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Ballistic transport in the one-dimensional Hubbard model: The hydrodynamic approach

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We outline a general formalism of hydrodynamics for quantum systems with multiple particle species which undergo completely elastic scattering. In the thermodynamic limit, the complete kinematic data of the problem consist of the particle content, the dispersion relations, and a universal dressing transformation which accounts for interparticle interactions. We consider quantum integrable models and we focus on the one-dimensional fermionic Hubbard model. By linearizing hydrodynamic equations, we provide exact closed-form expressions for Drude weights, generalized static charge susceptibilities, and charge-current correlators valid on the hydrodynamic scale, represented as integral kernels operating diagonally in the space of mode numbers of thermodynamic excitations. We find that, on hydrodynamic scales, Drude weights manifestly display Onsager reciprocal relations even for generic (i.e., noncanonical) equilibrium states, and establish a generalized detailed balance condition for a general quantum integrable model. We present exact analytic expressions for the general Drude weights in the Hubbard model, and explain how to reconcile different approaches for computing Drude weights from the previous literature.

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In the past few years, a lot of interest has been devoted to studying various paradigms of nonergodic many-body physics, such as quantum quenches, equilibration to generalized Gibbs ensembles, and the phenomenon of prethermalization [1–3]. One of the prominent recent results is the formalism of generalized hydrodynamics developed in Refs. [4,5], with a large number of subsequent studies investigating its various aspects and applications [6–13], including the exact computation of Drude weights in the Heisenberg model XXZ spin-$\frac{1}{2}$ chain [14]. In analogy to the conventional theory of hydrodynamics [15], the authors of Ref. [16] just recently obtained a closed formula for Drude weights expressed in terms of local equilibrium state functions for the case of an integrable Bose gas (Lieb-Liniger model) and conjectured that similar formulas may hold in quantum integrable models more generally. In this Rapid Communication, we go a step further and extend the formalism to integrable models which possess physical particles with internal degrees of freedom and are solvable by a *nested Bethe ansatz*. Nesting refers to the situation when physical degrees of freedom are associated with a higher rank symmetry group, leading to eigenfunctions with a hierarchical structure of internal quantum numbers and elementary excitations of different flavors. While studies of such models has been traditionally focused on the Gibbs equilibrium [17–22], they have also been recently studied in the nonequilibrium context [23,24].

The chief aspect in which interacting quantum integrable theories differ from widely studied noninteracting systems is the dressing of (quasi)particle excitations, i.e., a process in which the bare properties of particle-hole type excitations renormalize in the presence of interactions with a nontrivial reference (vacuum) state. The task of classifying excitations has been traditionally restricted to ground states for some of the simplest Bethe ansatz solvable models [25], and subsequently extended to some important examples of exactly solvable models of correlated electrons [19,20,26,27]. A comprehensive exposition of the dressing formalism for grand canonical ensembles in nested Bethe ansatz models can be found in Ref. [27].

Dressing formalism. Integrable theories exhibit a completely elastic (factorizable) scattering of particlelike excitations [28]. The properties of such excitations represent the *kinematic data* of the theory. In particular, in Bethe ansatz solvable models (see, e.g., Refs. [20,25]) thermodynamic excitations relative to a bare vacuum [29] can be inferred from the solutions to (nested) Bethe equations. The latter in a finite volume take the form $e^{ip_\alpha(u_k^{(\alpha)})}\prod_\beta\prod_{j=1}^{N_\beta}S_{\alpha\beta}(u_k^{(\alpha)},u_j^{(\beta)})=1$, imposing a single-valuedness of many-body eigenstates. Here, the sets of quantum numbers $\{u_k^{(\alpha)}\}$ are called the Bethe roots and represent rapidity variables for distinct species (or flavors) of elementary excitations. The number and types of excitations depend on the model and can be inferred with the aid of the representation theory of the underlying quantized Lie (super)algebra. Elementary excitations typically form complexes which are interpreted as bound states. The emergent thermodynamic particle content, which can be inferred by, e.g., analyzing the $L\to\infty$ limit of Bethe equations, is generally different from elementary excitations and is labeled by a pair of *mode numbers*, a particle type index a and a real rapidity variable u. The complete kinematic data are obtained from the bare momenta $k_a(u)$ and energies $e_a(u)$, and interparticle scattering phase shifts $\phi_{ab}(u,w)$. Once given these functions, no explicit operator representation of the Hamiltonian and its conservation laws is ever required. Here, we present the details of the entire formalism for the nontrivial case of the (fermionic) Hubbard model.

