Exact results for anomalous transport in one-dimensional Hamiltonian systems

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Anomalous transport in one-dimensional translation invariant Hamiltonian systems with short range interactions, is shown to belong in general to the KPZ universality class. Exact asymptotic forms for density-density and current-current time correlation functions and their Fourier transforms are given in terms of the Prähofer-Spohn scaling functions, obtained from their exact solution for the polynuclear growth model. The exponents of corrections to scaling are found as well, but not so the coefficients. For the Lévy flight representation of heat diffusion the jump distribution is given explicitly. Mode coupling theories developed previously are found to be adequate for weakly nonlinear chains, but in need of corrections for strongly anharmonic interparticle potentials.

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Since the discovery by Alder and Wainwright[1] of long-time tails in the Green-Kubo current-current time correlations, such as the velocity autocrrelation function it has been clear that transport in one and two dimensional Hamiltonian systems must be anomalous. one-dimensional systems have been studied extensively in the past decades, both by mode coupling techniques[2–5] and dynamical scaling[6], and also by computer simulations[2–5, 7]. Most studied are the exponents α describing the divergence of the coefficients of heat conduction and sound damping with system size L as L^α, and δ describing the power law $t^{-(1-\delta)}$ by which the corresponding current-current time correlation functions decay. For both exponents various values have been proposed, with $\alpha = \delta = 1/3$ being the most common recent ones.

Here I will argue that for generic Hamiltonian systems the long time behavior of the dynamics can be obtained *exactly* in terms of the scaling functions obtained by Prähofer and Spohn[8] for the polynuclear growth model, which is in the KPZ universality class. The value $\delta = 1/3$ is confirmed for both sound damping and heat conduction, whereas α equals 1/3 indeed for heat conduction, but it is 1/2 for sound damping. In addition the *coefficients* of size dependent transport coefficients and long-time current-current correlation functions are obtained exactly, as well as the scaling functions describing the asymptotic behaviors of the various density-density time correlation functions and their Fourier transforms.

More specifically, I have in mind classical one-dimensional N-particle systems described by a translation invariant Hamiltonian with short range interactions and periodic boundary conditions. To study these I will follow one of the ground-laying papers by Ernst, Hauge and Van Leeuwen[9]. Their basic assumption is that all slow variables of relevance for the long time behavior of hydrodynamics and related time correlation functions are the long-wave length Fourier components of the densities of conserved quantities, i.e. particle number, momentum and energy, plus products of these. For one-dimensional systems (and also for two-dimensional ones) their method has to be generalized somewhat: instead of assuming that the time correlation functions of hydrodynamic modes decay exponentially with time[5], one has to write down the mode coupling equations as a set of coupled nonlinear equations for these correlation functions that must be solved self-consistently[2–4].

EHvL define the hydrodynamic modes, to leading order in the wave number k as linear combinations of the Fourier transforms of the microscopic densities of particles, momentum and energy[16], $\rho^\mu(k,t) = \sum_{j=1}^{N} M_j^\mu \exp(-ikx_j) - \delta_{k0}\langle \hat{M}(k=0)\rangle$, with $M_j^\mu = 1, p_j, e_j$ for the particle density $n(k,t)$, the momentum density $g(k,t)$ and the energy density $e(k,t)$ respectively. Note that the energies and momenta of the particles are localized at the actual positions of the particles. For chains on which particles cannot pass each other, a natural alternative is localizing these densities at the average positions of the particles[2–4][17]. However, one can show that both approaches are equivalent, or at least so in their predictions of the long time dynamics[13]. The hydrodynamic modes are two sound modes[18] $a_1(k,t)$ and $a_{-1}(k,t)$ and a heat mode $a_H(k,t)$, given respectively, to leading order in k by

$$a_\sigma(k,t) = \left(\frac{\beta}{2\rho}\right)^{1/2} \left(c_0^{-1} p(k,t) + \sigma g(k,t)\right), \qquad (1)$$

$$a_H(k,t) = \left(\frac{\beta}{nTC_p}\right)^{1/2} (e(k,t) - hn(k,t)). \qquad (2)$$

Here, $\sigma=\pm1$, T is the equilibrium temperature, n the equilibrium number density and $\rho=nm$; $C_p=T(\partial s/\partial T)_p$ is the specific heat per particle at constant pressure p, with s the equilibrium entropy per particle; $c_0=(\partial p/\partial \rho)_s^{1/2}$ is the adiabatic sound velocity in the limit of zero wave number and h is the equilibrium enthalpy per particle. Furthermore,

$$p(k,t) = (\partial p/\partial e)_n e(k,t) + (\partial p/\partial n)_e n(k,t). \qquad (3)$$

The allowed values of k are of the form $k = \frac{2\pi n}{L}$. To leading order in k the hydrodynamic modes are normalized under the inner product $(f,g) = \frac{1}{L}\langle f^* g\rangle$, with $\langle\rangle$ a grand canonical equilibrium average.

