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Phys. Rev. Lett. **127**, 010601 — Published 2 July 2021

DOI: [10.1103/PhysRevLett.127.010601](https://doi.org/10.1103/PhysRevLett.127.010601)

Microscopic theory of fluctuating hydrodynamics in nonlinear lattices

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(Dated: June 1, 2021)

The theory of fluctuating hydrodynamics has been an important tool for analyzing macroscopic behavior in nonlinear lattices. However, despite its practical success, its microscopic derivation is still incomplete. In this work, we provide the microscopic derivation of fluctuating hydrodynamics, using the coarse-graining and projection technique; the equivalence of ensembles turns out to be critical. The Green-Kubo (GK) like formula for the bare transport coefficients are presented in a numerically computable form. Our numerical simulations show that the bare transport coefficients exist for a sufficiently large but finite coarse-graining length in the infinite lattice within the framework of the GK like formula. This demonstrates that the bare transport coefficients uniquely exist for each physical system.

Introduction.— Hydrodynamics is a universal theory that describes the flow of locally conserved quantities. In addition to the development of numerical computation of complicated flow in macroscopic systems [1], the concept of hydrodynamics has been extended to nano-fluids [2] and cold atomic systems [3–5], where the standard hydrodynamics in textbooks of fluid dynamics [6] cannot be directly applied. In particular, for low dimensional fluids, macroscopic transport coefficients such as heat conductivity diverge due to long-time tail in the correlation functions [7–11], which has been experimentally observed in low dimensional materials [12, 13]. Even for such anomalous transport, it has been recognized that fluctuating hydrodynamics (FH) [6, 14] can provide a quantitative prediction of dynamical phenomena assuming the form of the equations and choice of parameter values [8, 15–17]. A key drawback of the theory is the absence of a microscopic formula for the bare transport coefficients. A naive application of the standard Green-Kubo (GK) formula leads to a divergent answer. The detailed form of the transport coefficients is crucial for our understanding the strong finite-size effects seen in near-integrable models [18]. In order to deepen our understanding it is thus desirable to derive the FH from a microscopic mechanical model and to connect the parameter values in the hydrodynamic equations with those of the microscopic Hamiltonian.

Let q_n and p_n be variables that represent the position and momentum of the n th particle in a one-dimensional lattice. The Hamiltonian is generally described as

$$H = \sum_{n=1}^N p_n^2/2 + V(r_n), \quad r_n = q_{n+1} - q_n, \quad (1)$$

where the masses are set to unity and r_n is the stretch variable. The potential V depends solely on the stretch variables. Anomalous heat transport, which refers to the divergence of the heat conductivity, has been extensively studied for this Hamiltonian [9–11]. Since there

are three locally conserved quantities: the stretch, momentum, and energy, the long time and large distance behavior of the non-linear lattice may be described by the effective dynamics of their densities $u_a(x)$ at position x in the continuous picture, where the subscript a stands for the stretch ($a = r$), momentum ($a = p$) and energy ($a = \epsilon$). According to the FH theory for this system [16, 17], the time evolution of $u_a(x)$ near equilibrium is assumed to obey

$$\begin{aligned} \partial_t u_a = & -\partial_x [J_{a,\text{leq}}(u_r, u_p, u_\epsilon) \\ & - \sum_{a'=r,p,\epsilon} D_{a,a'} \partial_x u_{a'} + \xi_{a,x}(t)]. \end{aligned} \quad (2)$$

Here, $J_{a,\text{leq}}$ denotes the local equilibrium current which is given as a function of (u_r, u_p, u_ϵ) for each x . The functional form of $J_{a,\text{leq}}$ is determined from the local equilibrium thermodynamics or the local equilibrium distribution. The terms D and ξ , respectively, stand for dissipation and noise, which are both put by hand in order that the equilibrium properties are guaranteed, imposing the fluctuation dissipation relation [19]. Recently, in Ref. [17], Spohn has analyzed the local equilibrium current by transforming the three conserved variables into left and right moving sound modes, and a heat mode, and consequently derived the nontrivial connection to the Kardar-Parisi-Zhang equation of the nonlinear chains. In addition, through the mode-coupling calculation, the anomalous behavior in the current correlation has been clarified. Later, the scaling form of the space-time correlations arising from hydrodynamics has been numerically confirmed in many types of systems [20–25].

