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Nonequilibrium Invariant Measure under Heat Flow

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We provide an explicit representation of the nonequilibrium invariant measure for a chain of harmonic oscillators with conservative noise in the presence of stationary heat flow. By first determining the covariance matrix, we are able to express the measure as the product of Gaussian distributions aligned along some collective modes that are spatially localized with power-law tails. Numerical studies show that such a representation applies also to a purely deterministic model, the quartic Fermi-Pasta-Ulam chain.

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Characterizing the invariant measure of systems steadily kept out of equilibrium is one of the main challenges towards the construction of a nonequilibrium statistical thermodynamics. Some insight has been gained over the years mostly thanks to the solution of stochastic models [1]. In particular, heat conductivity in one-dimensional systems has played a prominent role, because its understanding would also imply giving a microscopic basis to the Fourier's law [2]. The first step dates back to 1967, when the problem of a harmonic chain in contact with two thermal reservoirs at different temperatures was solved exactly [3]. Unfortunately, the integrability of the underlying dynamics leads to several unphysical features (e.g., a vanishing temperature gradient) [2]. Later, purely stochastic models, where energy is assumed to diffuse between neighboring boxes (the oscillators), have been considered [4,5]. More recently, systems of harmonic oscillators exchanging energy with "conservative" noise have been proven to admit a unique stationary state with a constant heat flux and a linear temperature profile [6]. Admittedly, the leap from such class of models to even the simplest deterministic, nonlinear ones is still a challenge for the theory [7].

In this Letter we approach the problem of describing the invariant measure in terms of the spectral properties of the covariance matrix, i.e., at the level of two-point correlators of the relevant dynamical variables. This procedure is often referred to in data analysis as principal component analysis [8]. It amounts to expressing the initial distribution as the product of univariate Gaussians aligned along the eigenvectors of the covariance matrix and whose widths are given by the corresponding eigenvalues. The decomposition is exact for multivariate Gaussians (linear processes). In order to facilitate the comparison with the Gibbs equilibrium measure, it is convenient to express the covariance matrix in those variables that make it perfectly diagonal at equilibrium. At variance with purely diffusive models, the appearance of nondiagonal terms is crucially related to the onset of a nonzero heat flux and, in particular, to the existence of anomalous transport properties. Because of

the almost-diagonal structure, the eigenvectors are localized in space.

To illustrate the approach, we first introduce a stochastic model, closely related to the one presented in Ref. [9], in which coupled harmonic oscillators interact also by random pairwise collisions, each conserving both energy and momentum. Because of the linearity of the associated master equation, the equations for the two-point correlators are closed and can be computed exactly without any factorization assumption. Another useful property of the model is that it encompasses, as a limit case, an anomalous regime, in which the relevant transport coefficient, the thermal conductivity, diverges by virtue of total momentum conservation [10]. This allows comparing the cases of normal and anomalous conductivity. In order to test the generality of these results, we finally perform the same type of analysis by directly simulating a nonlinear deterministic model. In spite of the unavoidable statistical fluctuations, we find encouraging qualitative similarities.

The first model we deal with is a harmonic chain of N unit-mass particles, whose displacements and momenta are denoted by q_i and $p_i = \dot{q}_i$. The chain is in contact with stochastic Langevin heat baths at its extrema,

$$\begin{aligned} \dot{p}_i = & -kq_i + \omega^2(q_{i+1} - 2q_i + q_{i-1}) + \delta_{i,1}(\xi_+ - \lambda p_1) \\ & + \delta_{i,N}(\xi_- - \lambda p_N), \end{aligned} \quad (1)$$

where ξ_{\pm} 's are independent Wiener processes with zero mean and variance $2\lambda k_B T_{\pm}$, respectively. Fixed boundary conditions $q_0 = 0, q_{N+1} = 0$ are assumed. Besides satisfying dynamics (1), neighboring particles are assumed to randomly collide, and thereby to exchange their momenta, with a rate γ . As a result, the phase-space probability density $P(x, t)$, that we write in terms of the $2N$ -dimensional vector whose components x_{μ} are $(q_1, \dots, q_N, p_1, \dots, p_N)$, satisfies the master equation

$$\frac{\partial P}{\partial t} = (\mathbb{L} + \mathbb{L}_{\text{col}})P \quad . \quad (2)$$