The time correlation functions of the hydrodynamic modes satisfy linear equations involving memory kernels, viz.

$$\frac{\partial \hat{S}_\sigma(k,t)}{\partial\, t} = -i\sigma c_0 k \hat{S}_\sigma(k,t) - k^2 \int_0^t d\tau \hat{M}_\sigma(k,\tau)\hat{S}_\sigma(k,t-\tau), \tag{4}$$

$$\frac{\partial \hat{S}_H(k,t)}{\partial\, t} = -k^2 \int_0^t d\tau \hat{M}_H(k,\tau)\hat{S}_{H(k,t-\tau)}. \tag{5}$$

Here $\hat{S}_\sigma(k,t) = (a_\sigma(k,0), a_\sigma(k,t))$ etc. The memory kernels may be expressed through a diagrammatic mode coupling expansion as a sum of irreducible skeleton diagrams[10]. These consist of propagators, representing stationary density correlation functions $\hat{S}_\zeta(\ell, t_\alpha)$, and vertices representing the coupling of one propagator $\hat{S}(\ell, t_\alpha)$ to two propagators $\hat{S}_\mu(q, t_{\alpha'})$ and $\hat{S}_\nu(\ell - q, t_{\alpha''})$, with coupling strength $\ell W_\zeta^{\mu\nu}$. For the long time dynamics only a few of these 27 couplings are important; only couplings to two sound modes of the same sign or to two heat modes may give rise to long-lived perturbations, all other combinations of pairs of modes rapidly die out through oscillations. From EHvL[9] the relevant non-vanishing coupling strengths to leading order in k can be obtained as[19]

$$W_\sigma^{\sigma'\sigma'} = \frac{\sigma}{2(\rho\beta)^{1/2} c_0}\left(\frac{\partial c_0 n}{\partial n}\right)_s \tag{6}$$

$$W_\sigma^{HH} = \frac{-\sigma(\gamma-1)n}{2(\rho\beta)^{1/2} C_p}\left(\frac{\partial C_p}{\partial n}\right)_p \tag{7}$$

$$W_H^{\sigma\sigma} = \frac{\sigma k_B^{1/2} c_0}{(2nC_p)^{1/2}}. \tag{8}$$

Notice that $W_\sigma^{\sigma'\sigma'}$ does not depend on the value of σ'.

Now a central observation is the following: due to the first term on the right-hand side of Eq. (4) the sound-sound correlation functions will have their weights centered around the positions $x(t) = x(0) \pm c_0 t$, in other words, these functions will assume the forms $\hat{S}_\sigma(k,t) = \exp(-i\sigma c_0 kt)\hat{\Sigma}_\sigma(k,t)$, with $\hat{\Sigma}_\sigma(k,t)$ to a first approximation real non-oscillating functions. As a consequence the mode coupling contributions to $\hat{M}^\sigma$ are dominated by those diagrams in which all vertices are of the type $V_\sigma^{\sigma\sigma}$. All other contributions for at least some time will oscillate out of phase with the angular frequency $\sigma c_0 k$ of the sound mode under consideration. The remaining contributions, especially so if described in a coordinate frame comoving at the speed of sound, can be identified with the terms in a similar mode coupling expansion for the fluctuating Burgers equation[11],

