Dynamic Correlators of Fermi-Pasta-Ulam Chains and Nonlinear Fluctuating Hydrodynamics

Christian B. Mendl\textsuperscript{a}\textsuperscript{*} and Herbert Spohn\textsuperscript{a,\textsuperscript{b}\textsuperscript{†}}

\textsuperscript{a}Zentrum Mathematik, Technische Universität München, 85747 Garching, Germany and
\textsuperscript{b}Physik Department, Technische Universität München, 85747 Garching, Germany

(Dated: July 4, 2013)

We study the equilibrium time correlations for the conserved fields of classical anharmonic chains and argue that their dynamic correlator can be predicted on the basis of nonlinear fluctuating hydrodynamics. In fact our scheme is more general and would cover also other one-dimensional hamiltonian systems, for example classical and quantum fluids. Fluctuating hydrodynamics is a nonlinear system of conservation laws with noise. For a single mode it is equivalent to the noisy Burgers equation, for which explicit solutions are available. Our focus is the case of several modes. No exact solutions have been found so far and we rely on a one-loop approximation. The resulting mode-coupling equations have a quadratic memory kernel and describe the time evolving $3 \times 3$ correlator matrix of the locally conserved fields. Long time asymptotics is computed analytically and finite time properties are obtained through a numerical simulation of the mode-coupling equations.

PACS numbers: 05.60.Cd, 05.20.Jj, 05.70.Ln, 47.10.-g
To predict the dynamic correlator of anharmonic chains is still a theoretical challenge. In higher dimensions fluctuating hydrodynamics serves as a convenient starting point [1–3]. But, as recognized already in the 1970ies [4, 5], in one dimension, while the static correlations are of short range, the dynamic current-current correlations generically have an anomalously slow decay. In particular the transport coefficients, required as an input for fluctuating hydrodynamics, are divergent formal expressions. There have been huge efforts, both through theoretical investigations and numerical simulations, to more precisely characterize this “anomalous” behavior (for a partial list on FPU chains only, see [6–11]). Here we argue that, in one dimension, linear fluctuating hydrodynamics has to be extended to a nonlinear version, which will be outlined below. There have been earlier attempts [12, 13]. Our main advance is to treat the full system of coupled conserved modes and to run time-dependent numerical simulations of the respective mode-coupling equations. In our simulations we use the exact, microscopically computed parameters for the particular anharmonic chain under consideration. Thereby time-resolved predictions are provided which can be tested against molecular dynamics.

For anharmonic chains, the locally conserved fields are compression (or elongation), momentum, and energy. Fluctuating hydrodynamics provides a mesoscopic description of the dynamics of these fields. To illustrate the general framework it is instructive to first recall the simpler case of a single conserved field, here denoted by \( \tilde{u}(x,t) \), space \( x \in \mathbb{R} \), time \( t \). On the macroscopic scale it satisfies the conservation law

\[
\partial_t \tilde{u}(x,t) + \partial_x j(\tilde{u}(x,t)) = 0
\]  

with given current function \( j(\tilde{u}) \). We want to study the fluctuations relative to a uniform background \( u \), i.e. \( \tilde{u}(x,t) = u + u(x,t) \), hence expand (1) to second order in \( u \) and add dissipation plus noise, resulting in the Langevin equation

\[
\partial_t u + \partial_x \left( j'(u) u + \frac{1}{2} j''(u) u^2 - D \partial_x u + \xi \right) = 0 ,
\]  

where \( \xi(x,t) \) is space-time white noise of strength \( \sigma \). Since \( u \) models the deviations from uniformity, we consider the mean zero, space-time stationary process \( u(x,t) \) governed by (2). Then the spatial statistics at fixed time \( t \) is white noise, \( \langle u(x,t)u(x',t) \rangle = \chi \delta(x - x'), \chi = \sigma/2D \), which reflects that the static correlations of an underlying microscopic model decay exponentially fast. Of particular interest is the correlator \( S(x,t) = \langle u(x,t)u(0,0) \rangle \), \( S(x,0) = \]
χδ(x). Its large scale behavior will be dominated by the nonlinearity, but dissipation and noise are required to maintain the proper steady state. Eq. (2) is the noisy Burgers equation, equivalently the spatial derivative of the one-dimensional KPZ equation [14]. There is an exact computation of \( S(x, t) \) using replica [15]. In particular one knows the universal long time limit,

