PHYSICAL REVIEW E **87**, 050103(R) (2013)

Burnett coefficients in quantum many-body systems

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(Received 20 February 2013; published 30 May 2013)

The Burnett coefficient B is investigated for transport in one-dimensional quantum many-body systems. Extensive numerical computations in spin-1/2 chains suggest a linear growth with time, $B(t) \sim t$, for nonintegrable chains exhibiting diffusive transport. For integrable spin chains in the metallic regime, on the other hand, we find a cubic growth with time, $B(t) \sim -D_{\mathrm{m}}^2 t^3$, with the proportionality constant being simply a square of the Drude weight D_{m}. The results are corroborated with additional studies in noninteracting quantum chains and in the classical limit of large-spin chains.

DOI: 10.1103/PhysRevE.87.050103 PACS number(s): 05.60.Gg, 75.10.Pq, 05.70.Ln

Introduction. Understanding classical and quantum diffusion in deterministic Hamiltonian systems is one of the most ubiquitous problems of statistical physics [1]. In Fourier space of momentum q, diffusion is described by the well-known equation

$$\dot{\rho}_q(t) = -q^2 D(t)\, \rho_q(t), \quad D(t) = D, \tag{1}$$

and manifests as the simple exponential relaxation of a harmonic density profile at a characteristic time scale $\tau = 1/q^2 D$. The strict derivation of diffusion from truly microscopic principles remains a challenge to theorists [2], and the problem is often simplified to a mere calculation of the diffusion coefficient $D(t)$ in the limit $q = 0$ via the famous Green-Kubo formula [3]. It has become clear that $D(t)$ can diverge in integrable systems [4], $D(t) \propto t$ [5], due to the lack of sufficient scattering, which is a key issue for understanding large thermal spin transport in quantum magnets [6] or thermalization in cold atomic gases [7]. On the other hand, $D(t)$ is believed to be constant, $D(t) = D$, in generic nonintegrable systems as a consequence of microscopic Hamiltonian chaos [1]. This raises the important question of whether diffusion is the rule rather than the exception.

The existence of diffusion can only be clarified by taking into account finite momentum $q \neq 0$ [8,9]. The first higher order correction can be systematically described by the so-called Burnett coefficient $B(t)$ [1,10,11],

$$\dot{\rho}_q(t) = [-q^2 D(t) + q^4 B(t) + \cdots]\, \rho_q(t), \tag{2}$$

which may diverge even for dynamical processes with a constant $D(t)$ [10]. Even though Burnett coefficients have been extensively studied in the literature for various classical models, in particular for Lorentz-type gases [11,12], essentially nothing is known about Burnett coefficients in quantum systems.

In this Rapid Communication we do the first steps by calculating $B(t)$ numerically for various one-dimensional, integrable and nonintegrable models, including spin-1/2 XXZ chains, large-spin chains, and more abstract models of quantum transport. We generally observe the moderate divergence $B(t) \sim B' t$, for cases with a constant $D(t) \sim D$. At the characteristic time scale τ, this observation implies

$$\dot{\rho}_q(t = \tau) = [-q^2 D + q^2 B'/D + \cdots]\, \rho_q(t = \tau), \tag{3}$$

i.e., Burnett coefficients are a relevant correction at any finite momentum $q \neq 0$, which speed up or slow down the still diffusive relaxation (if $|B'| \lesssim D^2$). For ballistic cases with $D(t) \sim D_{\mathrm{m}}\, t$, on the other hand, we find the stronger divergence $B(t) \sim -D_{\mathrm{m}}^2 t^3$ with the Drude weight D_{m} as the constant of proportionality.