A distinguished feature of integrable systems is a macroscopic number of local conservation laws which can be formally expressed in terms of a discrete basis of local charges $Q_i=\sum_x q_i(x)$, with x labeling lattice sites. The associated currents $J_i=\sum_x j_i(x)$ are defined with the aid of the continuity equation, $\partial_t\hat{Q}_i+\partial_x\hat{J}_i=0$. The key concept of the hydrodynamic approach is the dressing of bare energies

$e_a \mapsto \varepsilon_a$ and momenta $k_a \mapsto p_a$ of particle excitations, which can be presented in a compact form,

$$\varepsilon'_a = \Omega_{ab} \star e'_b, \quad p'_a = \Omega_{ab} \star k'_b, \tag{1}$$

with convolution $(\Omega_{ab} \star f_b)(u) = \sum_b \int dw\, \Omega_{ab}(u,w) f_b(w)$. In interacting quantum integrable models solvable by a (nested) Bethe ansatz, the matrix convolution kernel Ω takes a *universal form*,

$$(\Omega^{-1})_{ab}(u,w) = \delta_{ab}\delta(u-w) + K_{ab}(u-w)\vartheta_b(w)\sigma_b, \tag{2}$$

with kernels $K_{ab}(u,w)$ defined as derivatives of the scattering phase shifts $\phi_{ab}(u,w) = \phi_{ab}(u-w)$, $K_{ab}(u) = \frac{1}{2\pi i}\partial_u \phi_{ab}(u)$, and $\sigma_a = \mathrm{sgn}[k'_a(u)]$. The (Fermi) filling functions $\vartheta_a(u)$ specify the fraction of occupied modes with rapidities inside a small interval around u.

The dispersion relations of excitations $\varepsilon_a(u)$ depend on a many-body vacuum which is uniquely specified by the rapidity distributions $\rho_a(u)$. In terms of (thermodynamic) particle excitations, the equilibrium averages of charge and current densities decompose as $q_i = \sum_a \int du\, q_{i,a}(u)\rho_a(u)$, $j_i = \sum_a \int du\, q_{i,a}(u) j_a(u)$, where $j_a(u) = \rho_a(u) v_a^{\mathrm{dr}}(u)$ are the current densities per mode [4,5]. The group velocities of propagating particles are thus state dependent, $v_a^{\mathrm{dr}}(u) = \varepsilon'_a(u)/p'_a(u)$.

We furthermore introduce the *effective charges* as the bare charges renormalized under transformation Ω, namely, the effective value of a local charge density q_i is obtained as

$$q_{a,i}^{\mathrm{eff}} = \Omega_{ab} \star q_{b,i} = \partial_{\mu_i} \log\left(\vartheta_a^{-1} - 1\right). \tag{3}$$

Here, the parameters μ_i are the chemical potentials of a local (generalized) equilibrium ensemble parametrized as $\hat{\varrho} \simeq \exp(-\sum_i \mu_i \hat{Q}_i)$ [30–32]. It is important to emphasize that despite the derivatives of dressed energies satisfying $\varepsilon'_a = \Omega_{ab} \star e'_b = (e'_a)^{\mathrm{eff}}$, the effective charges are *not* the proper dressed charges associated with an excitation, and specifically $\varepsilon_a \neq e_a^{\mathrm{eff}}$. We moreover note that with the aid of fusion identities among the scattering kernels, the transformation (2) can be decoupled to a quasilocal form in the mode space [cf. the Supplemental Material (SM) [33] for the explicit form for the Hubbard model].