Despite its success, the derivation of FH from Hamiltonian dynamics is still incomplete. In particular, let us focus on the parameter $D_{a,a'}$ which is referred to as the *bare transport coefficients* (Below, we use this terminology for all related quantities that are locally transformed). These should be distinguished from the macroscopic transport coefficients measured under non-equilibrium conditions,

such as heat conductivity. The latter corresponds to renormalized transport coefficients obtained by taking hydrodynamic fluctuations into account. The fundamental problem here is to derive the bare transport coefficients $D_{a,a'}$ from Hamiltonian dynamics. We remark that while the diffusion term formula for integrable chains has been studied in the framework of generalized hydrodynamics [26–28], it is unavailable for non-integrable systems in view of the fact that a simple application gives a divergence in this case. Hence, a more strict and general formulation is necessary to complete the FH theory.

Differences between microscopic expressions of bare transport coefficients and macroscopic transport coefficients have been addressed in the context of projection operator methods [29–32]. However, the debate remained formal, and the details on the bare transport coefficients could not be studied due to several uncontrolled functional forms that arise in the derivation. Note that in the mode-coupling calculations in Ref. [17], the assumption of finite bare transport coefficients are critical in deriving diverging heat conductivity. However, the existence of finite bare transport coefficients is still an open question especially in one dimension [16]. Here we show that a systematic application of the projection formalism and using ensemble equivalence technique lead to a modification of the standard Green-Kubo formula. This procedure leads to finite bare transport coefficients.

Coarse-graining and projection.— We consider the Hamiltonian (1) with the total number of sites N and we impose the periodic boundary conditions $r_{n+N} = r_n$ and $p_{n+N} = p_n$ for the stretch and the momentum variables, respectively [33]. In addition, we introduce the following notations to simply indicate phase-space-dependent conserved quantities at any site n :

$$\hat{c}_{r,n} := r_n, \quad \hat{c}_{p,n} := p_n, \quad \hat{c}_{\epsilon,n} := p_n^2/2 + V(r_n). \quad (3)$$

Throughout this study, the symbol $\hat{\cdot}$ on a variable implies that it is a function of the entire phase space Γ ($= (r_1, p_1, \dots, r_N, p_N)$) and hence, the detailed values are given once the phase space is specified. We also denote the current for the conserved quantities $\hat{c}_{a,n}$ at any site n by $\hat{j}_{a,n}$, which is given as $\hat{j}_{r,n} = -p_n$, $\hat{j}_{p,n} = -\partial V(r_{n-1})/\partial r_{n-1}$, and $\hat{j}_{\epsilon,n} = -p_n \partial V(r_{n-1})/\partial r_{n-1}$.

As a first step to obtain the hydrodynamics, we introduce a coarse-graining for conserved quantities:

$$\hat{u}_{r,x} := (1/\ell)(q_{G,x+1} - q_{G,x}),$$

$$\hat{u}_{b,x} := (1/\ell) \sum_{n=(x-1)\ell+1}^{x\ell} \hat{c}_{b,n}, \quad (b = p, \epsilon), \quad (4)$$

$$\hat{\mathcal{J}}_{r,x} := -\hat{u}_{p,x},$$

$$\hat{\mathcal{J}}_{b,x} := \hat{j}_{b,(x-1)\ell+1}, \quad (b = p, \epsilon), \quad (5)$$

where the number ℓ is the coarse-graining length and hence, we set the total number of sites N to a multiple