The first term accounts for both the deterministic force and

the coupling with the heat baths and is given by

$$\mathbb{L}P = \sum_{\mu,\nu} \left[a_{\mu\nu} \frac{\partial}{\partial x_\mu} (x_\nu P) + \frac{d_{\mu\nu}}{2} \frac{\partial^2 P}{\partial x_\mu \partial x_\nu} \right] \quad (3)$$

where $a_{\mu\nu}$ and $d_{\mu\nu}$ are elements of the $2N \times 2N$ matrices \mathbf{a} and \mathbf{d} that we write in terms of $N \times N$ blocks

$$\mathbf{a} = \begin{pmatrix} \mathbf{0} & -\mathbf{I} \\ \omega^2 \mathbf{g} + k\mathbf{I} & \lambda \mathbf{r} \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 2\lambda k_B T (\mathbf{r} + \eta \mathbf{s}) \end{pmatrix} \quad (4)$$

with \mathbf{I} , $\mathbf{0}$ being the identity and null matrices, respectively, $r_{ij} = \delta_{ij}(\delta_{i1} + \delta_{iN})$, $s_{ij} = \delta_{ij}(\delta_{i1} - \delta_{iN})$ and $g_{ij} = 2\delta_{ij} - \delta_{i+1,j} - \delta_{i,j+1}$. Moreover, we let $T = (T_+ + T_-)/2$ and $\eta = (T_+ - T_-)/T$. The collisional term is

$$\mathbb{L}_{\text{col}}P = \gamma \sum_i [P(\dots p_{i+1}, p_i \dots) - P(\dots p_i, p_{i+1} \dots)]. \quad (5)$$

For $k = \gamma = 0$ the model reduces to the one of Ref. [3], where it was showed that the nonequilibrium measure is a multivariate Gaussian and all the second moments were exactly determined.

By denoting with $\langle \cdot \rangle$ the average over P , the covariance matrix $c_{\mu\nu} = \langle x_\mu x_\nu \rangle$ can be written as four $N \times N$ blocks,

$$\mathbf{c} = \begin{pmatrix} \mathbf{u} & \mathbf{z} \\ \mathbf{z}^\dagger & \mathbf{v} \end{pmatrix} \quad (6)$$

with $u_{ij} = \langle q_i q_j \rangle$, $v_{ij} = \langle p_i p_j \rangle$, $z_{ij} = \langle q_i p_j \rangle$; the symbol \dagger denotes the transpose and we also assume $\langle x_\mu \rangle = 0$. The evolution equation is obtained by multiplying both sides of Eq. (2) by $x_k x_l$ and thereby integrating,

$$\dot{\mathbf{c}} = \mathbf{d} - \mathbf{a}\mathbf{c} - \mathbf{c}\mathbf{a}^\dagger + \dot{\mathbf{c}}_{\text{col}}. \quad (7)$$

The first three terms on the right-hand side are associated with the operator (3) and are the same found in Ref. [3]. The contribution due to collisions (5) is

$$\dot{\mathbf{c}}_{\text{col}} = -\gamma \begin{pmatrix} \mathbf{0} & \mathbf{z}\mathbf{g} \\ \mathbf{g}\mathbf{z}^\dagger & \mathbf{w} \end{pmatrix} \quad (8)$$

where the auxiliary $N \times N$ matrix \mathbf{w} is defined by

$$w_{ij} \equiv \begin{cases} v_{i+1j} + v_{i-1j} + v_{ij-1} + v_{ij+1} - 4v_{ij} & |i-j| > 1 \\ v_{i\pm 1j} + v_{ij\mp 1} - 2v_{ij} & i-j = \pm 1 \\ v_{i-1j-1} + v_{i+1j+1} - 2v_{ij} & i=j. \end{cases}$$

The matrices \mathbf{u} and \mathbf{v} are symmetric by construction, and one can easily check that \mathbf{z} is antisymmetric in the stationary state.

Observables.—The most relevant observables are the kinetic temperature field $T_i = \langle p_i^2 \rangle = v_{ii}$ and the local energy current J_i , that can be written as the sum of two contributions, $J_i = J_i^d + J_i^c$, where

$$J_i^d = \omega^2 \langle q_{i-1} p_i \rangle = \omega^2 z_{i-1,i}, \quad (9)$$

$$J_i^c = \frac{\gamma}{2} [\langle p_i^2 \rangle - \langle p_{i-1}^2 \rangle] = \frac{\gamma}{2} [v_{i,i} - v_{i-1,i-1}] \quad (10)$$

are the deterministic contribution (due to the springs) and the stochastic one (due to collisions), respectively.