Drude weights. In this Rapid Communication, we shall mainly be concerned with general off-diagonal Drude weights

$$\mathcal{D}^{(i,j)} = \frac{\beta}{2} \lim_{t\to\infty} \int_{\tau=0}^{t} d\tau \langle \hat{J}_i(\tau)\hat{j}_j(0)\rangle_{\mathrm{c}}, \tag{4}$$

which represent the magnitudes of the singular parts of the zero-frequency generalized conductivities [34,35], $\mathrm{Re}\,\sigma_{ij}(\omega) = 2\pi\,\mathcal{D}^{(i,j)}\delta(\omega) + \sigma_{ij}^{\mathrm{reg}}(\omega)$. We use $\langle\cdot\rangle_{\mathrm{c}}$ to denote the connected part of the equilibrium expectation values. Although we shall restrict ourselves to grand canonical equilibria, our formalism applies (without modifications) to general local equilibrium states.

An exact representation for $\mathcal{D}^{(i,j)}$ can be given in terms of the static covariance matrix $\mathcal{C}$, $\mathcal{C}_{ij} = \langle Q_i q_j\rangle_{\mathrm{c}}$, with diagonal components $\chi_i = \mathcal{C}_{ii}$ representing (generalized) static susceptibilities, and charge-current correlators (overlaps) $\mathcal{O}$, $\mathcal{O}_{ij} = \langle Q_i j_j\rangle_{\mathrm{c}}$. Explicit expressions in terms of thermodynamic state functions can be found in Ref. [33]. The time-averaged current-current correlator Eq. (4) can be projected onto the subspace formed by local conserved quantities which yields the well-known Mazur-Suzuki equality [36,37] and proves useful for bounding dynamical susceptibilities [38]. In matrix notation the latter reads $\mathcal{D}^{(i,j)} = \frac{\beta}{2}\mathcal{O}_{ik}(\mathcal{C}^{-1})_{kl}\mathcal{O}_{lj}$ [39].

A central result of our work is that on the hydrodynamic scale, static charge-charge, charge-current correlations, and generic Drude weights all assume a universal mode decomposition (writing formally $\mathcal{A} \in \{\mathcal{C},\mathcal{D},\mathcal{O}\}$),

$$\mathcal{A}_{ij} = \sum_a \int du\, q_{a,i}^{\mathrm{eff}}(u) A_a(u) q_{a,j}^{\mathrm{eff}}(u), \tag{5}$$

which has exactly the same form as in the case of a single-component interacting integrable Bose gas derived in a recent paper [16]. Importantly, in the above formula the kernels $A_a(u)$ and effective charges $q_{a,i}^{\mathrm{eff}}$ are expressible in terms of the properties of equilibrium states which can be efficiently computed within the thermodynamic Bethe ansatz (TBA) method [40–42]. It is noteworthy that Eq. (5) is written solely in the mode space, i.e., it acts (diagonally) on particle labels and rapidities, and that no explicit knowledge of a complete set of local charges is ever required in a computation. Indeed, the thermodynamic expectation values of local charges are expressible as *linear* functionals of particles' rapidity distributions (see, e.g., Refs. [32,43]) which are a natural extension of momentum distribution functions of free theories [44].