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\kappa}{2}\frac{\partial \rho^2}{\partial x} + \frac{D}{A}\frac{\partial^2 \rho}{\partial x^2} + \frac{\partial \eta}{\partial x}, \tag{9}$$

with A=$\hat{S}(0,0)$, the density-density time correlation function $\hat{S}(k,t)$ defined as

$$\hat{S}(k,t) = \int_{-\infty}^{\infty} dx e^{-ikx} S(x,t) \equiv \int_{-\infty}^{\infty} dx e^{-ikx}\langle \rho(0,0)\rho(x,t)\rangle$$

and $\eta(x,t)$ representing gaussian white noise with $\langle \eta(x,t)\eta(x',t')\rangle$=$D\delta(x-x')\delta(t-t')$. The brackets denote an average over the stationary distribution of the density field. This is similar to the hydrodynamic equations, but simpler because there is only one conservation law. The function $\hat{S}(k,t)$ satifies an equation similar to Eqs. (4,5), of the form

$$\frac{\partial \hat{S}_B(k,t)}{\partial t} = -k^2 \int_0^t d\tau \hat{M}_B(k,\tau)\hat{S}_B(k,t-\tau). \tag{10}$$

The mode coupling expansion for this memory kernel has exactly the same structure as the set of dominant terms for the sound mode memory kernel; all propagators correspond to the same type of correlation function and all vertices carry the same weight factor W, in the case of the Burgers equation given by $W_B = \kappa\sqrt{2A}$.

From their exact solution of the polynuclear growth model[8] Prähofer and Spohn obtained exact expressions for the long time, respectively small frequency behavior of the function $\hat{S}_B(k,t)$ and its temporal Fourier transform $\tilde{S}_B(k,\omega)$. These are of the form[12]

$$\hat{S}_B(k,t) = A\hat{f}_{PS}\left((2A\kappa^2 t^2)^{1/3} k\right) \tag{11}$$

$$\tilde{S}_B(k,\omega) = \sqrt{\frac{A}{2\kappa^2 |k|^3}}\mathring{f}_{PS}\left(\frac{\omega}{(2A\kappa^2)^{1/2}|k|^{3/2}}\right), \tag{12}$$

with the functions $\hat{f}_{PS}$ and $\mathring{f}_{PS}$ defined in Eqs. ((5.20) and (5.24) of Ref.[8]. From Eq. 10 one may obtain expressions for the memory kernel in terms of these scaling functions. For the full Fourier transform one obtains

$$\tilde{M}(k,\omega) = \sqrt{2A\kappa^2} M_{PS}\left(k, \frac{\omega}{\sqrt{2A\kappa^2}}\right), \tag{13}$$

with

$$\tilde{M}_{PS}(k,\omega) = \frac{i\omega}{k^2} + \left(\sqrt{k}\mathring{f}_{PS}^{+}\left(\frac{\omega}{|k|^{3/2}}\right)\right)^{-1}, \tag{14}$$

where $\mathring{f}_{PS}^{+}(\omega) = \int_0^\infty dt \exp(i\omega t)\hat{f}_{PS}(t^{2/3})$.

The corresponding expressions for the long time behavior of the sound modes are

$$\hat{S}_\sigma(k,t) = \exp(-i\sigma c_0 kt)\hat{f}_{PS}\left((V_s t)^{2/3} k\right), \tag{15}$$

$$\hat{M}_\sigma(k,t) = V_s \exp(-i\sigma c_0 kt)\hat{M}_{PS}(k, V_s t), \tag{16}$$

with $V_s = W_\sigma^{\sigma\sigma}$.

Next, I consider the wave number dependent sound damping constant $\Gamma(k) = 2\tilde{M}_\sigma(k,0)$ and define the sound currents as $\hat{J}_\sigma(k,t) = \left(\frac{\beta}{2\rho}\right)^{1/2} \sigma \hat{J}_l(k,t) + \frac{1}{c_0}\hat{J}_H(k,t) - \sigma \left(\frac{\partial p}{\partial n}\right)_e$, where $\hat{J}_l(k,t)$ and $\hat{J}_H(k,t)$ are the longitudinal current and the heat current[9], denoted by EHvL as J_l and J_λ respectively. Eq. (5.28) of Ref.[8] can now be used to obtain the leading small-k behavior of $\Gamma(k)$ and long time behavior of $\langle \hat{J}_\sigma(0,0)\hat{J}_\sigma(0,t)\rangle$ as

$$\Gamma(k) = \frac{16}{19.444}\sqrt{\frac{V_s^2}{|k|}} \tag{17}$$

$$\frac{1}{L}\langle \hat{J}_\sigma(0,t)\hat{J}_\sigma(0,0)\rangle = \frac{2.1056}{4\sqrt{3}\Gamma_E(1/3)}\left(\frac{V_s^2}{t}\right)^{2/3}, \tag{18}$$

with Γ_E Euler's gamma function[20].