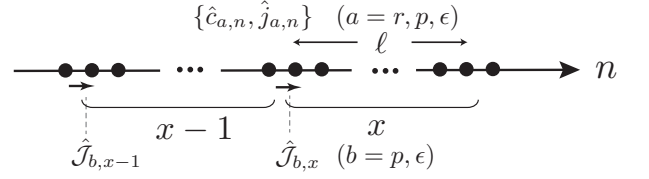


FIG. 1. Schematic of the coarse-graining. We define the x -coordinate with a unit of ℓ sites. The coarse-grained currents $\hat{\mathcal{J}}_{p,x}$ and $\hat{\mathcal{J}}_{\epsilon,x}$ are locally defined between the blocks.

of ℓ , and $x = 1, \dots, N/\ell$. The variable $q_{G,x}$ is the position of center of mass for the x th coarse-graining block defined as $q_{G,x} = (1/\ell) \sum_{n=(x-1)\ell+1}^{x\ell} q_n$. Note that the coarse-grained stretch variable $\hat{u}_{r,x}$ is a function of microscopic stretch variables $\hat{c}_{r,n}$ [34]. One can easily check that the coarse-grained variable \hat{u} is again a conserved quantity; i.e., the summation of the variables over x is conserved. The coarse-grained current denoted by $\hat{\mathcal{J}}_{a,x}$ is connected to the variable $\hat{u}_{a,x}$ through the continuity equation, i.e., $\partial_t \hat{u}_{a,x}^t = \{\hat{u}_{a,x}^t, \hat{H}\} = -\nabla_x \hat{\mathcal{J}}_{a,x}^t$, where the superscript t implies the time-dependence and $\{\dots, \dots\}$ is the Poisson bracket and the derivative is defined as $\nabla_x A_x := (1/\ell)(A_{x+1} - A_x)$ for an arbitrary function A_x . For large ℓ , the variable $\hat{u}_{a,x}$ becomes a macroscopic variable, while the currents $\hat{\mathcal{J}}_{p,x}$ and $\hat{\mathcal{J}}_{\epsilon,x}$ are microscopic variables defined locally at the boundaries between coarse-graining blocks. See Fig. 1.

Each macrostate defined by the set $\hat{u}_{a,x}$ corresponds to a large number of microstates and so the evolution of $\hat{u}_{a,x}$ is not deterministic. The internal degrees of freedom serve like a heat bath providing dissipation and noise that drives the “slow” hydrodynamic fields. As we now show, the projection formalism allows us to efficiently derive a Fokker-Planck equation for the fields and from this identify the Langevin equations that gives us the required FH in Eqs. (2). Let $\hat{\rho}_t$ be the full phase space density obeying the standard Liouville equation, $\partial_t \hat{\rho}_t = \{\hat{H}, \hat{\rho}_t\} =: \mathbb{L} \hat{\rho}_t$. Then, we define the following distribution of the coarse-grained variables:

$$f_t(u) := \int d\Gamma \hat{\rho}_t(\Gamma) \prod_{a=r,p,\epsilon} \prod_{x=1}^{N/\ell} \delta(\hat{u}_{a,x}(\Gamma) - u_{a,x}), \quad (6)$$

where the integral is defined over the entire phase space. This is the distribution that the variable $\{\hat{u}_{a,x}\}$ takes the c -number value $\{u_{a,x}\}$. The evolution of f_t is given by:

$$\partial_t f_t(u) = \partial_t \int d\Gamma \hat{\rho}_t(\Gamma) \prod_{a,x} \delta(\hat{u}_{a,x}(\Gamma) - u_{a,x})$$

$$= \int d\Gamma \hat{\rho}_t(\Gamma) \sum_{a',x'} \nabla_{x'} \hat{\mathcal{J}}_{a',x'}(\Gamma) \frac{\delta}{\delta u_{a',x'}} \prod_{a,x} \delta(\hat{u}_{a,x}(\Gamma) - u_{a,x}).$$

