp peaks shift to smaller frequencies as system size increases. An extrapolation of $\sigma_{\text{reg}}(\omega)$ to zero frequency is thus difficult to control.

The behavior of $\sigma_{\text{reg}}(\omega)$ computed using the L -independent FT strategy, by contrast, is a very smooth function that strongly resembles the optical conductivity of a typical diffusive system. This is clearly related to the fast initial decay of $C(t)$ [see the data shown in Fig. 1(b)], and the corresponding establishment of the plateau in the integrated quantity $\mathcal{D}(t)$, which consequently allows us to estimate the dc limit under the assumption that no additional time dependence emerges in $C(t)$ at very long times and large systems. We thus propose that whenever such a plateau is present in $\mathcal{D}(t)$, the cleanest way of computing $\sigma_{\text{reg}}(\omega)$ is the L -independent FT, in line with the reasoning of Refs. [64,67,84].

Figure 6 shows data for $U/t_h = 4$ as an example for a case, in which no clear plateau in $\mathcal{D}(t)$ can be resolved with the accessible system sizes. Here, we thus compute $\sigma_{\text{reg}}(\omega)$ from the full available time series of $C(t)$, which is shown in Fig. 6(b). The optical conductivity has a broad maximum at $\omega/t_h \sim U/t_h$ and an additional low-frequency peak at $\omega/t_h \sim 1$ whose position shifts to small frequencies as L increases. The data would suggest a small or vanishing dc conductivity, which we believe does not reflect the behavior of an infinitely large system [compare Fig. 4(b)], since the low-frequency finite-size effects likely screen the correct low-frequency dependence.

V. RESULTS FOR THE MASS-IMBALANCED CASE

In this section, we present our results for the mass-imbalanced cases $\eta = t_{\downarrow}/t_{\uparrow} < 1$, where the model is nonintegrable. We start with the case $\eta = 0$, the Falicov-Kimball

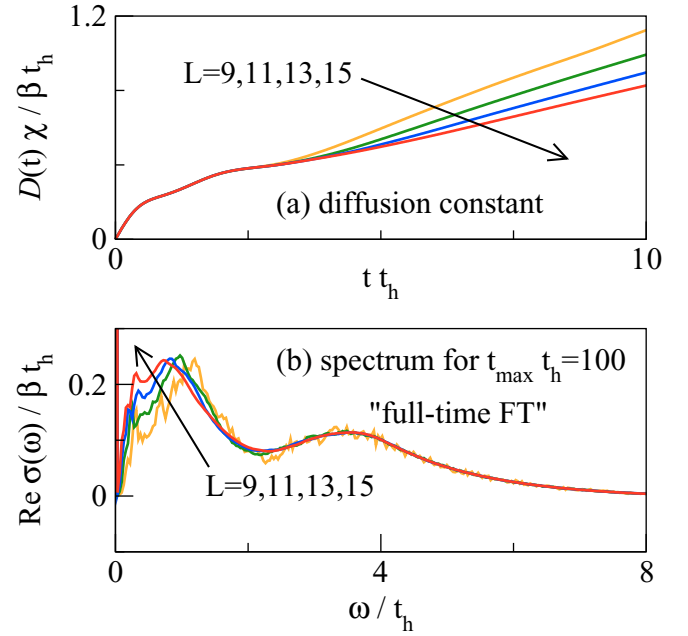


FIG. 6. (Color online) The same information as shown in Fig. 4, yet here for $U/t_h = 4$. Extracting $\text{Re } \sigma(\omega)$ via the L -independent FT strategy is not applicable here, since $\mathcal{D}(t)$ does not exhibit a clear plateau [see (a)], due to the long-time tail in $C(t)$. This plateau will also not occur for $L = 18$. Thus, in (b), we present $\text{Re } \sigma(\omega)$ obtained from a full-time FT, which thus results in strong finite-size effects at small frequencies.

limit, and discuss the emergence of Anderson localization in this limit. Then we turn to the case of $\eta \sim 1/2$ and study both Drude weight and optical conductivity. Finally, we summarize the scaling of the diffusion constant as a function of η in the η region accessible to our numerical method.

A. Falicov-Kimball limit

In the Falicov-Kimball limit $\eta = 0$ the model simplifies to

$$h_l = -t_{\uparrow}(c_{l,\uparrow}^{\dagger}c_{l+1,\uparrow} + \text{H.c.}) + U\left(n_{l,\uparrow} - \frac{1}{2}\right)\left(n_{l,\downarrow} - \frac{1}{2}\right). \quad (26)$$

For this simplified model all $n_{l,\downarrow}$ commute with all local Hamiltonians h_l and with each other,

$$[h_l, n_{k,\downarrow}] = [n_{l,\downarrow}, n_{k,\downarrow}] = 0, \quad (27)$$

$l, k = 1, \dots, L$. Each $(n_{l,\downarrow} - 1/2)$ is thus conserved and yields a good quantum number $\epsilon_l = \pm 1/2$, with 2^L different sequences,

$$\epsilon(m) = (\epsilon_1(m), \dots, \epsilon_L(m)), \quad (28)$$

$m = 1, \dots, 2^L$. As a consequence, the full Hamiltonian $H = \sum_l h_l$ can be rewritten as a sum of 2^L uncoupled Hamiltonians $H(m) = \sum_l h_l(m)$, where

$$h_l(m) = -t_{\uparrow}(c_{l,\uparrow}^{\dagger}c_{l+1,\uparrow} + \text{H.c.}) + U \epsilon_l(m) \left(n_{l,\uparrow} - \frac{1}{2}\right), \quad (29)$$

and the U part becomes a site-dependent potential given by the sequence $\epsilon(m)$. For many m , $\epsilon(m)$ can be understood as a