Diffusion and Burnett coefficient. Following Refs. [10,12,13] the quantum Burnett coefficient $B(t)$ may be introduced by formally expanding the decay rate of density-density correlation functions in q. This expansion leads to the time-dependent diffusion coefficient

$$D(t) = \frac{1}{\chi} \int_0^t dt_1\ f(t_1), \quad f(t_1) = \langle J(0) J(t_1) \rangle, \tag{4}$$

given as a time integral over the two-point correlation function of the current operator $J(t)$ in the Heisenberg picture, where $\langle \bullet \rangle = \mathrm{tr}(\bullet)/\mathrm{dim}$ denotes an equilibrium expectation at high temperatures, as considered in this Rapid Communication. The further occurring prefactor χ is a constant and denotes the "static susceptibility" [14].

The time-dependent Burnett coefficient is the *difference* between two contributions,

$$B(t) = I_4(t) - I_{2-2}(t), \tag{5}$$

where the first term $I_4(t)$ is given by

$$I_4(t) = \frac{2}{\chi} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3\ \langle J(0) J(t_1) J(t_2) J(t_3) \rangle \tag{6}$$

as a triple-time integral over the *time-ordered* four-point current autocorrelation function. The second term

$$I_{2-2}(t) = \frac{2}{\chi} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3\ [f(t_1) f(t_2 - t_3) + f(t_2) f(t_1 - t_3) + f(t_3) f(t_1 - t_2)] \tag{7}$$

is a similar time-ordered integral but over products of two-point correlations [15]. Conveniently, this contribution can be rewritten as $I_{2-2}(t) = 2\chi D(t) \int_0^t dt_1 D(t_1)$, particularly

unveiling the linear increase $I_{2-2}(t) \propto t$ in the case of a existent diffusion constant. However, despite the apparent divergence of $I_{2-2}(t)$ in that case, the Burnett coefficient can still remain finite, as discussed in the following. To this end, assume for the moment that (i) the two-point correlation $f(t)$ is a δ function $\delta(t)$ and that (ii) the four-point correlation $\langle J(0)J(t_1)J(t_2)J(t_3)\rangle$ can be factorized as $f(t_3)f(t_1-t_2)$. Then the contributions $I_{2-2}(t)$ and $I_4(t)$ are identical and, as a consequence, the Burnett coefficient vanishes exactly. Giving up the assumption (i) by broadening the δ function still allows for a finite Burnett coefficient. While the assumption (ii) appears to be crucial, it may be fulfilled for a nonintegrable model with J, in the energy eigenbasis, being a random Hermitian matrix and, consequently, J^2 being close to proportional to an identity matrix.

Anisotropic spin-1/2 Heisenberg chain. We are going to investigate the transport of magnetization in the spin-1/2 XXZ model as a paradigmatic example of an interacting *many*-particle quantum system in one dimension. The XXZ Hamiltonian is given by

$$H = \sum_{r=1}^{L} \left(S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta\, S_r^z S_{r+1}^z \right), \tag{8}$$

where $S_r^{x,y,z}$ are the components of spin-1/2 operators at site r, L is the number of sites arranged periodically, $L+1 \equiv 1$, and Δ is the anisotropy. The magnetization current

$$J = \sum_{r=1}^{L} \left(S_r^x S_{r+1}^y - S_r^y S_{r+1}^x \right) \tag{9}$$

commutes with H in the noninteracting case $\Delta = 0$. In that case (due to $\langle J^2\rangle = L/8$, $\langle J^4\rangle = 3(L^2-L)/64$, and $\chi = L/4$), one obtains directly $D(t) = t/2$ and $B(t) = -t^3/16$, which for $\Delta > 0$ remains only an approximation at short times, in agreement with Eq. (4) of Ref. [9]. Remarkably, at $\Delta = 0$ a series expansion of density autocorrelations (Bessel functions [16]) leads also to $q^2 D(t)$ and $-q^4 B(t)$ as the leading terms, a convincing consistency check of the present approach.