Linearized hydrodynamics. The hydrodynamic approach [4,5] is based on the notion of local quasistationary states, characterized by the local continuity equation in the mode space $\partial_t \rho_a(u) + \partial_x j_a(u) = 0$. In the simplest scenario, one can think of a quantum quench in which an inhomogeneous initial state is initialized as two homogeneous equilibrated macroscopic regions brought in contact at $t = 0$ (see Refs. [45–47]). In such a scenario, an emergent nonequilibrium state remains confined to the light cone region determined by the particles' dressed velocities, leading eventually to a quasistationary state which depends on the ray coordinate $\zeta = x/t$ and is determined by the condition of the vanishing convective derivative $[\partial_t + v_a^{\mathrm{dr}}(u)\partial_x]\vartheta_a(u) = 0$.

The setting proves particularly useful for studying nonequilibrium transport properties and, in particular, the computation of Drude weights. The latter can be conveniently defined as asymptotic current rates in the limit of vanishing bias $\delta\mu_j$ (while keeping other chemical potentials fixed),

$$\mathcal{D}^{(i,j)} = \frac{\beta}{2} \lim_{\delta\mu_j\to 0} \frac{\partial}{\partial\,\delta\mu_j} \lim_{t\to\infty} \frac{J_i(t)}{t}. \tag{6}$$

The above prescription has been initially used in Ref. [50] and employed in a recent numerical study [48], while an analogous formula already appeared in an earlier work [39]. Equation (6) has been recently evaluated in Refs. [14,51] using the hydrodynamic approach, transforming it first in the light cone coordinates, $\mathcal{D}^{(i,j)} = (\beta/2)\lim_{\delta\mu_j\to 0}\int d\zeta\, \partial j_i(\zeta)/\partial\delta\mu_j$, and then computing quasistationary currents which are generated by joining together two nearly identical equilibrium states, i.e., imposing a small chemical potential drop at the origin $\mu_i^{\mathrm{L}} = \mu_i + \delta\mu_i/2$ and $\mu_i^{\mathrm{R}} = \mu_i - \delta\mu_i/2$. Here, $\delta\mu_i$ has the role of a thermodynamic force, e.g., to study energy transport we identify $\mu_e = \beta$.

Just very recently in Ref. [16] the authors applied Eq. (6) to the Lieb-Liniger model and obtained closed-form expressions analogous to Eq. (5). Below, we generalize this result to interacting quantum models which involve multiple species of excitations and internal degrees of freedom. It is quite remarkable, however, that the final outcome remains a bilinear functional operating diagonally in the mode-number space, while the effect of interparticle interactions gets absorbed into a universal renormalization of bare charges [see Eq. (3)].

Equation (6) indicates that Drude weights are expressible as the variation of the equilibrium expectation values of *total* current [14] with respect to thermodynamic forces $\delta\mu_j$, $\mathcal{D}^{(i,j)} = \frac{\beta}{2}(\partial J_i/\partial\,\delta\mu_j)_{\delta\mu_j=0} = \frac{\beta}{2}\sum_a \iint d\zeta\, du\, q_{a,i}(u;\zeta)[\partial j_a(u;\zeta)/\partial\,\delta\mu_j]_{\delta\mu_j=0}$, being the susceptibility of a system to develop ballistic currents. On each ray ζ, the averages of the particle current densities are given by [4] $j_a(\zeta) = [\sigma_a\vartheta_a^{-1}(\zeta)\delta_{ab} + K_{ab}]^{-1} \star e'_b(\zeta)$, where rapidity dependence has been suppressed for brevity. Given the filling functions inside the light cone $\vartheta_a(u;\zeta) = \vartheta_a^{\rm L}(u) + \Theta(v_a^{\rm dr}(u) - \zeta)[\vartheta_a^{\rm R}(u) - \vartheta_a^{\rm L}(u)]$, with the left/right boundary conditions $\vartheta_a^{\rm L,R}$, and neglecting corrections of order $O(\delta\mu^2)$, one can integrate out the dependence on the light cone coordinates (see SM [33] for details). This leads to the form of Eq. (5), with