\[
S(x, t) = \chi(\lambda_B |t|)^{-2/3} f_{\text{KPZ}} \left( (\lambda_B |t|)^{-2/3} (x - j'(u)t) \right),
\]

valid for large \( x, t \) with \( \lambda_B = \sqrt{2 \chi |j''(u)|} \). Because of the nonlinearity the spreading is faster than diffusive. Note that \( D, \sigma \) appear in Eq. (3) only through the static susceptibility \( \chi \). Identical scaling properties have been derived also for stochastic lattice gases [16, 17]. The universal scaling function \( f_{\text{KPZ}} \) can be written in terms of a Fredholm determinant and has been computed with great precision [18]. Interpreting the \( u \)-field as the slope of a moving front, Eq. (3) and related predictions have been confirmed for growth processes in the plane, both in experiments on slow combustions fronts [19] and on turbulent liquid crystals [20] and numerically through Monte Carlo simulations of Eden cluster growth [21].

To handle anharmonic chains, we have to extend the above scheme to several components. We use \( \alpha \) as mode index. Then Eq. (1) generalizes to

\[
\partial_t \bar{u}_\alpha + \partial_x j_\alpha(\bar{u}) = 0, \quad \alpha = 1, \ldots, n,
\]

\( \bar{u} = (u_1, \ldots, u_n) \). Expanding as \( \bar{u}_\alpha = u_\alpha + u_\alpha \), the coefficients of the linearized equation are

\[
A_{\alpha\beta}(\bar{u}) = \frac{\partial j_\alpha(\bar{u})}{\partial u_\beta}
\]

and the coefficients of the quadratic part are given by the Hessians

\[
H^\alpha_{\beta\gamma}(\bar{u}) = \frac{\partial^2 j_\alpha(\bar{u})}{\partial u_\beta \partial u_\gamma}.
\]

Since the background \( \bar{u} \) is already prescribed, we will suppress it in our notation. It is assumed that the equal time correlations decay rapidly. Hence \( u_\alpha(x, t) \) at fixed \( t \) is modeled as white noise with covariance \( \langle u_\alpha(x, t)u_\beta(x', t) \rangle = C_{\alpha\beta}\delta(x - x') \), where \( C \) is the \( n \times n \) susceptibility matrix, \( C_{\alpha\beta} = C_{\beta\alpha} \). As valid in great generality [22], and as can be verified directly for anharmonic chains, it holds

\[
AC = CA^T,
\]

transpose denoted by \( ^T \), which implies that \( A \) has real eigenvalues. It turns out to be crucial to switch to normal modes, \( \bar{\phi} \), defined by \( \bar{\phi} = R\bar{u} \). We require the normal mode \( \phi_\alpha \) to have a
definite propagation velocity, $c_\alpha$, and the modes to be statistically uncorrelated. Hence the similarity matrix $R$ has to satisfy $RAR^{-1} = \text{diag}(c_1, \ldots, c_n)$ and $RCR^T = 1$, where both properties together determine $R$ uniquely up to an overall sign.

We now expand in Eq. (4) to second order in $\vec{u}$, transform to normal modes, and add dissipation plus noise, resulting in the statistical field theory

$$
\partial_t \phi_\alpha + \partial_x (c_\alpha \phi_\alpha + \langle \phi | G^\alpha \vec{\phi} \rangle - \partial_x (D \phi)_\alpha + \xi_\alpha) = 0,
$$

(8)

$\alpha = 1, \ldots, n$, where

$$
G^\alpha = \sum_{\alpha'=1}^n \frac{1}{2} R_{\alpha\alpha'} (R^{-1})^T H^{\alpha'} R^{-1}.
$$

(9)

The diffusion matrix $D$ is positive definite. $\xi_\alpha(x,t)$ is space-time white noise with strength

$$
\langle \xi_\alpha(x,t) \xi_\beta(x',t') \rangle = 2 D_{\alpha\beta} \delta(x-x') \delta(t-t').
$$