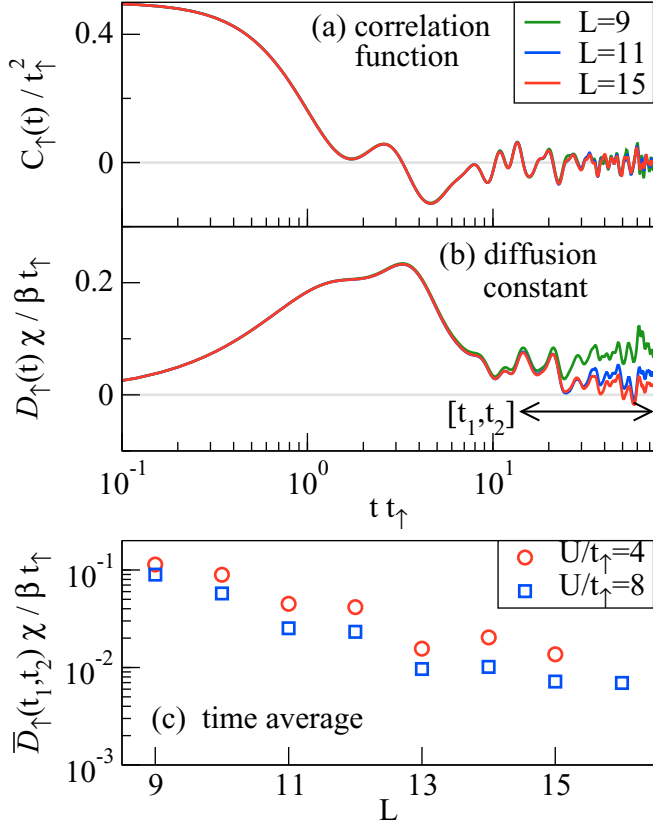


FIG. 7. (Color online) (a) Real-time decay of the current autocorrelation function $C_{\uparrow}(t)$ of the light \uparrow component for $U/t_{\uparrow} = 4$, strong imbalance $\eta = t_{\downarrow}/t_{\uparrow} = 0$, $L = 9, 11, 15$, and high temperatures $\beta t_{\uparrow} \rightarrow 0$. Since $C_{\uparrow}(t)$ is highly oscillating after the initial decay, also the time-dependent diffusion constant $D_{\uparrow}(t)$ does so in (b). Consequently, the usual extraction of a diffusion constant would depend on the specific point in time considered. However, the time average still yields a reasonable diffusion constant. (c) Finite-size scaling of the time average for $U/t_{\uparrow} = 4, 8$, as resulting from the time interval $[t_1, t_2] = [12.5, 75]$, in a semi-log plot. Apparently, the scaling is nontrivial, but the decrease is consistent with insulating behavior in the thermodynamic limit $L \rightarrow \infty$.

sequence of random numbers drawn from a binary distribution $[-1/2, 1/2]$. Therefore, remarkably, many uncoupled Hamiltonians $H(m)$ can be interpreted also as the single-particle, Anderson problem for on-site disorder of strength U . Note that translation invariance is typically broken for a given m but restored by sampling over m . Note further that *all* m contribute at finite temperatures.

Due to the analogy to the single-particle, Anderson problem and the strict one-dimensionality of the lattice, one expects perfectly insulating behavior in the thermodynamic limit $L \rightarrow \infty$ at all temperatures. Early on, this expectation has been verified in numerical calculations of the optical conductivity [85,86] for $\beta t_{\uparrow} > 0$ and values of U where the localization length does not exceed lattice sizes accessible. Yet, the high-temperature limit $\beta t_{\uparrow} \rightarrow 0$ has not been studied.

In Fig. 7(a) we show our results for the time-dependent current autocorrelation function $C_{\uparrow}(t)$ for $\beta t_{\uparrow} \rightarrow 0$, $U/t_{\uparrow} = 4$, and different $L = 9, 11, 15$. Clearly, $C_{\uparrow}(t)$ decays rapidly on a rather short time scale $t/t_{\uparrow} \sim 1$. After this initial decay