The leading higher order corrections are obtained by replacing in the diagrammatic expansion of the memory kernel just one pair of vertices of type $V_\sigma^{\sigma\sigma}$ by vertices of type $V_\sigma^{-\sigma-\sigma}$ or V_σ^{HH}. Note this can only be done by having the new vertices connected by the same pair of propagators. One easily shows that all these terms add contributions proportional to $|k|^{-1/3}$ to $\Gamma(k)$ and contributions proportional to $t^{-7/9}$ to the current-current correlation function. Since there are infinitely many such contributions, there seems to be no straightforward way of determining the coefficients exactly. However, estimates based on the simplest contributing diagrams can be made[13]. Further corrections obtain from terms with $4, 6, \cdots$ vertices of type $V_\sigma^{-\sigma-\sigma}$ or V_σ^{HH}. Each of these appears to be of the form $Ck^{-\mu}$ for $\Gamma(k)$ and $Dt^{-\nu}$ for the current correlation function, with C and D constants and μ and ν of the form $\mu = 1/3 - \sum_{j=2}^{\infty} m_j (2/3)^j$ and $\nu = 2/3 + \sum_{j=2}^{\infty} 2n_j (2/3)^j$ respectively, with m_j and n_j natural numbers. Again, for each exponent there is an infinity of contributing terms.

The leading long time behavior of $\hat{S}_H(k,t)$ is determined in similar way by the sum of all contributions to $\hat{M}^H(k,t)$ where the first and last vertex are of type $V_H^{\sigma\sigma}$ and all other vertices are of type $V_\sigma^{\sigma\sigma}$, all with the same value of σ. These terms do contain an oscillating factor $\exp(-i\sigma c_0 k t)$, but these oscillations are much slower than the oscillations in any of the other terms. Since we have to include the contributions to $\hat{M}^H$ of either sign of σ, we cannot express $\hat{S}_H$ directly in terms of the Prähofer-Spohn scaling functions, but we can do so immediately for the memory kernel. A simple analysis yields to leading order

$$\hat{M}_H(k,t) = 2\frac{V_H^2}{V_s}\cos(\sigma c_0 k t)\hat{M}_{PS}(k, V_s t), \tag{19}$$

with $V_H = |W_H^{\sigma\sigma}|$. For the k-dependent heat conduction coefficient and the heat current time correlation function this leads to the expressions

$$\lambda(k) = nC_p D_T(k) = 2nC_p\left(\frac{V_H}{V_s}\right)^2 V_s^{4/3}\frac{2.1056}{4\sqrt{3}(c_0|k|)^{1/3}}, \tag{20}$$

$$\frac{1}{L}\langle \hat{J}_H(0,t)\hat{J}_H(0,0)\rangle = 2nC_p\left(\frac{V_H}{V_s}\right)^2\frac{2.1056}{\Gamma_E(1/3)}\left(\frac{V_s^2}{t}\right)^{2/3}. \tag{21}$$

Higher order corrections may be obtained in similar way as for the sound modes.

The analysis presented here clearly shows that for long times the dynamics of 1d hydrodynamic systems to leading order belongs to the KPZ universality class and can be described exactly by means of the Prähofer-Spohn scaling functions. However, the correction terms decay only slightly faster with time and in most cases will not be negligible.

The dynamic structure factor $\tilde{S}(k,\omega)$, i.e. the spatio-temporal Fourier transform of the density-density time correlation function exhibits Brillouin peaks at $\omega = \pm c_0 k$ and a central Rayleigh peak, as ususal, but, due to the anomalous transport the width and inverse height of the Brillouin peaks scale with k as $|k|^{3/2}$ and those of the Rayleigh peak with $|k|^{5/3}$, in contrast to the usual scaling with k^2. Also, the shape of these peaks is not Lorentzian, but is given through the Prähofer-Spohn scaling functions as

$$\begin{aligned}
\tilde{S}(k,\omega) &= \sum_\sigma (\hat{n}(0), \hat{a}_\sigma(0))^2 \tilde{S}_\sigma(k,\omega) \\
&\quad + (\hat{n}(0), \hat{a}_H(0))^2 \tilde{S}_H(k,\omega), \quad \text{with} \\
\tilde{S}_\sigma(k,\omega) &= 2(V_s|k|^3)^{-1/2}\mathring{f}_{PS}\left(\frac{\omega - i\sigma c_0 k}{(V_s|k|^3)^{1/2}}\right), \\
\tilde{S}_H(k,\omega) &= \frac{1}{-i\omega + k^2\frac{V_H^2}{V_s}\sum_\sigma \tilde{M}_{PS}\left(k, \frac{\omega - i\sigma c_0 k}{V_s}\right)} + cc.
\end{aligned}$$