Coordinate change.—In the perspective of better understanding the differences between the equilibrium and non-equilibrium invariant measure, it is convenient to choose new variables Q_i, P_i in such a way that the equilibrium covariance matrix becomes fully diagonal. This is accomplished by the linear transformation

$$Q_i = a q_{i+1} - b q_i; \quad P_i = p_i \quad (11)$$

with $a = [\omega^2 + k/2 + (\omega^2 k + k^2/4)^{1/2}]^{1/2}$, $b = \omega^2/a$. Moreover, in analogy to Eq. (6), we introduce a new covariance matrix \mathbf{C} whose components \mathbf{U} , \mathbf{V} , and \mathbf{Z} are given by $U_{ij} = \langle Q_i Q_j \rangle$, $V_{ij} = \langle P_i P_j \rangle$, and $Z_{ij} = \langle Q_i P_j \rangle$.

Numerical solution.—The stationary solution of Eq. (7) can be efficiently computed by exploiting the sparsity of the corresponding linear problem, as well as the symmetries of the unknowns \mathbf{u} , \mathbf{v} and \mathbf{z} . The elements of \mathbf{C} can be thereby obtained from transformation (11). The diagonal elements of \mathbf{C} correspond to the temperature profile. This is illustrated in Fig. 1(a), where both V_{ii} and U_{ii} are plotted versus $y \equiv 2i/N - 1$ for $k = 2$ and different system sizes. The linear profile confirms the validity of Fourier's law, as expected in the presence of an on-site potential [2]. All the other \mathbf{C} elements are of order $\mathcal{O}(1/N)$ and proportional to the temperature difference ΔT and are, therefore, scaled accordingly in the other panels of Fig. 1. The upper-diagonal of \mathbf{Z} is plotted in panel (b); because of the anti-symmetry of \mathbf{z} , $Z_{i-1,i}$ coincides with the deterministic component J_i^d of the flux [see Eq. (9)]. The singular behavior at the extrema is a consequence of J_i^d vanishing at the boundaries, where the particles are not free to move.

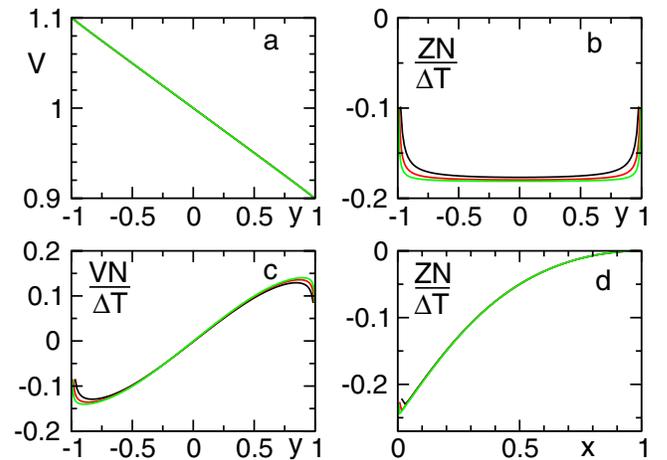


FIG. 1 (color online). Some elements of the covariance matrix \mathbf{C} (properly normalized) for $k = 2$, $\omega = 1$, $\gamma = 1$, $\lambda = 1$, $T_+ = 1.1$, $T_- = 0.9$ and different chain sizes $N = 128, 256, 512$; (a) $U_{i,i} = V_{i,i} = T_i$, (b) $NZ_{i,i+1}/\Delta T$, (c) $NV_{i,i+1}/\Delta T$, (d) $NZ_{i,N+1-i}$ (antidiagonal).

The behavior of \mathbf{V} along the upper diagonal is presented in Fig. 1(c); it basically quantifies the $1/N$ finite-size deviations exhibited by the temperature profile. Finally, the dependence of \mathbf{Z} along the principal antidiagonal [$x = (i - j)/N$] is shown in Fig. 1(d), where one can notice a slow decay of the correlations. This is analogous to what found in purely stochastic models [5,11] and is believed to be a generic feature of nonequilibrium stationary states [1].

Principal component analysis.—Once the covariance matrix is known, it is natural to determine its eigenvalues $\lambda^{(\nu)}$ ($\nu = 1, \dots, 2N$)—that we assume to be ordered from the largest to the smallest one—and the corresponding normalized eigenvectors, that are denoted as $(\phi_1^{(\nu)}, \dots, \phi_N^{(\nu)}, \psi_1^{(\nu)}, \dots, \psi_N^{(\nu)})$. Since \mathbf{C} is “almost diagonal”, $\lambda^{(\nu)}$ yields the temperature profile and each of the two eigenvector components are localized. A less obvious fact is that the eigenvalues come in almost degenerate pairs (the relative difference being much smaller than $1/N$) and that the ϕ and ψ components of corresponding eigenvectors are localized around the same site $m = \nu/2$ [see Fig. 2(a), where the ψ components are plotted for $\nu = 100, 101$]. We interpret this by saying that any pair $(\nu, \nu + 1)$ of eigenvectors identifies a single, localized, degree of freedom at equilibrium with a “temperature” $\lambda^{(\nu)}$.