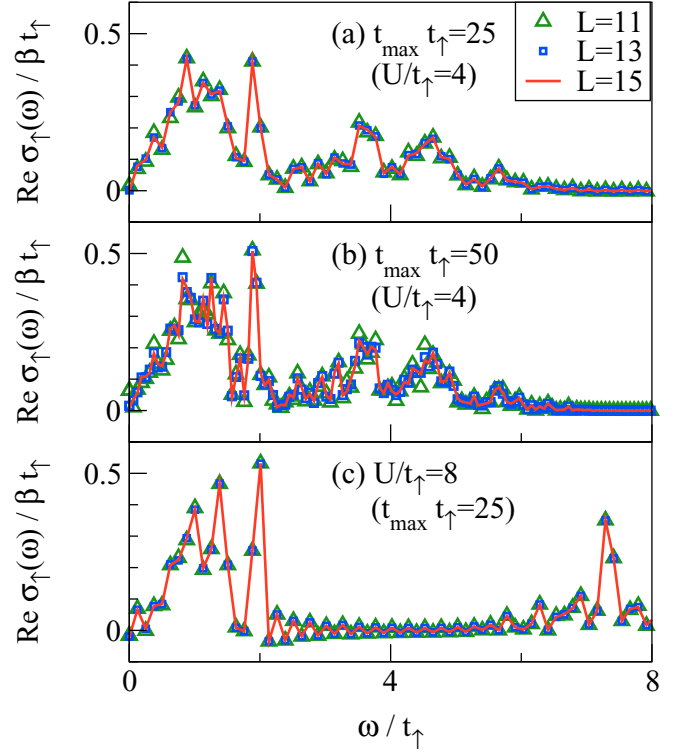


FIG. 8. (Color online) Frequency dependence of the optical conductivity $\text{Re } \sigma_{\uparrow}(\omega)$ for (a) $t_{\max} t_{\uparrow} = 25$, (b) $t_{\max} t_{\uparrow} = 50$ for $U/t_{\uparrow} = 4$, strong imbalance $\eta = t_{\downarrow}/t_{\uparrow} = 0$, different $L = 11, 13, 15$, and high temperatures $\beta t_{\uparrow} \rightarrow 0$. (c) Shows (a) for $U/t_{\uparrow} = 8$. The overall structure is independent of t_{\max} and L . For the dependence of the dc limit $\text{Re } \sigma_{\uparrow}(\omega \rightarrow 0)$ on L and t_{\max} , see $\bar{D}_{\uparrow}(t_1, t_2)$ discussed before.

$C_{\uparrow}(t)$ approaches zero from the negative side but still shows small oscillations. Note that these oscillations are no finite-size effects since curves for $L = 11$ and 15 are practically identical to each other for the long times $t/t_{\uparrow} \sim 75$ depicted in the figure. This curve for $C_{\uparrow}(t)$ yields the time-dependent diffusion constant $D_{\uparrow}(t)$ shown in Fig. 7(b). After the initial increase of $D_{\uparrow}(t)$ we find a strong decrease related to the region where $C_{\uparrow}(t)$ is negative. Necessarily, $D_{\uparrow}(t)$ also shows small oscillations not related to finite-size effects, as evident from comparing $L = 11$ and 15 again.

The long-time oscillations of $D_{\uparrow}(t)$ indicate that the dynamical process cannot be described by a diffusion constant in the strict sense. However, to extract an effective diffusion constant, we average $D_{\uparrow}(t)$ over the long-time interval $[t_1, t_2] = [12.5, 75]$. In Fig. 7(c) we depict the resulting $\bar{D}_{\uparrow}(t_1, t_2)$ as a function of L for $U/t_{\uparrow} = 4, 8$ in a semi-log plot. Apparently, this time-averaged quantity decreases as system size increases and may eventually become zero in the thermodynamic limit $L \rightarrow \infty$. Note that the scaling for small L is partially related to tiny finite-size Drude weights D_{\uparrow} , entering $D_{\uparrow}(t)$ via the relation $D_{\uparrow}(t) \propto D_{\uparrow} t$ in the long-time limit.

Next we turn to the optical conductivity. Since $C_{\uparrow}(t)$ and $D_{\uparrow}(t)$ do not become constant in the long-time limit, the finite-time Fourier transform necessarily depends on the specific time interval chosen. Thus, we show in Figs. 8(a) and 8(b) the Fourier transform of $U/t_{\uparrow} = 4$ data for $t_{\max} t_{\uparrow} = 25$ and 50 , where times $t \leq t_{\max}$ were considered in the Fourier

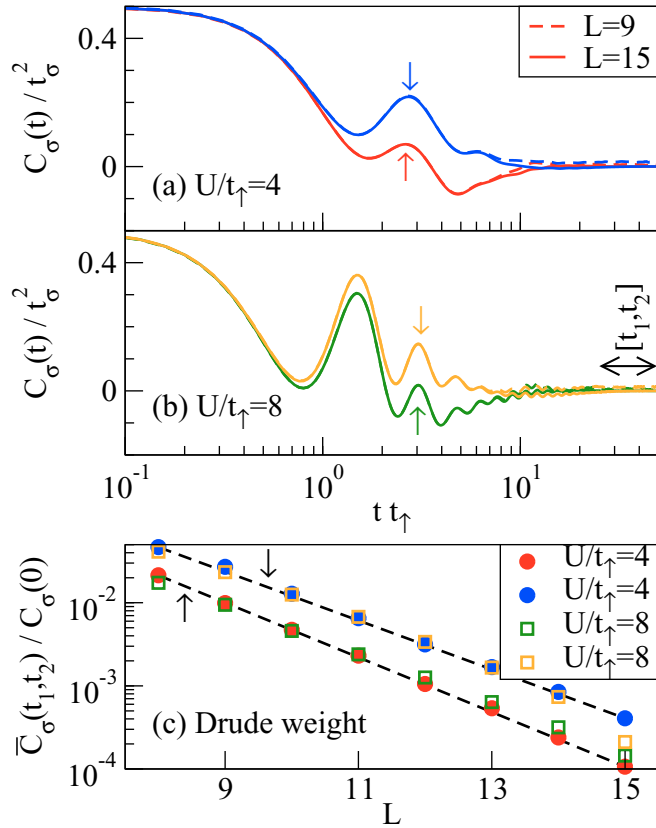


FIG. 9. (Color online) Real-time decay of the current autocorrelation function $C_\sigma(t)$ for (a) $U/t_\uparrow = 4$, (b) $U/t_\uparrow = 8$ for $\eta = t_\downarrow/t_\uparrow = 0.4$, both components $\sigma = \uparrow, \downarrow$, two $L = 9, 15$, and high temperatures $\beta t_\uparrow \rightarrow 0$. (c) Finite-size scaling of the Drude weight $\bar{C}_\sigma(t_1, t_2)$, as extracted from the time interval $[t_1 t_\uparrow, t_2 t_\uparrow] = [25, 50]$, in a semi-log plot. As a guide to the eyes, exponentials (dashed lines) are indicated.

transformation. While Figs. 8(a) and 8(b) differ with respect to details, the overall structure does not depend on the specific choice of t_{\max} . In particular, the limit $\omega \rightarrow 0$ is consistent with a vanishing dc conductivity. Note that this limit coincides with $D_\uparrow(t)$ evaluated at $t t_\uparrow = 25$ and 50 , respectively. Similarly, our results indicate a vanishing dc conductivity for $U/t_\uparrow = 8$, as shown in Fig. 8(c). The small negative spectral weight is an artifact of the finite-time Fourier transform used and depends on the specific choice of t_{\max} .