In the metallic regime, $0 < |\Delta| < 1$, the magnetization current is still partially conserved such that the two-point correlation $f(t)$ does not decay to zero but remains at a finite Drude weight $D_{\rm m} = \lim_{t\to\infty} f(t)$, $0 < D_{\rm m} < 1/8$, recently proven by establishing positive lower bounds in the thermodynamic limit [4]. This finite Drude weight implies the linear increase of the diffusion coefficient at long times, $D(t) \propto 4D_{\rm m}t$, just as in the case of $\Delta = 0$. By factoring the four-point correlation at long times [17], one derives the asymptotics of the Burnett coefficient as

$$B(t) \simeq -4D_{\rm m}^2 t^3 . \tag{10}$$

In Fig. 1 we demonstrate this result by numerically simulating $B(t)$ for finite length $L = 10,\ldots,18$ using *all* invariant subspaces (translation, magnetization) and also using fourth-order Runge-Kutta integration for generating time order [15] (step size $\delta t = 0.02$). While Fig. 1 clearly shows for $\Delta = 0.5$ a stronger than quadratic increase of $B(t)$ with time, it also is consistent with $B(t) \sim -(0.63)^2 t^3/16$ at long times, e.g., 63% of the Drude weight in the case of $\Delta = 0$. Remarkably, the exact Drude weight at $\Delta = 0.5$ for finite $L = 18$ (20) is 63%

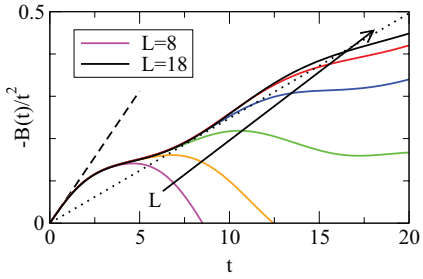

FIG. 1. (Color online) Burnett coefficient $B(t)$, divided by t^2, for the spin-1/2 XXZ chain at $\Delta = 0.5$ for $L = 8,10,\ldots,18$ and all magnetization sectors. At short times or at $\Delta = 0$ (free fermions), $B(t)/t^2$ is given by the function $-t/16$ (dashed curve). In addition, a function $-(0.63)^2 t/16$ is indicated (dotted curve); see prediction (10).

(62%) of the Drude weight at $\Delta = 0$, while the lower bound in the thermodynamic limit is 56% [4].

Eventually, we discuss the regime $\Delta > 1$, where Drude weights are expected to vanish in the thermodynamic limit and strong evidence of magnetization diffusion has been found in nonequilibrium bath scenarios on the basis of the Lindblad equation [19,20]. The diffusion coefficient has been shown to behave as $D(t > 3.0/\Delta) \approx 0.88/\Delta$ at vanishing [5] and finite momentum [9]. We focus on the Burnett coefficient $B(t)$ in this Rapid Communication. Figure 2(a) shows numerical results summarizing an order of a CPU-year of simulations and plotting, for convenience, $|dB(t)/dt|$ in a log-log scale. Several comments are in order: First, after the already discussed t^3 behavior at short times, the Burnett coefficient changes its sign, visible as the zero drop in Fig. 2(a), and indicates a correction towards an insulator. Second, curves for $L \geqslant 12$ have converged for times after the zero drop and show at least the tendency to form a plateau at $t \sim 4$ for $L \to \infty$, then indicating a linearly increasing Burnett coefficient $B(t) \propto t$. Third, even though a possible plateau is not pronounced yet, the contributions $I_4(t)$ and $I_{2-2}(t)$ increase linearly with time at $t \sim 4$; see the inset of Fig. 2(a). Notably, the Burnett coefficient turns out to be the *small* difference between both contributions, which by themselves diverge with L. This divergence does not appear in the modular quantum system, discussed later. Finally, we show in Fig. 2(b) numerical results for the modified *nonintegrable* XXZ model $H + \Delta_2 \sum_r S_r^z S_{r+2}^z$ with $\Delta_2 = 0.5$. While the overall structure of $|dB(t)/dt|$ is similar, an emerging plateau is more clearly visible for the accessible lengths, hence pointing towards a linearly increasing Burnett coefficient again. Summarizing, a linear asymptotic scaling $B(t) \propto t$ is clearly suggested in either integrable or nonintegrable regimes with a finite diffusion constant.