(10)

As before, since $\vec{\phi}$ models the deviation from uniformity, we consider the mean zero, stationary process $\vec{\phi}(x,t)$ governed by (8). In the linear case, $G^\alpha = 0$, $\vec{\phi}(x,t)$ is a Gaussian process, which for fixed $t$ has white noise statistics with independent components of unit strength, as imposed by $RCR^T = 1$. Note that nonlinear fluctuating hydrodynamics requires as only microscopic input the average currents $j_\alpha$, more precisely $A, H^\alpha$, and the susceptibility $C$.

Coupled Langevin equations of the form (8) have been proposed and studied before in disguise. Introducing the height $h_\alpha$ through $\partial_x h_\alpha = u_\alpha$, Eq. (8) turns into the coupled KPZ equations in one dimension, which describe dynamic roughening of directed lines [23], sedimenting colloidal suspensions [24, 25], stochastic lattice gases [22, 26], and magnetohydrodynamics [27, 28].

Equipped with the above frame, let us turn to anharmonic chains, for which purpose we first have to figure out the conserved fields and their macroscopic Euler equations. The chain consists of $N$ particles, position $q_j$, momentum $p_j$, $j = 1, \ldots, N$, unit mass, and is governed by the Hamiltonian

$$
H = \sum_{j=1}^N \left( \frac{1}{2} p_j^2 + V(q_{j+1} - q_j) \right),
$$

(11)

where periodic boundary conditions of the form $q_{N+1} = q_1 + L$ are imposed. A prototypical potential is the FPU choice $V(y) = \frac{1}{2} y^2 + \frac{1}{3} a y^3 + \frac{1}{4} y^4$. The locally conserved microscopic fields are compression $r_j = q_{j+1} - q_j$, momentum $p_j$, and energy $e_j = \frac{1}{2} p_j^2 + V(r_j)$. Following
our blueprint we collect them as the three-vector $\vec{g}$ with $g_1(j,t) = r_j(t)$, $g_2(j,t) = p_j(t)$, and $g_3(j,t) = e_j(t)$. In a microcanonical simulation one fixes the length (compression) per particle, $\ell$, as $L = N\ell$, the momentum per particle, $u$, as $\sum_{j=1}^{N} p_j = Nu$, and the energy per particle, $\epsilon$, as $H = N\epsilon$. Computationally, it is convenient to switch to the grand canonical pressure ensemble. Then $\ell$ is conjugate to the pressure $p$ and the internal energy $\epsilon$ to the inverse temperature $\beta$. In the grand canonical ensemble, $\{r_j, p_j\}$ become independent random variables. The distribution of $p_j$ is a Maxwellian shifted by $u$, and the distribution of $r_j$ is given by $Z^{-1}\exp[-\beta(V(y) + py)] = \langle\cdot\rangle_{p,\beta}$ with partition function $Z = \int dy \exp[-\beta(V(y) + py)]$. Clearly the pressure equals the average force acting on a specified particle. The microcanonical and grand canonical parameters are related through

$$\ell = \langle y \rangle_{p,\beta}, \quad \epsilon = \frac{1}{2\beta} + \langle V(y) \rangle_{p,\beta}.$$  \hfill (12)

On the hydrodynamic scale the average conserved fields $\langle g_\alpha(j,t) \rangle$ are slowly varying and approximated by the continuum fields $\bar{u}_\alpha(x,t)$, where $x$ stands for the continuum approximation of the particle index $j$. From the microscopic conservation laws one deduces the hydrodynamic currents

$$j_\ell = -u, \quad j_u = p(\ell, \epsilon - \frac{1}{2}u^2), \quad j_\epsilon = up(\ell, \epsilon - \frac{1}{2}u^2),$$  \hfill (13)

which, when inserted in Eq. (4), result in the Euler hydrodynamics of the anharmonic chain. Without loss of generality the equilibrium state of the chain is taken at $u = 0$. The similarity transformation $R$, the velocities $c_\alpha$, and the coupling coefficients $G^\alpha$ are computed in terms of at most third order cumulants involving $y, V(y)$ with average $\langle\cdot\rangle_{p,\beta}$. These integrals and the somewhat unwieldy required substitutions are easily performed using Mathematica. There are three modes: the heat mode, $\alpha = 0$, with velocity $c_0 = 0$ and two sound modes, $\alpha = \pm 1$, with velocity $c_\sigma = \sigma c$, $\sigma = \pm 1$, where $c$ is the sound speed,

$$c^2 = -\partial_\ell p + p\partial_\epsilon p.$$  \hfill (14)