We now use the crucial idea of defining a projection operator [29, 35] \mathcal{P} which projects any function \hat{A} onto the

coarse-grained conserved variables as

$$\mathcal{P}\hat{A}(\Gamma) = \int d\Gamma' \hat{A}(\Gamma') \prod_{a,x} \delta(\hat{u}_{a,x}(\Gamma') - \hat{u}_{a,x}(\Gamma)) / \hat{\Omega}(\hat{u}), \quad (7)$$

where the normalization $\hat{\Omega}(\hat{u})$ is defined as $\hat{\Omega}(\hat{u}) = \int d\Gamma' \prod_{a,x} \delta(\hat{u}_{a,x}(\Gamma') - \hat{u}_{a,x}(\Gamma))$. If different phase-space points give the same value in the coarse-grained variables, projected observables also yield the same value between these phase-space points. The projection redefines a function in terms of coarse-grained conserved quantities. The projection enables us to write $\hat{\rho}_t = \mathcal{P}\hat{\rho}_t + \mathcal{Q}\hat{\rho}_t$, where $\mathcal{Q} = 1 - \mathcal{P}$, which separate the evolution into slow part following the conserved fields and a fast part from the internal degrees. Then from a straightforward calculation which involves using the Markovian approximation (Sec.III in the supplementary material (SM) [33]), we obtain the Fokker-Planck equation for the distribution $f_t(u)$ (Eq. (S.19) in SM [33]). Finally using standard procedure we find the corresponding Langevin equation (Eqs. (S.21-S.31) in SM [33]):

$$\begin{aligned} \partial_t u_{a,x} = & -\nabla_x \left[\langle \hat{\mathcal{J}}_{a,x} \rangle_{\text{LM}}^u - \sum_{a'} D_{a,a'}^{(A)} \nabla_x u_{a',x} \right. \\ & \left. - \sum_{a'} D_{a,a'}^{(S)} \nabla_x u_{a',x} + \xi_{a,x}(t) \right], \quad (8) \end{aligned}$$

where the term $\xi_{a,x}(t)$ is the noise at time t satisfying the fluctuation dissipation relation $\langle \langle \xi_{a,x}(t) \xi_{a',x'}(t') \rangle \rangle = 2K_{a,a'} \delta_{a,a'} \delta_{x,x'} \delta(t-t')$ with the bare transport coefficient given explicitly below in (10). The first line indicates the reversible terms, while the second indicates the irreversible terms consisting of noises and bare transport coefficients. The term $\langle \hat{\mathcal{J}}_{a,x} \rangle_{\text{LM}}^u$ is the local equilibrium current in (2), which turns out to be given as the average with respect to the local microcanonical ensemble $\hat{\rho}_{\text{LM}}$:

$$\hat{\rho}_{\text{LM}} := \prod_{a,x} \delta(\hat{u}_{a,x} - u_{a,x}) / \Omega(u), \quad (9)$$

which is the distribution for the values $\{u_{a,x}\}$ on the phase space. The denominator is a normalization defined as $\Omega(u) = \int d\Gamma \prod_{a,x} \delta(\hat{u}_{a,x}(\Gamma) - u_{a,x})$. The bare transport coefficient is expressed in terms of the Green-Kubo (GK) like formula as:

$$\begin{aligned} D_{a,a'}^{(S,A)} &= \sum_{a''} (1/2) (K_{a,a''} \pm K_{a'',a}) \Lambda_{a',a''}, \\ K_{a,a'} &= \int_0^\infty ds C_{a,a'}(s), \\ C_{a,a'}(s) &= (\ell/N) \langle \left(\sum_x \mathcal{Q} \hat{\mathcal{J}}_{a,x} \right) (e^{s\mathbb{L}} \sum_{x'} \mathcal{Q} \hat{\mathcal{J}}_{a',x'}) \rangle_{\text{eq}}, \end{aligned} \quad (10)$$

where $\langle \dots \rangle_{\text{eq}}$ is the average over the equilibrium distribution $\hat{\rho}_{\text{eq}} = e^{-\sum_n (\hat{c}_{\epsilon,n} + P_0 \hat{c}_{r,n}) / T} / Z$ with the normalization factor Z , since we assume that the dynamics is near equilibrium. Here, the temperature T and the pressure P_0 are determined by a given initial state through the

total energy and length. The inverse susceptibility matrix element $\Lambda_{a,a'}$ is explicitly computable (Sec.VII.A in SM [33]). We note that $\mathcal{P}\hat{u}_{p,x} = \hat{u}_{p,x}$, and hence we have $K_{r,a} = K_{a,r} = 0$. This property as well as Λ determines the matrix structure of the diffusion matrix D [33].