The eigenvector spatial structure can be fruitfully illustrated by plotting $\rho_i^{(\nu)} = [\phi_i^{(\nu)}]^2 + [\psi_i^{(\nu)}]^2 + [\phi_i^{(\nu+1)}]^2 + [\psi_i^{(\nu+1)}]^2$. In Fig. 2(b), we see that the vector width does not depend on the system size, which only determines the

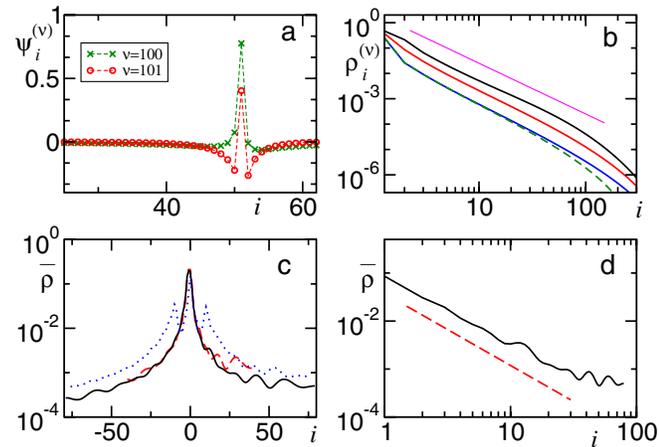


FIG. 2 (color online). Localized structure of the eigenvectors of \mathbf{C} . The upper panels correspond to the model and parameter values of Fig. 1: (a) ψ components of the vectors $\nu = 100, 101$ for $N = 200$; (b) the squared envelope $\rho_i^{(\nu)}$ defined in the text for $N = 400$ with $\gamma = 2$ (dashed line) and $N = 800$ with $\gamma = 0.5, 1, 2$ (solid lines from top to bottom). (c) $\bar{\rho} = \sum_{\nu_2=\nu_1}^{\nu_2} \rho_i^{(\nu)}$: FPU model for $N = 511, \nu_1 = 150, \nu_2 = 350$ (dotted line), unpinning case ($\gamma = 0.4$) for $N = 512, \nu_1 = 150, \nu_2 = 350$ (solid line) and $N = 256, \nu_1 = 75, \nu_2 = 175$ (dashed line); (d) same data in log-log scale for the unpinning case ($N = 512$). The straight lines have a slope -2 in (b) and -1.5 in (d).

extension of the tails. Moreover, Fig. 2(b) shows also that the squared envelope decays as a power-law from its localization center, $\rho_i^{(\nu)} \approx [\ell/|i - m|]^2$ [12]. This defines a typical length ℓ that can be interpreted as the minimal size of the spatial region that is necessary to ensure a local thermal equilibrium, a sort of mean free path. This interpretation is supported by the fact that ℓ decreases upon increasing the strength γ of the stochastic process, which is the only thermalization mechanism in the bulk.

The unpinning case.—The limit case of vanishing pinning force, $k = 0$, is of particular interest. Indeed, here the total momentum is conserved and we expect an anomalous behavior, i.e., a diverging finite-size thermal conductivity [2,10]. As shown in Fig. 3(a) the temperature profile (solid line) is no more linear. Remarkably, we find also that all the nondiagonal elements are in this case of order $\mathcal{O}(1/\sqrt{N})$ [see the solid lines in Fig. 3(b)–3(d)]. In particular, through Eq. (9) this implies that the heat conductivity diverges as \sqrt{N} , in agreement with the linear response prediction [9]. This observation is supported by analytical arguments based on an expansion of Eq. (7) in the smallness parameter $1/\sqrt{N}$ [13]. A second remarkable difference with the case $k > 0$ is the exponential decay of the off-diagonal terms, the decay length scaling as \sqrt{N} . For instance, in Fig. 3(d) (solid line) the elements along the antidiagonal of the matrix \mathbf{Z} are plotted versus $x\sqrt{N} = (i - j)/\sqrt{N}$; similar curves are obtained for the same elements of the matrices \mathbf{U} and \mathbf{V} .