To summarize, our $\beta t_\uparrow \rightarrow 0$ results are consistent with the interpretation of the model in terms of the single-particle, Anderson problem in one spatial dimension.

B. Intermediate imbalance

Next we discuss the region $0 < \eta < 1$, where the model still is nonintegrable but the interpretation of the model in terms of the single-particle Anderson problem is not possible any more. In fact, in this η region, we deal with a many-particle problem.

We start with intermediate imbalance $\eta = 0.4$. In Fig. 9(a) we depict our results for the time-dependent current autocorrelation function $C_\sigma(t)$ for the light ($\sigma = \uparrow$) and the heavy ($\sigma = \downarrow$) component for $U/t_\uparrow = 4$ and $L = 9, 15$, still in the high-temperature limit $\beta t_\uparrow \rightarrow 0$. In Fig. 9(b) we additionally

show results for $U/t_\uparrow = 8$. For both components, $C_\sigma(t)$ decays fast on a time scale $t t_\uparrow \sim 1$ but revivals appear afterward. While these revivals are equally pronounced for $\sigma = \uparrow$ and \downarrow , only $C_\uparrow(t)$ becomes negative in the time interval $t t_\uparrow \sim 2.5$. However, any revivals eventually disappear and $C_\sigma(t)$ decays fully to approximately zero for $\sigma = \uparrow$ and \downarrow . When comparing curves for $L = 9$ and 15 , it is also evident that finite-size effects are small on the physically relevant time scale. Thus, we are able to obtain information on $C_\sigma(t)$ in the thermodynamic limit $L \rightarrow \infty$ without invoking intricate extrapolations.

It is also evident from Figs. 9(a) and 9(b) that Drude weights D_σ are small, i.e., there is no long-time saturation of $C_\sigma(t)$ at a significant positive value. However, it is instructive to discuss the actual value of the Drude weights in more detail. In Fig. 9(c) we show the finite-size scaling of $\bar{C}_\sigma(t_1, t_2)$, as extracted from the time interval $[t_1 t_\uparrow, t_2 t_\uparrow] = [25, 50]$, for $\sigma = \uparrow, \downarrow$ and $U/t_\uparrow = 4, 8$ in a semi-log plot. Interestingly, \bar{C}_σ is larger for $\sigma = \downarrow$ and does not depend on U . In all cases, the finite-size scaling of \bar{C}_σ is remarkably well described by a simple exponential decrease over three orders of magnitude, with a relative value $\bar{C}_\sigma/C_\sigma(0) < 10^{-3}$ at $L = 15$. This exponential decrease is expected for strongly nonintegrable models [47,56] and, moreover, is in accord with the eigenstate thermalization hypothesis [50,57].

Since finite-size effects are small and $C_\sigma(t)$ decays to approximately zero, we can accurately determine the optical conductivity by Fourier transforming data for finite L and t . In Figs. 10(a) and 10(b) we show the finite-time optical conductivity $\text{Re } \sigma_\sigma(\omega)$ at $U/t_\uparrow = 8$ for the light and heavy component, respectively. As expected, $\text{Re } \sigma_\sigma(\omega)$ does neither depend on t_{\max} nor L and is a smooth function of frequency ω . Similarly to the integrable case $\eta = 0$, we find a broad maximum at $\omega/t_\uparrow \sim U/t_\uparrow$ for both σ . In contrast, the position of the additional peak at low ω depends on σ but is roughly independent of U , as shown in Fig. 10(c). Most importantly, the dc conductivity is finite and its actual value is, relative to the amplitude of the low- ω peak, larger for the heavy component $\sigma = \downarrow$. As a function of U , this dc conductivity decreases but is still finite for all U depicted; see Fig. 10(c). Therefore, at $\eta = 0.4$, we can exclude the existence of an insulator in the high-temperature limit $\beta t_\uparrow \rightarrow 0$.

C. Scaling of diffusion constant and dc conductivity

We eventually discuss the scaling of transport coefficients as a function of imbalance $\eta = t_\downarrow/t_\uparrow$. For the η discussed below, extracting the dc conductivity $\sigma_{\sigma, \text{dc}}$ as $\text{Re } \sigma_\sigma(\omega \rightarrow 0)$ for finite L is equivalent to determining the plateau value of the time-dependent diffusion constant $\mathcal{D}_\sigma(t)$. Therefore, we focus on an analysis of $\mathcal{D}_\sigma(t)$, which can be concisely summarized for various η .