Computable expressions from the ensemble equivalence.— Let us consider how to practically compute the local microcanonical average on the local equilibrium current term, $\langle \hat{\mathcal{J}}_{a,x} \rangle_{\text{LM}}^u$, and the projected current that appears in the GK like formula, $\mathcal{P}\hat{\mathcal{J}}_{a,x}$. From the expressions of local microcanonical ensemble and the projection, we can exactly find simple expressions for the component $a = r$: $\langle \hat{\mathcal{J}}_{r,x} \rangle_{\text{LM}}^u = -u_{p,x}$, and $\mathcal{P}\hat{\mathcal{J}}_{r,x} = -\hat{u}_{p,x}$. Hence, the main focus here is on $\langle \hat{\mathcal{J}}_{b,x} \rangle_{\text{LM}}^u$ and $\mathcal{P}\hat{\mathcal{J}}_{b,x}$ with the components $b = p$ and ϵ . As we outline the underlying physics below, we can expand these terms with respect to coarse-grained quantities and variables:

$$\begin{aligned} \langle \hat{\mathcal{J}}_{b,x} \rangle_{\text{LM}}^u &\sim A_{b,a} \delta u_{a,x} + (1/2) H_{a,a'}^b \delta u_{a,x} \delta u_{a',x} + \dots, \\ (\mathcal{P}\hat{\mathcal{J}}_{b,x}) &\sim A_{b,a} \delta \hat{u}_{a,x} + (1/2) H_{a,a'}^b \delta \hat{u}_{a,x} \delta \hat{u}_{a',x} + \dots, \end{aligned} \quad (11)$$

where \hat{u} is defined as $\hat{u}_{r,x} := (1/\ell) \sum_{n=(x-1)\ell+1}^{x\ell} r_n$ and $\hat{u}_{b',x} := \hat{u}_{b',x}$ with $b' = p, \epsilon$. In the above expansions, the same subscripts are summed. The symbol $\delta \dots$ implies the deviation from the equilibrium value. The matrix elements in \mathbf{A} [36] and \mathbf{H} are identical to coefficients in the local equilibrium currents of the nonlinear FH in Ref. [17].

We now outline the underlying mechanism leading to the above computable expressions. It is convenient to discuss $\langle \hat{\mathcal{J}}_{b,x} \rangle_{\text{LM}}^u$ first. Note that the coarse-grained currents are defined at local sites in the coarse-graining block with the length ℓ , as depicted in Fig.1, while the coarse-grained variable \hat{u} is a hydrodynamic variable for sufficiently large ℓ . We then employ the standard argument in statistical physics; the microcanonical average can be accurately replaced by the canonical average to calculate local observables, as long as the size is large. Leaving the detailed justification in SM [33], we can use the following *ensemble equivalence* for large ℓ to describe the zeroth order of the gradient expansion in terms of the hydrodynamic motions

$$\hat{\rho}_{\text{LM}} \cong \hat{\rho}_{\text{LG}}, \quad (12)$$

where $\hat{\rho}_{\text{LG}}$ is the local Gibbs ensemble defined as

$$\hat{\rho}_{\text{LG}} = \prod_x \hat{\rho}_{\text{LG}}^{(x)}, \quad \hat{\rho}_{\text{LG}}^{(x)} = e^{-\sum_{a=r,p,\epsilon} \lambda_{a,x}(t) \hat{u}_{a,x}} / Z_x. \quad (13)$$

Here, Z_x is the normalization, and the parameter $\lambda_{a,x}$ is a conjugate parameter to the variable $\hat{u}_{a,x}$ that is determined through the condition $\langle \hat{u}_{a,x} \rangle_{\text{LG}} = u_{a,x}$, where $\langle \dots \rangle_{\text{LG}}$ is an average with the local Gibbs ensemble. This argument systematically yields the expansion for the local equilibrium current in (11). Next, we can similarly discuss the projected current that appears in the GK