On the other hand, the principal component analysis reveals that the eigenvalues still appear in almost degenerate pairs and the eigenvectors are localized [see Fig. 2(c)], although the tails decay with a slower power-law exponent, close to 1.5 [see Fig. 2(d)].

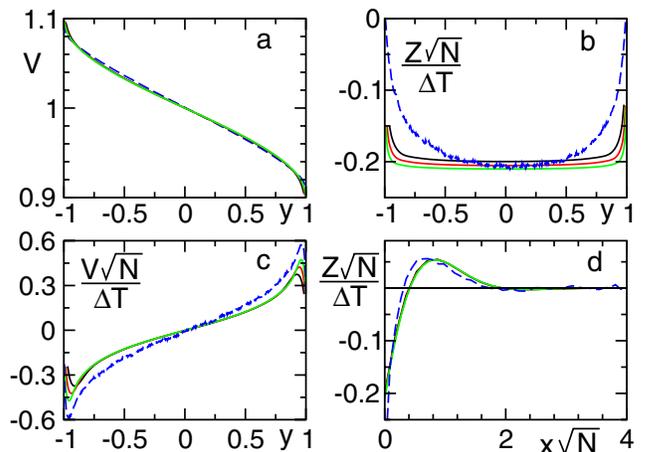


FIG. 3 (color online). The same matrix elements as in Fig. 1 in the absence of an on-site potential $k = 0$ and for $\gamma = 0.4$. The three solid lines refer to $N = 128, 256, 512$. The dashed lines are obtained by simulation of a chain of 511 quartic FPU oscillators.

Comparison with a nonlinear model.—In order to assess the generality of the scenario resulting from the stochastic model, it is crucial to investigate also a nonlinear deterministic model. We have considered the Fermi-Pasta-Ulam (FPU) chain with a purely quartic interparticle potential $(q_{i+1} - q_i)^4/4$ [14]. We have implemented Eq. (1), by working with stochastic heat baths in the limit of a small mass for the reservoir's particles [2]. This choice allows us to use a symplectic integrator and thereby to use “large” time steps (10^{-2}), still obtaining accurate results. The covariance matrix is then estimated by time averaging and is thus affected by the unavoidable statistical fluctuations (we have sampled about 5×10^7 data points separated by one time unit). For a meaningful comparison, the Q variables (11) are chosen to be $\Omega_i(q_{i+1} - q_i)$, where Ω_i is a renormalized frequency that can be determined by imposing that the effective harmonic potential energy equals the kinetic energy. The homogeneity of the potential suggests setting $\Omega_i = \zeta T_i^{1/4}$; we have found that the best overlap between kinetic and potential energy is obtained for $\zeta = 1.4$ [15]. The results obtained for a chain of 511 oscillators are plotted in Fig. 3 (dashed lines), where the same \sqrt{N} scaling of variables as in the unpinned stochastic model is implicitly assumed. Even though we should notice that $\gamma = 0.4$ for the stochastic model has been selected to yield the best agreement with the temperature profile of the FPU model, the similarity between the deterministic and the stochastic model is quite striking and extends to the temperature deviations as well as to the behavior of the off-diagonal terms. The only elements that are significantly different are the upper-diagonal terms of \mathbf{Z} [see Fig. 3(b)]. Statistical fluctuations prevent an accurate analysis of the single eigenvectors. In order to reduce their effects, we have decided to average a subset of eigenvectors around their localization center. The results presented in Fig. 2(c) (the average, denoted by $\bar{\rho}$, is performed over the eigenvectors from 150 to 350) reveal that also the eigenvectors of the FPU model are localized (the side peaks seem to be a finite-size effect, as they tend to disappear upon increasing the system size). A quantitative analysis of the decay rate is out of question.

The study of the above models has shown that the key features of nonequilibrium steady states are captured by principal component analysis and are contained in the statement that, the invariant measure can be effectively approximated as the product of independent Gaussians for the collective, localized mode amplitudes. The variances are the local temperatures.

In order to further explore the validity of this claim, we have studied the fluctuations of the single mode amplitudes and the correlations between pairs of such modes, going beyond the second cumulants. Within the numerical accuracy, we have not found any deviation from the assumption

of a purely Gaussian distribution, even in the FPU model. We can also conjecture that the Gaussian assumption should become exact in the thermodynamic limit for model (1). We want to point out that, to our knowledge, this is the first case where an explicit nontrivial, even if approximate, representation of the nonequilibrium invariant measure is given for Hamiltonian models. As a further development, the stochastic model should be modified to reproduce quantitatively the universal scaling laws predicted for a generic system [10], as well as to analyze the corresponding modifications on the structure of the measure.

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