In Fig. 11(a) we show the time-dependent diffusion constant $\mathcal{D}_\uparrow(t)$ of the light component for different $\eta = 0.7, \dots, 0.2$, a single $U/t_\uparrow = 8$, and fixed system size $L = 14$. In Fig. 11(b) we show $\mathcal{D}_\downarrow(t)$ of the heavy component for the same set of parameters. Several comments are in order. First, for both $\sigma = \uparrow, \downarrow$, a plateau of $\mathcal{D}_\sigma(t)$ is clearly visible at times $t t_\uparrow \sim 15$ for imbalances $0.3 \leq \eta \leq 0.6$. We have checked that the plateau values $\mathcal{D}_\sigma \chi$ coincide with the dc conductivity $\sigma_{\sigma, \text{dc}}$, cf. Fig. 10 for $\eta = 0.4$, even though not shown explicitly for all

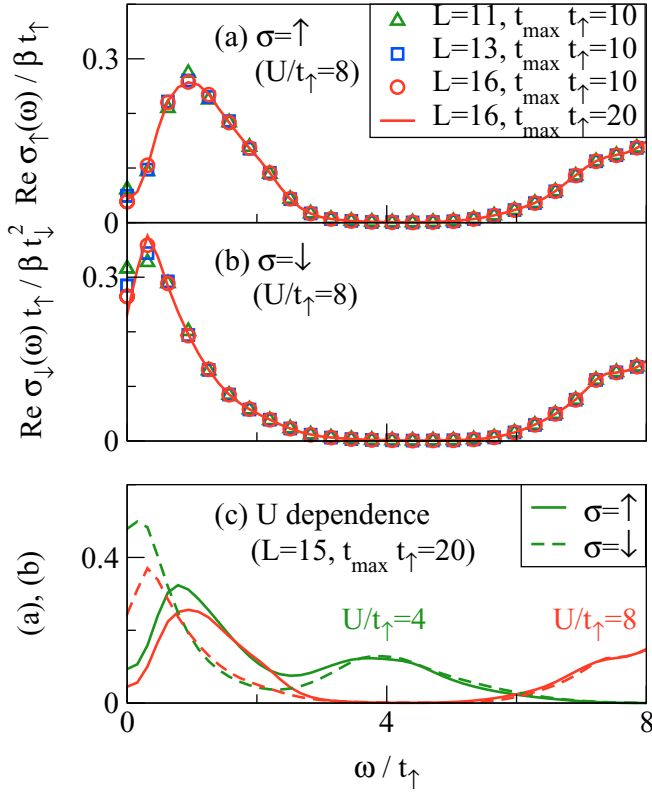


FIG. 10. (Color online) Frequency dependence of the optical conductivity $\text{Re } \sigma_\sigma(\omega)$ for the (a) light component $\sigma = \uparrow$, (b) heavy component $\sigma = \downarrow$ for $U/t_\uparrow = 8$, $\eta = t_\downarrow/t_\uparrow = 0.4$, and high temperatures $\beta t_\uparrow \rightarrow 0$, as resulting from different $L = 11, 13, 16$ and $t_{\max} t_\uparrow = 10, 20$. The independence of L and t_{\max} is evident. (c) U dependence of $\text{Re } \sigma_\sigma(\omega)$ for a large $L = 15$ and long $t_{\max} t_\uparrow = 20$. A peak at $\omega/t_\uparrow = U/t_\uparrow$ is clearly visible.

η . Second, for $\eta > 0.6$, $\mathcal{D}_\sigma(t) \propto D_\sigma t$ due to strong finite-size Drude weights D_σ in the vicinity of the integrable point $\eta = 1$; cf. Fig. 6. These finite-size effects prevent us from determining the diffusion constant in the thermodynamic limit $L \rightarrow \infty$. Third, for $\eta < 0.3$, $\mathcal{D}_\uparrow(t)$ of the light component develops the small oscillations around zero discussed in the context of the Falicov-Kimball limit $\eta = 0$. These oscillations prevent us from determining the diffusion constant with sufficiently high accuracy. Fourth, $\mathcal{D}_\uparrow(t)$ is much more sensitive to varying η than $\mathcal{D}_\downarrow(t)$. Note, however, that we depict $\mathcal{D}_\downarrow(t)/t_\downarrow^2$ rather than $\mathcal{D}_\downarrow(t)$. In this way, we do not show the trivial scaling $\mathcal{D}_\downarrow(t) \propto t_\downarrow^2$ resulting from the static scaling of the current operator $j_\downarrow \propto t_\downarrow$.

In Fig. 11(c) we depict the η dependence of the plateau values \mathcal{D}_σ , visible for $L = 14$, in a semi-log plot. While we find $\mathcal{D}_\downarrow/t_\downarrow^2 \approx \text{const.}$, we observe a decrease of \mathcal{D}_\uparrow as η decreases, consistent with a simple exponential function. If we assume that this scaling continues to small η beyond the η range accessible, this assumption would imply the absence of a diffusion-localization transition at $\eta \neq 0$, consistent with the conclusions of [63]. However, based on our results in Fig. 11(c), we cannot exclude the onset of many-body localization and a sudden drop of \mathcal{D}_\uparrow to zero at finite but small η , as suggested in previous works [60,61]. Nevertheless,