Heisenberg chains in the large-spin limit. In addition we present results on the classical limit of the considered spin chains, where we focus on the case $\Delta = 1.5$ and $\Delta_2 = 0.5$ only. In that limit the magnetization current is a function of classical unit (angular momentum) vectors. We obtain their dynamics by numerically integrating the corresponding Hamiltonian equations of motion. Formally, the diffusion coefficient in Eq. (4) and the Burnett coefficient in Eq. (5) remain defined the same way, but the equilibrium average at high temperatures is now performed by sampling over a set

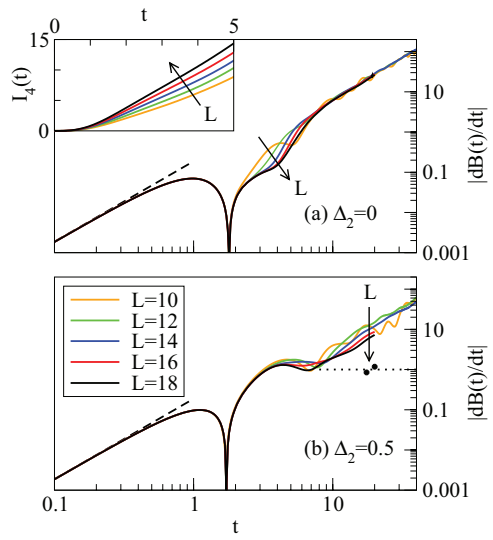

FIG. 2. (Color online) Absolute value of the derivated Burnett coefficient, $|dB(t)/dt|$, for the spin-1/2 XXZ chain at $\Delta = 1.5$ (a), and for its nonintegrable modification with $\Delta_2 = 0.5$ (b). Numerical results (solid curves) for $L = 10, 12, \ldots, 18$ are shown in a log-log plot. In addition to the short-time behavior (dashed curves), the long-time behavior is extrapolated in panel (b) using the observed exponential scaling with L (dotted curve). Inset: The contribution $I_4(t)$ by itself increases with L.

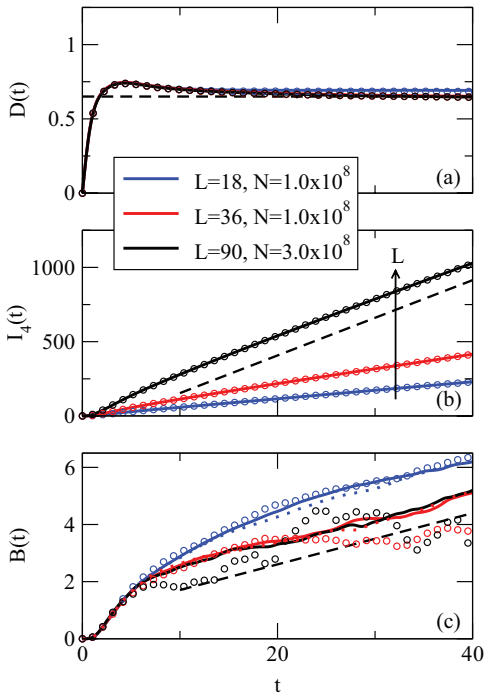

FIG. 3. (Color online) Classical (a) diffusion coefficient $D(t)$, (b) the contribution $I_4(t)$, and (c) Burnett coefficient $B(t)$ for the XXZ model at $\Delta = 1.5$ with $\Delta_2 = 0.5$. Numerical results (solid curves) on finite length $L = 18$, 36, 90 are obtained by numerically integrating the Hamiltonian equations of motion (fixed step size $\delta t = 0.05$) and by averaging over $N \sim 10^8$ completely random initial states. The average over only $N = 10^7 \ll 10^8$ is also indicated (symbols). In panel (c) results for a 2.5× smaller time step are shown (dotted curves). Straight lines (dashed curves) serve as guides to the eye.