$$D_a(u) = \rho_a(u)(1-\vartheta_a(u))\big(v_a^{\rm dr}(u)\big)^2. \tag{7}$$

On detailed balance. The symmetry under exchanging indices i and j in representation (5), $\mathcal{D}^{(i,j)} = \mathcal{D}^{(j,i)}$, indicates that the Onsager reciprocal relations [52] remain valid for any stationary state, not only in thermal Gibbs equilibrium. This is indeed a general property of the hydrodynamic equation of motion [15]. Moreover, we here show that in a general local equilibrium state of an integrable quantum model, there exists a generalized *detailed balance* condition on the hydrodynamic scale (i.e., for small κ and ω), similarly as in the Lieb-Liniger model found recently in Refs. [53,54]. More specifically, given a conserved quantity of the model $\hat{Q} = \sum_x \hat{q}_x$, the corresponding dynamical structure factor defined as $\mathcal{S}_{\hat{q}}(\kappa,\omega) = \sum_x \int dt e^{i(\kappa x-\omega t)}\langle\hat{q}_x(t)\hat{q}_0(0)\rangle$ decomposes in terms of individual particle contributions, $\mathcal{S}_{\hat{q}}(\kappa,\omega) = \sum_a \mathcal{S}_{\hat{q},a}(\kappa,\omega)$. In the low-momentum limit $\kappa\to 0$, each term is determined by a single matrix element of a particle-hole excitation on a reference equilibrium state [33]. Therefore, following the logic presented in Ref. [53], we derive the following generalized reversibility property,

$$\mathcal{S}_{\hat{q},a}(\kappa,-\omega) = e^{-\mathcal{F}_a(k,\omega)}\mathcal{S}_{\hat{q},a}(\kappa,\omega) + O(\kappa^2), \tag{8}$$

with $\mathcal{F}_a(\kappa,\omega) = \kappa\frac{\partial}{\partial p_a(u)}\log[\vartheta_a^{-1}(u)-1]$, with u fixed by the energy constraint $v_a^{\rm dr}(u)\kappa = \omega$. In the case of thermal (canonical) equilibrium, given by $\vartheta_a = [1+\exp(\beta\,\varepsilon_a + \sum_i \mu_{a,i}n_a)]^{-1}$, we have $\mathcal{F}_a(\kappa,\omega) = \beta\omega$, which is the usual detailed balance relation.

Hubbard model. The Hamiltonian of the one-dimensional (1D) Hubbard model [55,56] is given as

$$\hat{H} = \sum_{x=1}^{L}\hat{T}_{x,x+1} + 4\mathrm{u}\sum_{x=1}^{L}\hat{V}_{x,x+1}, \tag{9}$$

where $\hat{T}_{x,x+1} = -\sum_{\sigma=\uparrow,\downarrow}\hat{c}^\dagger_{x,\sigma}\hat{c}_{x+1,\sigma} + \hat{c}^\dagger_{x+1,\sigma}\hat{c}_{x,\sigma}$ is electron hopping and $\hat{V}_{x,x+1} = (\hat{n}_{x,\uparrow}-\frac{1}{2})(\hat{n}_{x,\downarrow}-\frac{1}{2})$ is the Coulomb interaction. This model has received a lot of attention in the past decades [17,57–60] as well as in the last years [48,61–73]. We consider the repulsive case $\mathrm{u}\geqslant 0$, featuring a u-dependent charge gap and gapless spin degrees of freedom.

The Hubbard model is diagonalized by means of a nested Bethe ansatz [17,20]. Eigenstates in a finite system of length L are characterized by quantum numbers which are solutions to the Lieb-Wu equations [74] (cf. SM [33]) The model involves two elementary degrees of freedom; the physical particles are momentum-carrying electrons, while spin degrees of freedom represent internal (nondynamical) excitations described by auxiliary quantum numbers. In a thermodynamic system one finds various types of charge and/or spin-carrying bound states. Specifically, the thermodynamic particle content of the Hubbard model has been derived in Ref. [75] (see also Refs. [20,27]) and comprises (i) spin-up momentum-carrying electronic excitations which carry a unit bare (electronic) charge, (ii) spin-singlet electronic bound states, and (iii) charge-neutral *nondynamical* spin-carrying magnonic