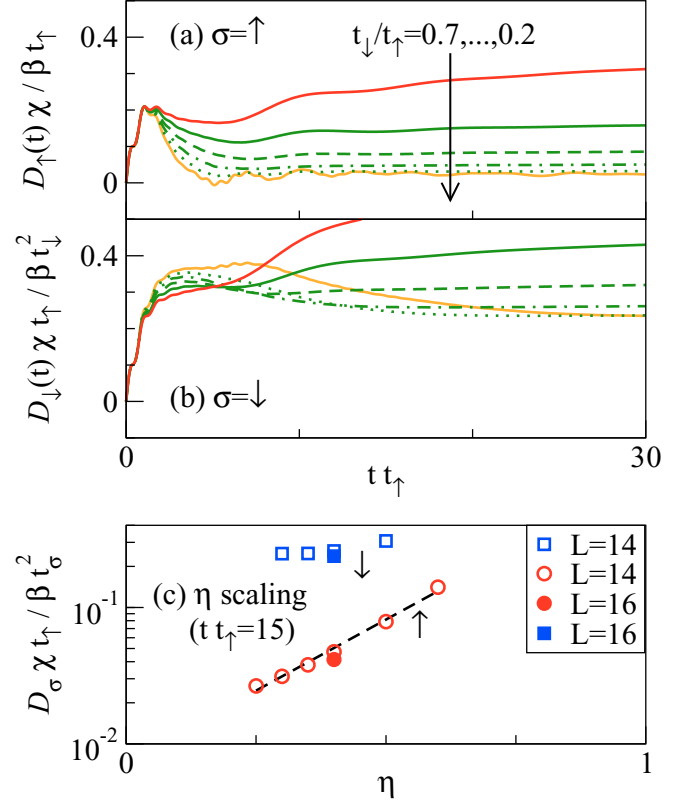


FIG. 11. (Color online) Time dependence of the diffusion constant $\mathcal{D}_\sigma(t)$ for (a) $\sigma = \uparrow$, (b) $\sigma = \downarrow$ for various $\eta = t_\downarrow/t_\uparrow = 0.7, \dots, 0.2$, a single $U/t_\uparrow = 8$, fixed $L = 14$, and high temperature $\beta t_\uparrow \rightarrow 0$. Apparently, $\mathcal{D}_\uparrow(t)$ is very sensitive to varying η , in contrast to $\mathcal{D}_\downarrow(t)$. For imbalance $\eta \leq 0.6$, a plateau of $\mathcal{D}_\sigma(t)$ already can be seen for the L depicted. (c) η scaling of the plateau value for both components, as extracted at the point $t t_\uparrow = 15$, in a semi-log plot. As a guide to the eyes, an exponential (dashed line) is indicated. Note that $\mathcal{D}_\sigma \chi = \sigma_{\sigma, \text{dc}}$.

we can constrain the existence of a possibly localized regime to $\eta \ll 0.25$.

VI. SUMMARY AND OUTLOOK

In this work we studied finite-temperature charge transport in the one-dimensional repulsive Hubbard model at half filling. Using the method of dynamical quantum typicality, we were able to access system sizes much larger than what can be reached with full exact diagonalization, and with no restriction on the accessible time scales. This allowed us to extract the finite-size dependent Drude weight from the time dependence of current autocorrelation functions. The analysis of the finite-size dependencies indicated a vanishing Drude weight in the thermodynamic limit, in agreement with [25]. We further computed the optical conductivity and provided evidence that it is (i) a smooth function of ω at low frequencies and in the thermodynamic limit and (ii) that the dc conductivity is indeed finite, the latter in agreement with [26].

As an example of a nonintegrable model, we considered the mass-imbalanced Hubbard chain. This model has recently been discussed in the context of many-body localization in

translationally invariant systems [60,61,63]. We demonstrated the absence of a Drude weight for large L , as expected for a nonintegrable system. Our results for inverse mass ratios of $\eta \gtrsim 0.25$ indicated a small dc conductivity, that appears to vanish exponentially fast as a function of decreasing η . At intermediate η , the system is thus a normal diffusive conductor, while at small η , the emergence of small long-time oscillations in the current autocorrelation function give rise to slightly anomalous transport, in line with the conclusions of Ref. [63].

Extensions of our work comprise the study of finite-temperature charge and spin transport in one-dimensional strongly correlated electron systems. For instance, there is an intriguing prediction on the role of spin drag in one dimension, which has been claimed to give rise to diffusive spin transport, while charge transport remains ballistic at finite temperature

[87]. Such questions as well as other effects due to a coupling of the various transport channels in the Hubbard model and its variants constitute a rich playground for future work.

ACKNOWLEDGMENTS

We thank C. Karrasch for sending us tDMRG data and very helpful comments. We gratefully acknowledge the computing time granted by the JARA-HPC Vergabegremium and provided on the JARA-HPC Partition part of the supercomputer JUQUEEN at Forschungszentrum Jülich. R.S. thanks the Arnold-Sommerfeld-Center for Theoretical Physics, LMU Munich, for its kind hospitality. This work was also supported in part by National Science Foundation Grant No. PHYS-1066293 and the hospitality of the Aspen Center for Physics.