The microscopic equilibrium time correlations of the conserved fields in normal mode representation are defined by ($\sharp$ signals normal mode)

$$S_{\alpha\beta}^\sharp(j,t) = \langle (R\vec{g})_\alpha(j,t)(R\vec{g})_\beta(0,0) \rangle_c,$$  \hfill (15)

the index $c$ standing for connected. Our central claim is that the normal mode correlations of the chain are approximated for large $x,t$ as

$$S_{\alpha\beta}^\sharp(j,t) \simeq \langle \phi_\alpha(x,t)\phi_\beta(0,0) \rangle = S_{\alpha\beta}^{\phi\phi}(x,t).$$  \hfill (16)
This leaves us with the task to work out the correlator $S^{\phi\phi}$ for the stochastic field theory (8). With no exact solution at hand, we rely on the mode-coupling equations in one-loop approximation. But before, since the three modes travel with distinct velocities, for long times only the self-coupling will contribute. Since $G_{11}^1 = -G_{-1-1}^{-1}$ and generically $G_{11}^1 \neq 0$, the two sound modes are expected to satisfy the KPZ scaling (3) with $\chi = 1$, $j'(u) = \sigma c$ and $\lambda_B = 2\sqrt{2}|G_{\sigma\sigma}^{\sigma}|$, $\sigma = \pm 1$. The decoupling of modes is convincingly confirmed in a two-component lattice gas [22]. For the heat mode our argument fails, since $G_{00}^{0} = 0$ always. Note that for the popular case of an even potential, $V(y) = V(-y)$, at $p = 0$ also $G_{11}^1 = 0$ implying that all three modes are non-KPZ.

The derivation of the mode-coupling equations is presented in [29]. Numerically one observes that, while off-diagonal elements of $S_{\alpha\beta}^{\delta}$ develop immediately, they decay fairly rapidly. Thus we may invoke the diagonal approximation, $S_{\alpha\beta}^{\delta}(x,t) \simeq \delta_{\alpha\beta} f_\alpha(x,t)$ in position space. Switching to Fourier space and adopting the standard conventions for discrete Fourier transforms, the mode-coupling equations then read

$$\partial_t \hat{f}_\alpha(k,t) = -ic_\alpha \sin(2\pi k) \hat{f}_\alpha(k,t) - 2(1 - \cos(2\pi k))$$

$$\times \left( D_\alpha \hat{f}_\alpha(k,t) + \int_0^t ds \hat{M}_{\alpha\alpha}(k,s) \hat{f}_\alpha(k,t-s) \right),$$

where $\hat{M}_{\alpha\alpha}(k,s)$ is the mode coupling function and $D_\alpha$ is the mode-derivative operator.
\[ \alpha = 1, \ldots, n, \] with memory kernel

\[
\hat{M}_{\alpha\alpha}(k, t) = 2 \sum_{\beta, \gamma=1}^{n} (G_{\beta\gamma}^\alpha)^2 \int_{-\frac{1}{2}}^{\frac{1}{2}} dq \, \hat{f}_\beta(k - q, t) \hat{f}_\gamma(q, t).
\] (18)

The special case \( n = 1 \) is discussed already in [30], see [31] for a first numerical integration. In Fig. 1 we display a time sequence for a single mode with \( G_{11}^1 = \frac{1}{2} \). For \( t \geq 32 \) the scaled

![Graphs of S_{aa}(x,t) for different times (a) t = 12, (b) t = 32, (c) t = 64, (d) heat mode, (e) right sound mode.](image)

FIG. 2. (Color online) Time sequence of normal mode correlations for the FPU chain with \( a = 2, p = 1, \beta = 0, \) and \( u = 0 \) (a), (b), (c). Magnification of the central heat mode peak (d) and the right sound mode peak (e) in suitably rescaled coordinates.

solution remains stationary. The asymptotic scaling function differs from \( f_{\text{KPZ}} \) by a few percent only. On this basis we expect that such a precision extends to several modes.