of completely random initial configurations; see Ref. [18], for instance. While the required number of initial states decreases with the chain length L for the evaluation of the diffusion coefficient [21], the situation turns out to be different for the evaluation of the Burnett coefficient. As in the quantum case, the Burnett coefficient is the *small* difference between two contributions, which by themselves diverge with L. Thus, errors due to insufficient averaging increase with L and can only be compensated by taking into account more initial configurations. Approximately $N \approx 10^8$ initial states are already required for a chain of length $L = 90$, taking about a CPU-year of computation time. In Fig. 3 we summarize these results for three different sizes $L = 18$, 36, 90. Apparently, $D(t \gtrsim 10)$ becomes independent of time for all considered lengths $L \geqslant 18$. Remarkably, the quantitative value $D \approx 0.65$ is close to the expectation for the diffusion constant in the quantum case [21]. Furthermore, $B(t \gtrsim 10)$ is observed to increase linearly in time, at least for the largest two sizes $L \geqslant 36$. The latter observation indicates the linear divergence of the Burnett coefficient in diffusive classical spin chains. This is in clear agreement with the finite-size results in the quantum case (see Fig. 2), indicating that the underlying mechanism "survives" the transition to the classical limit.

Modular quantum system. Due to a delicate counterbalance of the terms I_4 and I_{2-2}, the calculation of Burnett coefficients for many-body systems is extremely demanding. Thus, in order to corroborate our prediction that $B(t) \propto t$ for one-dimensional lattice systems with finite diffusion constants, we make another numerical experiment in a single-particle diffusive quantum system—the so-called *modular quantum system* [5,22]. Each of the L local modules features an identical spectrum, consisting of n equidistant levels in a band with the width $\delta\epsilon$. Therefore, the local Hamiltonian at the position r is given by $h_r = \sum_\mu \mu\, \delta\epsilon/n\, |r,\mu\rangle\langle r,\mu|$ in the one-particle basis $|r,\mu\rangle$. The nearest-neighbor interaction between two local modules at the positions r and $r+1$ is $v_r = \lambda\, m_r + \text{H.c.}$,

$$m_r = \sum_{\mu,\nu} c_{\mu,\nu}\, |r,\mu\rangle\langle r+1,\nu| \tag{11}$$

with the overall coupling strength λ. The r-independent coefficients $c_{\mu,\nu}$ are a *single* realization of complex, random, and uncorrelated numbers: Their real and imaginary part are both chosen corresponding to a Gaussian distribution with the mean 0 and the variance 1/2. Of particular interest is the probability for finding the particle somewhere within the rth local module. The associated local current is $j_r = \imath\, \lambda\, m_r + \text{H.c.}$ with a form very similar to v_r, e.g., almost completely random (apart from the translation invariance and the necessary Hermitian property).

The modular quantum system is one of the few quantum models which have been reliably shown to exhibit diffusion with a finite diffusion constant, reading $D^{\text{w}}_{\text{th}}(t > \pi/\delta\epsilon) = 2\pi\lambda^2 n/\delta\epsilon$ for weak coupling [22] and $D^{\text{s}}_{\text{th}} = (t > 1/\lambda\sqrt{2n}) = \lambda\sqrt{\pi n/2}$ for strong coupling [5]. One might expect a finite Burnett coefficient due to both the presence of diffusion and the random elements of the current. For instance, because J^2 is close to an identity matrix, one may be tempted to factorize as $\langle J(0)J(t_1)J(t_2)J(t_3)\rangle = f(t_3)f(t_1 - t_2)$, then allowing for