-
- [1] E. Dagotto, *Rev. Mod. Phys.* **66**, 763 (1994).
 - [2] P. A. Lee, N. Nagaosa, and X.-G. Wen, *Rev. Mod. Phys.* **78**, 17 (2006).
 - [3] T. Esslinger, *Annu. Rev. Condens. Matt. Phys.* **1**, 129 (2010).
 - [4] F. H. L. Essler, H. Frahm, F. Göhmann, A. Klümper, and V. E. Korepin, *The One-Dimensional Hubbard Model* (Cambridge University Press, Cambridge, 2005).
 - [5] D. Jerome, *Chem. Rev.* **104**, 5565 (2004).
 - [6] V. Vescoli, L. Degiorgi, W. Henderson, G. Grüner, K. P. Starkey, and L. K. Montgomery, *Science* **21**, 1155 (1998).
 - [7] T. Hasegawa, S. Kagoshima, T. Mochida, S. Sugiura, and Y. Iwasa, *Solid State Commun.* **103**, 489 (1997).
 - [8] R. Claessen, M. Sing, U. Schwingenschlög, P. Blaha, M. Dressel, and C. S. Jacobsen, *Phys. Rev. Lett.* **88**, 096402 (2002).
 - [9] S. Wall, D. Brida, S. R. Clark, H. P. Ehrke, D. Jaksch, A. Ardavan, S. Bonora, H. Uemura, Y. Takahashi, T. Hasegawa, H. Okamoto, G. Cerullo, and A. Cavalleri, *Nature Phys.* **7**, 114 (2011).
 - [10] M. Bockrath, D. H. Cobden, J. Lu, A. G. Rinzler, R. E. Smalley, L. Balents, and P. L. McEuen, *Nature (London)* **397**, 598 (1999).
 - [11] H. Ishii, H. Kataura, H. Shiozawa, H. Yoshioka, H. Otsubo, Y. Takayama, T. Miyahara, S. Suzuki, Y. Achiba, M. Nakatake, T. Narimura, M. Higashiguchi, K. Shimada, H. Namatame, and M. Taniguchi, *Nature (London)* **426**, 540 (2003).
 - [12] V. V. Deshpande, B. Chandra, R. Caldwell, D. Novikov, J. Hone, and M. Bockrath, *Science* **323**, 106 (2009).
 - [13] D. Pertot, A. Sheikhan, E. Cocchi, L. A. Miller, J. E. Bohn, M. Koschorreck, M. Köhl, and C. Kollath, *Phys. Rev. Lett.* **113**, 170403 (2014).
 - [14] U. Schneider, L. Hackermüller, J. P. Ronzheimer, S. Will, S. Braun, T. Best, I. Bloch, E. Demler, S. Mandt, D. Rasch, and A. Rosch, *Nature Phys.* **8**, 213 (2012).
 - [15] X. Zotos and P. Prelovšek, *Strong Interactions in Low Dimensions*, edited by D. Baeriswyl and L. Degiorgi (Kluwer Academic Publishers, Dordrecht, 2004), pp. 347–382.
 - [16] F. Heidrich-Meisner, A. Honecker, and W. Brenig, *Eur. J. Phys. Special Topics* **151**, 135 (2007).
 - [17] S. Kirchner, H. G. Evertz, and W. Hanke, *Phys. Rev. B* **59**, 1825 (1999).
 - [18] X. Zotos, F. Naef, and P. Prelovšek, *Phys. Rev. B* **55**, 11029 (1997).
 - [19] C. Karrasch, D. M. Kennes, and F. Heidrich-Meisner, *arXiv:1506.05788*.
 - [20] T. Prosen, *Phys. Rev. Lett.* **106**, 217206 (2011).
 - [21] T. Prosen and E. Ilievski, *Phys. Rev. Lett.* **111**, 057203 (2013).
 - [22] M. Mierzejewski, P. Prelovšek, and T. Prosen, *Phys. Rev. Lett.* **114**, 140601 (2015).
 - [23] S. Fujimoto and N. Kawakami, *J. Phys. A: Math. Gen.* **31**, 465 (1997).
 - [24] N. M. R. Peres, R. G. Dias, P. D. Sacramento, and J. M. P. Carmelo, *Phys. Rev. B* **61**, 5169 (2000).
 - [25] J. M. P. Carmelo, S.-J. Gu, and P. Sacramento, *Annals of Physics* **339**, 484 (2013).
 - [26] C. Karrasch, D. M. Kennes, and J. E. Moore, *Phys. Rev. B* **90**, 155104 (2014).
 - [27] X. Zotos and P. Prelovšek, *Phys. Rev. B* **53**, 983 (1996).
 - [28] B. N. Narozhny, A. J. Millis, and N. Andrei, *Phys. Rev. B* **58**, R2921 (1998).
 - [29] F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, *Phys. Rev. B* **68**, 134436 (2003).
 - [30] J. Herbrych, P. Prelovšek, and X. Zotos, *Phys. Rev. B* **84**, 155125 (2011).
 - [31] C. Karrasch, J. H. Bardarson, and J. E. Moore, *Phys. Rev. Lett.* **108**, 227206 (2012).
 - [32] C. Karrasch, J. Hauschild, S. Langer, and F. Heidrich-Meisner, *Phys. Rev. B* **87**, 245128 (2013).
 - [33] R. Steinigeweg, J. Gemmer, and W. Brenig, *Phys. Rev. Lett.* **112**, 120601 (2014).
 - [34] X. Zotos, *Phys. Rev. Lett.* **82**, 1764 (1999).
 - [35] J. Benz, T. Fukui, A. Klümper, and C. Scheeren, *J. Phys. Soc. Jpn. Suppl.* **74**, 181 (2005).
 - [36] M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, *Phys. Rev. Lett.* **98**, 050405 (2007).
 - [37] M. Mierzejewski, P. Prelovšek, and T. Prosen, *Phys. Rev. Lett.* **113**, 020602 (2014).
 - [38] P. Prelovšek, S. El Shawish, X. Zotos, and M. W. Long, *Phys. Rev. B* **70**, 205129 (2004).
 - [39] R. Steinigeweg and W. Brenig, *Phys. Rev. Lett.* **107**, 250602 (2011).
 - [40] R. Steinigeweg, J. Herbrych, P. Prelovšek, and M. Mierzejewski, *Phys. Rev. B* **85**, 214409 (2012).
 - [41] T. Giamarchi, *Phys. Rev. B* **44**, 2905 (1991).