As a representative example for anharmonic chains we choose the FPU potential with \( a = 2 \) and \( u = 0, p = 1, \beta = 2, \) resulting in \( c = 1.455 \), which are commonly used parameters in molecular dynamics simulations. \( V(y) + py \) has a single minimum at \( y = -1.755 \). We stress that simulations can be performed for any choice of the potential and thermodynamic parameters at minimal numerical efforts. With the theoretically determined velocities and
couplings, the mode-coupling equations are iterated in time, using Fourier space representation as in (17), in such a way that the values of the memory kernel $\hat{M}_{\alpha\alpha'}(k, s)$ for $s < t$ can be stored and re-used. No diagonal approximation is invoked. The time and momentum variables are discretized by a uniform grid. In Fig. 2 the grey vertical lines at $\pm ct$ indicate the predicted position of the sound mode peaks. The off-diagonal elements of $S^{\phi}$ are essentially zero. In the time sequence we display the superimposed diagonal normal mode correlations (area 1 under each curve). More details are provided in the blow-up. For the heat mode one observes oscillations which move away from the center and eventually die out. The tail of the heat mode is cut at the location of the sound mode. At the longest available time the sound modes are still asymmetric and have not yet reached their asymptotic shape.

Theoretically the scaling function for the heat mode can be obtained by inserting the known asymptotic form of $f_{\pm 1}$ in (18) with $\alpha = 0$. Solving the then linear memory equation (17) results in the symmetric Levy 5/3 distribution, $f_0(k, t) = \exp[-|k|^{5/3}\lambda_0|t|]$ with computable non-universal coefficient $\lambda_0$. The Levy 5/3 for the heat mode peak has been observed in molecular dynamics for the hard point potential, $V(y) = 0$ for $0 < y < a$ and $V(y) = \infty$ otherwise, with a suitable choice of thermodynamic parameters [32]. Note that the slow tails of the Levy distribution are cut by the sound mode.

Based on these and further simulations of the mode-coupling equations for anharmonic chains, the following qualitative picture for the motion of the normal mode peaks in index number space seems to emerge. The sound modes “rapidly” decay to a shape function which is centered at $\sigma ct$ and varies on the scale $t^{2/3}$. The shape function itself is still slowly varying. The couplings $G^{0}_{\sigma\sigma}$ determine the scaling of the heat mode. Since only the integral over the square of the shape function is involved, the heat mode rapidly achieves its asymptotic shape in the range $\{|x| \leq ct\}$ and with a still slowly varying non-universal constant. The slow motion of the sound modes is governed by $G^{0}_{00}$ and $G^{\sigma}_{-\sigma-\sigma}$. Assuming already the validity of overall scaling picture, the size of these corrections is estimated to be of the order $t^{-1/15}$, resp. $t^{-1/9}$, relative to the leading term which signals that $f_{KPZ}$ is approached rather slowly. Of course, only a qualitative guideline is presented. For the precise dynamics all velocities and couplings have to be used.

**Conclusions.** We developed a nonlinear extension of fluctuating hydrodynamics applicable to one-dimensional systems, in principle including classical fluids, quantum fluids [33–35], and quantum spin chains. Already at the level of the one-loop approximation it is crucial to
maintain the couplings between all conserved modes. As applied to anharmonic chains, the numerical solutions of the mode-coupling equations provide a realistic picture of the correlation dynamics and, on the limited time scale simulated, are consistent with the analytical computations and also with molecular dynamics, as far as available.

We thank Henk van Beijeren, Patrik Ferrari, Tomohiro Sasamoto, and Hong Zhao for most useful comments. The research is supported by the DFG project SP 181/29-1.

* mendl@ma.tum.de
† spohn@ma.tum.de

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