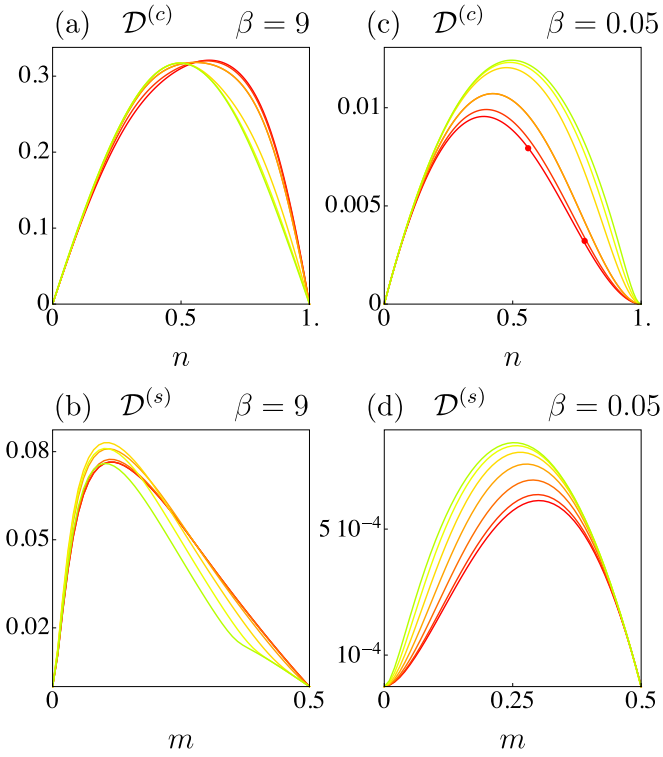

FIG. 1. Charge Drude $\mathcal{D}^{(c)} \equiv \mathcal{D}^{(c,c)}$ and spin Drude $\mathcal{D}^{(s)} \equiv \mathcal{D}^{(s,s)}$ weights as functions of magnetization density $\langle\hat{S}^z\rangle/L = m$ or electron filling $\langle\hat{N}\rangle/L = n$, shown for different values of chemical potentials: Ranging from red to green, with integer $k = 0,\ldots,6$, chemical potentials are parametrized in each plot as (a) $B = 2k$, (b) $\mu = 30+5k$, (c) $B = k$, (d) $\mu = k$. Red dots are DRMG numerical computations reported in Ref. [48]. Notice that charge and spin Drude weights are exactly zero at vanishing chemical potentials $\mu = 0$ ($n = 1$) and $B = 0$ ($m = \frac{1}{2}$), respectively, which is a consequence of the particle-hole symmetry of the Gibbs ensemble [14]. From the viewpoint of dressing excitations, this can now be understood as the vanishing of the effective charge/spin [see Eq. (5)].