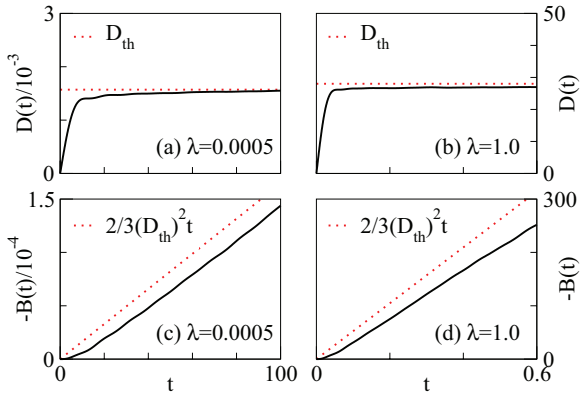

FIG. 4. (Color online) Diffusion coefficient $D(t)$ and Burnett coefficient $B(t)$ for the modular quantum system at coupling (a), (c) $\lambda = 0.0005$ and (b), (d) $\lambda = 1.0$. (Other parameters: $n = 500$, $\delta\epsilon = 0.5$.) Numerical results (solid curves) on arbitrary length L are shown for a *representative* translation subspace (momentum $k = \pi/5$). Results agree well with the theoretical predictions (dotted curves).

a finite Burnett coefficient. However, the latter factorization already fails when all time arguments are equal. In fact, $\langle J^4\rangle = 2f(0)^2 = 8\lambda^4 n^2$, resulting from an additional *coherent* sum over the off-diagonal elements of J^2. Instead, fulfilling the static property, we may choose the *unbiased* factorization of $\langle J(0)J(t_1)J(t_2)J(t_3)\rangle$ into $2/3[f(t_1)f(t_2-t_3)+f(t_2)f(t_1-t_3)+f(t_3)f(t_1-t_2)]$, yielding the relation $I_4(t) = 2/3 I_{2-2}(t)$ between the two contributions to $B(t)$. Therefore, noting that $\chi = 1$, this choice leads to the *linearly* increasing Burnett coefficient

$$B(t > \tau) \simeq -\tfrac{2}{3} D_{\rm th}^2 t. \tag{12}$$

For verification, we present in Fig. 4 numerical results on $D(t)$ and $B(t)$. Because the linear growth of the Hilbert space with L is compensated by translation invariance, the dimension of a momentum k subspace is only set by the level number n, chosen as $n = 500$ to ensure a sufficient number of states. Since we do not find a significant dependence on k, Fig. 4 depicts numerical results for a single k subspace. The quantitative agreement with the theoretical predictions on $D(t)$ and $B(t)$ clearly demonstrates a linearly increasing Burnett coefficient despite the existence of a diffusion constant, which is in agreement with the previous results on spin chains, but much clearer due to computational simplicity of the model.

Conclusion. In this Rapid Communication we presented extensive numerical and theoretical investigations of Burnett coefficients in quantum chains. We conjectured and supported the general statement that in the thermodynamic limit Burnett coefficients diverge linearly, $B(t) \propto t$, in diffusive regimes with finite diffusion constants. Recall that this linear divergence is still consistent with diffusion but causes Burnett coefficients to be a relevant correction at arbitrary small momentum. In ballistic regimes with positive Drude weights, on the other hand, we demonstrated the cubic divergence $B(t) \propto t^3$. This behavior is remarkably different than for Lorentz billiard-type classical systems and and calls for a deeper theoretical analysis.

Acknowledgment. Financial support by the grant P1-0044 of Slovenian research agency is gratefully acknowledged.

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[14] We define the "static susceptibility" as the square of the conserved quantity [5], e.g., $\chi = \langle (S^z)^2\rangle$ for spin transport with S^z being the conserved magnetization.
[15] The time order of $I_4(t)$ can be determined by numerically solving a set of coupled differential equations for auxiliary operators $M_i(t)$,

$$I_4(t) = \frac{2}{\chi}\langle J(0)M_3(t)\rangle, \quad \dot{M}_i(t) = J(t)M_{i-1}(t),$$

where $M_0(t) = 1$. Here, we use full exact diagonalization of H to evaluate $J(t)$ in the Heisenberg picture and a fourth-order Runge-Kutta integration.
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