In previous mode coupling analyses Delfini et al.[2] and Wang and Li[4] assumed the sound modes were linear combinations of momentum density and displacement field (equivalent to number density in the absence of transversal modes), without contributions from the energy density. As can be seen from Eq. (3) this is justified if $(\partial p/\partial e)_n = 0$ or equivalently, if $C_p = C_v$. This is the case for harmonic chains, so it will be a good approximation for weakly anharmonic chains. For general potentials this approximation will not be justified.

Cipriani et al. argue that energy transport in anharmonic chains can be mapped to a Lévy flight process[14]. The present analysis confirms this picture and allows one to make it very concrete; the kernel $K(x,t)$ describing the probability distribution for a flight leading to a displacement x over a time t, to leading order in t can be identified as

$$K(x,t) = \frac{V_H^2}{V_s}\frac{\partial^2}{\partial x^2}M_{PS}(|x-c_0t|,V_st). \quad (22)$$

Exceptional behavior will be found if the mode coupling amplitude V_s vanishes. Obviously the condition for this is $\frac{n}{c_0}\left(\frac{\partial c_0}{\partial n}\right)_s = -1$. This condition is satisfied for harmonic chains and in general for potentials that are even as function of the deviations of the particle positions from their equilibrium values (this includes the FPU-β model). For non-integrable models it may be satisfied on certain lines in the phase diagram. On those lines no KPZ behavior is found and the anomalous transport behavior is different. As discussed by Delfini et al.[3], the mode coupling under these conditions is dominated by the coupling of a sound mode to three sound modes of the same type. Sound damping becomes almost normal. It is still superdiffusive, but only logarithmically so. The k-dependent heat conduction coefficient diverges roughly as $|k|^{-1/2}$ and the heat current time correlation function decays as $t^{-1/2}$, both up to logarithmic corrections. A similar situation appears to arise on the addition of transversal degrees of freedom, with a transversal sound velocity that differs from the longitudinal one. Their currents have zero coupling to pairs of transverse modes and are dominated by the coupling to triplets of these. This should be taken into account in applications to real physical systems, such as nanotubes.

In stationary states the $k^{\alpha-2}$ behavior of the Rayleigh peak implies a nonlinear temperature profile with, for large systems a cusp of form $|x-x_0|^{1-\alpha}$ (the inverse Fourier transform) near a boundary located at x_0. Such nonlinear profiles have been observed regularly in simulations, but so far I have nowhere seen mention of this simple interpretation.

Like in the case of the fluctuating Burgers equation, the mode coupling equations can also be obtained from fluctuating nonlinear hydrodynamic equations[15]. Since their structure remains exactly the same, all the results obtained above hold for all one-dimensional systems satisfying fluctuating hydrodynamic equations with *finite* transport coefficients. The asymptotic long time behavior of density-density and current-current time correlation functions is independent of the values of the transport coefficients, again like for the fluctuating Burgers equation. This argument suggests transport coeffients in nonlinear transport equations may be finite even if the corresponding Green-Kubo integrals are divergent. Whether this actually will occur for one and two dimensional Hamiltonian systems, as far as I know is an open question.

More detailed derivations of the results presented here will be published elsewhere. Besides comparisons to existing numerical results, new Molecular Dynamics simulations will be performed. Applications to quantum systems will also be studied. They look feasible but will require careful consideration of all quantum aspects.

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[16] The sign convention used here for the spatial Fourier transforms is opposite to that used by Prähofer and Spohn, but the same as that used by Ernst, Hauge and Van Leeuwen[9]. Since the scaling functions obtained by Prähofer and Spohn are even in k this is of no severe consequence.
[17] Both groups use the displacement field instead of the number density, but since the latter is the divergence of the former, both are equivalent.
[18] I use $\sigma = \pm 1$ for right respectively left moving sound modes, rather than positive respectively negative frequency, as is conventional.
[19] For obtaining Eq. (7) from the EHvL expression some thermodynamics is required.
[20] Similar expressions may be obtained for the wave number dependent diffusion coefficient and for the current-current time correlation function of the fluctuating Burgers equation.