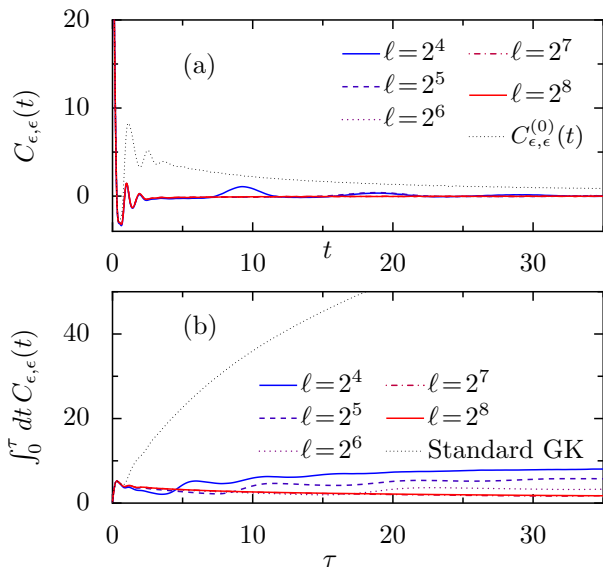


FIG. 2. Numerical demonstration of the GK like formula (10) for the element (ϵ, ϵ) . Parameters: $k_3 = 2.0, k_4 = 1.0, T = 3.0$ and $N = 2^{15}$. (a): The correlations as a function of time for different ℓ . $C_{\epsilon,\epsilon}^{(0)}$ is the standard energy current correlation for obtaining the macroscopic heat conductivity. (b): Integration of the correlations up to τ . ‘Standard GK’ (black dotted line) implies $\int_0^\tau dt C_{\epsilon,\epsilon}^{(0)}(t)$, which shows clear divergence. The integration for finite ℓ shows the convergence, where the saturated values are plotted in Fig.3.

like formula. We note that $\langle \hat{\mathcal{J}}_{a,x} \rangle_{LM}^u$ can be obtained in $\mathcal{P}\hat{\mathcal{J}}_{a,x}$ by replacing a phase-space-dependent variable $\hat{u}_{a,x}$ by a c -number value $u_{a,x}$ (see definitions (7) and (9)). This indicates that the projected current is accurately computable with the ensemble equivalence technique as above, which leads to the expansion in (11) [33].

Numerical investigation.— In the remainder of this paper, we perform a numerical calculation in order to see how unique bare transport coefficients emerge. We use the Fermi-Pasta-Ulam-Tsingou (FPUT) chain with the potential term:

$$V(r) = (1/2)r^2 + (k_3/3)r^3 + (k_4/4)r^4. \quad (14)$$

We remark that the hydrodynamics behavior has been numerically checked in this model [20].

We show the typical behavior of the correlation function $C_{a,a'}(t)$. Here, we present the most important element, the energy-energy current correlation function $C_{\epsilon,\epsilon}(t)$ because the standard energy current correlation for obtaining macroscopic transport coefficient shows a power-law decay at long times, resulting in a diverging heat conductivity. We present the other elements in SM [33]. In Fig.2(a), we show the time-dependence of $C_{\epsilon,\epsilon}(t)$ for many values of ℓ for the system size $N = 2^{15}$ and temperature $T = 3.0$ without pressure; the system parameters are $(k_3, k_4) = (2.0, 1.0)$ [37]. For small ℓ , we observe small humps in the time-domain. These humps occur every ℓ/c where c is the sound velocity ($c \sim 1.54$)