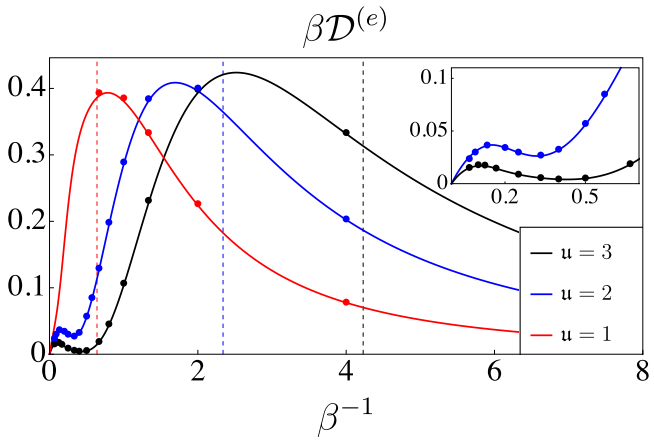

FIG. 2. Thermal Drude weight $\mathcal{D}^{(e)} \equiv \mathcal{D}^{(e,e)}$ (rescaled by β) as a function of temperature $1/\beta$, presented for three different values of coupling u. The dotted vertical lines represent the charge gap. The inset plot magnifies the region around $1/\beta \sim 0$. Our results confirm the presence of the low-temperature bump in the thermal Drude weight which comes from the dominant spin-carrying excitations, suggested and observed numerically in Refs. [48,49]. The dots drawn on top of the theoretical predictions (solid curves) are the results of numerical DMRG calculations presented in Ref. [48].

excitations. A detailed description of the particle content and other information, including explicit expressions for their bare momenta, energies, scattering phases, and the dressing transformation, are reported in SM [33].

Numerical results. We present the temperature dependence of charge and spin (see Fig. 1) and thermal Drude weights (see Fig. 2) in grand canonical equilibrium $\hat{\varrho}_{\rm GCE} \simeq \exp(-\beta\,\hat{H} - \mu\,\hat{N} + B\,\hat{S}^z)$, where $\hat{N} = \sum_{x=1}^{L}(\hat{c}^\dagger_{x,\uparrow}\hat{c}_{x,\uparrow} + \hat{c}^\dagger_{x,\downarrow}\hat{c}_{x,\downarrow})$ is the total electron charge, and $\hat{S}^z = \frac{1}{2}\sum_{x=1}^{L}(\hat{c}^\dagger_{x,\uparrow}\hat{c}_{i,\uparrow} - \hat{c}^\dagger_{x,\downarrow}\hat{c}_{x,\downarrow})$ the total magnetization. We compared our data with the recent density matrix renormalization group (DMRG) computation presented in Refs. [48,72]. Most notably, at low temperatures appreciably below the charge gap, we confirm the "Hubbard to Heisenberg crossover" in the thermal Drude weight observed previously in Refs. [48,49] (see Fig. 2). In Ref. [33] we also present an exact computation of the asymptotic charge and current profiles inside a light cone and make comparisons with the numerical results of Ref. [72].

Conclusions. We presented a general theoretical and computational framework to access the singular components (Drude weights) of generalized transport coefficients in quantum integrable models. We exemplified our approach by computing the exact numerical values of (diagonal) charge, spin, and thermal Drude weights in the one-dimensional fermionic Hubbard model in grand canonical equilibrium at finite temperatures and chemical potentials. Using the two-partition protocol, we additionally computed the quasistationary energy and charge density profile and the corresponding current [33].

Our results finally permit us to establish the equivalence of various approaches for computing the spin Drude weight employed in the previous literature: (i) using projections onto local conserved subspaces by virtue of the Mazur-Suzuki equality [38,76,77], (ii) taking the linear-response limit of the asymptotic current rates [14,51], and (iii) computing the energy-level curvatures [78–81] under the twisted boundary conditions in accordance with the Kohn formula [82]. The latter has been evaluated within the TBA framework in Refs. [79,80], yielding a closed formula expressed in terms of filling functions, magnonic dispersion relations, and $\mathcal{O}(1/L)$ corrections to the Bethe spectrum induced by the twist. Remarkably, however, it is easy to see that the twist dependence of the energy levels can be directly linked to the effective spin as given by Eq. (2). This in turn reconciles the results of Ref. [80] with Eq. (7), representing the equilibrium analog of definition (6) used previously in Refs. [14,51] (further details are given in SM [33], which also includes Refs. [83–94]).

Finally, our results show that a generalized version of the detailed balance [53,54,95] is valid on hydrodynamic scales in any stationary state.

As a future task, it would be interesting to find an extension of the presented approach which would allow resolving the diffusive time scale from the microscopic picture (see, e.g., Refs. [96,97]).

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