- [42] J. Sirker, R. G. Pereira, and I. Affleck, *Phys. Rev. Lett.* **103**, 216602 (2009).
- [43] J. Sirker, R. G. Pereira, and I. Affleck, *Phys. Rev. B* **83**, 035115 (2011).
- [44] G. Uhrig and D. Vollhardt, *Phys. Rev. B* **52**, 5617 (1995).
- [45] T. Prosen, *Phys. Rev. E* **89**, 012142 (2014).
- [46] T. Prosen and M. Žnidarič, *Phys. Rev. B* **86**, 125118 (2012).
- [47] R. Steinigeweg, F. Heidrich-Meisner, J. Gemmer, K. Michielsen, and H. De Raedt, *Phys. Rev. B* **90**, 094417 (2014).
- [48] R. Steinigeweg, J. Gemmer, and W. Brenig, *Phys. Rev. B* **91**, 104404 (2015).
- [49] R. Steinigeweg, J. Herbrych, X. Zotos, and W. Brenig, [arXiv:1503.03871](https://arxiv.org/abs/1503.03871).
- [50] R. Steinigeweg, J. Herbrych, and P. Prelovšek, *Phys. Rev. E* **87**, 012118 (2013).
- [51] J. V. Alvarez and C. Gros, *Phys. Rev. Lett.* **89**, 156603 (2002).
- [52] X. Zotos, *Phys. Rev. Lett.* **92**, 067202 (2004).
- [53] P. Jung, R. W. Helmes, and A. Rosch, *Phys. Rev. Lett.* **96**, 067202 (2006).
- [54] M. Žnidarič, *Phys. Rev. Lett.* **110**, 070602 (2013).
- [55] M. Žnidarič, *Phys. Rev. B* **88**, 205135 (2013).
- [56] F. Heidrich-Meisner, A. Honecker, D. C. Cabra, and W. Brenig, *Phys. Rev. Lett.* **92**, 069703 (2004).
- [57] W. Beugeling, R. Moessner, and M. Haque, *Phys. Rev. E* **89**, 042112 (2014).
- [58] R. Vosk and E. Altman, *Annu. Rev. Condens. Matter Phys.* **6**, 383 (2015).
- [59] R. Nandikishore and D. Huse, *Annu. Rev. Condens. Matter Phys.* **6**, 15 (2015).
- [60] M. Schiulaz and M. Müller, *AIP Conf. Proc.* **1610**, 11 (2014).
- [61] T. Grover and M. P. A. Fisher, *J. Stat. Mech.* (2014) P10010.
- [62] W. De Roeck and F. Huveneers, *Commun. Math. Phys.* **332**, 1017 (2014).
- [63] N. Y. Yao, C. R. Laumann, J. I. Cirac, M. D. Lukin, and J. E. Moore, [arXiv:1410.7407](https://arxiv.org/abs/1410.7407).
- [64] R. Steinigeweg and J. Gemmer, *Phys. Rev. B* **80**, 184402 (2009).
- [65] S. Langer, F. Heidrich-Meisner, J. Gemmer, I. P. McCulloch, and U. Schollwöck, *Phys. Rev. B* **79**, 214409 (2009).
- [66] S. Langer, M. Heyl, I. P. McCulloch, and F. Heidrich-Meisner, *Phys. Rev. B* **84**, 205115 (2011).
- [67] C. Karrasch, J. E. Moore, and F. Heidrich-Meisner, *Phys. Rev. B* **89**, 075139 (2014).
- [68] C. Bartsch and J. Gemmer, *Phys. Rev. Lett.* **102**, 110403 (2009).
- [69] C. Bartsch and J. Gemmer, *Europhys. Lett.* **96**, 60008 (2011).
- [70] J. Gemmer and G. Mahler, *Eur. Phys. J. B* **31**, 249 (2003).
- [71] S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghì, *Phys. Rev. Lett.* **96**, 050403 (2006).
- [72] P. Reimann, *Phys. Rev. Lett.* **99**, 160404 (2007).
- [73] S. Popescu, A. J. Short, and A. Winter, *Nature Phys.* **2**, 754 (2006).
- [74] S. R. White, *Phys. Rev. Lett.* **102**, 190601 (2009).
- [75] S. Sugiura and A. Shimizu, *Phys. Rev. Lett.* **108**, 240401 (2012).
- [76] A. Hams and H. De Raedt, *Phys. Rev. E* **62**, 4365 (2000).
- [77] T. A. Elsayed and B. V. Fine, *Phys. Rev. Lett.* **110**, 070404 (2013).
- [78] K. De Raedt, K. Michielsen, H. De Raedt, B. Trieu, G. Arnold, M. Richter, T. Lippert, H. Watanabe, and N. Ito, *Comput. Phys. Commun.* **176**, 121 (2007).
- [79] F. Jin, H. De Raedt, S. Yuan, M. I. Katsnelson, S. Miyashita, and K. Michielsen, *J. Phys. Soc. Jpn.* **79**, 124005 (2010).
- [80] J. M. Deutsch, *Phys. Rev. A* **43**, 2046 (1991).
- [81] M. Srednicki, *Phys. Rev. E* **50**, 888 (1994).
- [82] M. Rigol, V. Dunjko, and M. Olshanii, *Nature (London)* **452**, 854 (2008).
- [83] V. Alba, *Phys. Rev. B* **91**, 155123 (2015).
- [84] C. Karrasch, D. M. Kennes, and F. Heidrich-Meisner, *Phys. Rev. B* **91**, 115130 (2015).
- [85] P. de Vries, K. Michielsen, and H. De Raedt, *Z. Phys. B* **92**, 353 (1993).
- [86] P. de Vries, K. Michielsen, and H. De Raedt, *Z. Phys. B* **95**, 475 (1994).
- [87] M. Polini and G. Vignale, *Phys. Rev. Lett.* **98**, 266403 (2007).