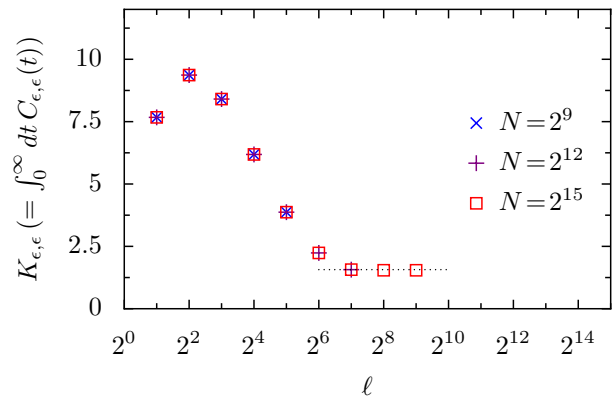


FIG. 3. Bare transport coefficients versus coarse-graining length ℓ . For same system parameters in Fig.2, we computed the integration of the GK like formula with different ℓ for three system sizes: $N = 2^9, 2^{12}$ and 2^{15} . The values for the same ℓ do not differ between different N , and eventually saturate for sufficiently large ℓ . This implies that the bare transport coefficients for each system can be uniquely determined for $1 \ll \ell \ll N$. The integration are performed up to $\tau = 100$ as in Fig.2(b) for all cases.

reflected from the sound propagation [38]. As ℓ increases, the amplitudes of humps decrease and the overall functional structures collapses onto the same curve, where finite values are seen only at the small-time scale. For comparison, we also show the standard energy current correlation denoted by $C_{\epsilon,\epsilon}^{(0)}(t)$, which corresponds to $C_{\epsilon,\epsilon}(t)$ with $\ell = 1$ where the projection contains only the first order dropping the higher orders. In Fig.2(b), integration up to τ is shown for the correlation functions in Fig.2(a). The integration of standard energy current correlation denoted by ‘Standard GK’ is also presented, which shows a clear divergence. In contrast, the integral of $C_{\epsilon,\epsilon}(t)$ with finite ℓ converges for sufficiently large ℓ . The main contribution in the saturated integration is given from the short-time behavior in the correlation.

In Fig.3, we show the bare transport coefficients $K_{\epsilon,\epsilon}$ computed via the GK like formula for different coarse-graining lengths ℓ . Particularly, we consider three different system sizes, $N = 2^9, 2^{12}$ and 2^{15} , and compute the bare transport coefficients for different ℓ . The figure shows that the same coarse-graining length give same values even when the system sizes are different. For sufficiently large coarse-graining length, the bare transport coefficients are uniquely determined. We stress that the order of limitation in the formula (10) is critical, i.e., $K_{a,a'} = \lim_{\tau \rightarrow \infty} \lim_{N \rightarrow \infty} \int_0^\tau ds C_{a,a'}(s)$ with the condition $1 \ll \ell \ll N$. Using the saturated functional form for sufficiently large ℓ , one can estimate the values of bare transport coefficients ($K_{p,p}, K_{p,\epsilon} (= -K_{\epsilon,p}), K_{\epsilon,\epsilon}$) $\sim (0.2 \times 10, 0.2 \times 10^{-2}, 0.1 \times 10)$.

Summary.— To summarize, we presented a microscopic theory to derive fluctuating hydrodynamics (FH) in nonlinear lattices. The formalism presented here is

quite general and it would be an interesting problem to compare the results of the lattice system to fluid systems that have been studied so far [39–43]. We hope that the microscopic theory presented here can provide a resolution of some of the open issues in low-dimensional transport [18] and useful information for other applications [44], and also gives a possibility to extend the FH to other classes of many-body systems such as [45–47].

ACKNOWLEDGEMENT

K.S. was supported by Grants-in-Aid for Scientific Research (JP16H02211, JP19H05603, JP19H05791). M.H. was supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Award Number DE-FG0201ER41195, and the RIKEN iTHEMS Program (in particular iTHEMS STAMP working group). A.D. acknowledges support of the Department of Atomic Energy, Government of India, under project no.12-R&D-TFR-5.10-1100. S.S. was supported by KAKENHI (JP17H01148, JP19H05496, JP19H05795). We are grateful to C. Bernardin, B. M. Itami, H. Nakano, M. Sasada, and H. Spohn for their valuable comments.

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