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Self-consistent mode-coupling approach to one-dimensional heat transport

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In the present Rapid Communication we present an analytical and numerical solution of the self-consistent mode-coupling equations for the problem of heat conductivity in one-dimensional systems. Such a solution leads us to propose a different scenario to accommodate the known results obtained so far for this problem. More precisely, we conjecture that the universality class is determined by the leading order of the nonlinear interaction potential. Moreover, our analysis allows us to determine the memory kernel, whose expression puts on a more firm basis the previously conjectured connection between anomalous heat conductivity and anomalous diffusion.

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It is well known that relaxation and transport phenomena in reduced spatial dimensions ($d<3$) are often qualitatively different from their three-dimensional counterparts. This is a documented effect, for example, in single-filing systems, where particle diffusion does not follow Fick's law [1]. Another related phenomenon is the enhancement of vibrational energy transmission in quasi- one-dimensional (1D) systems like polymers [2] or individual carbon nanotubes [3]. The specific instance of anomalous thermal conduction in low-dimensional many-particle systems has recently received a renewed attention [4]. Anomalous behavior means both a divergence of the finite-size conductivity $\kappa(L)\propto L^{\alpha}$ in the large-size limit $L\to\infty$ and a nonintegrable decay of equilibrium correlations of the energy current (the Green-Kubo integrand) $\langle J(t)J(0)\rangle\propto t^{-(1-\alpha)}$ at large times $t\to\infty$ (with $0\leq\alpha<1$). Simulations [5] and theoretical arguments [6] indicate that anomalies should occur generically in $d\leq 2$ whenever momentum is conserved.

The importance of predicting the scaling behavior (i.e., the value of α) is twofold: (i) on a basic ground, to classify the ingredients (e.g., symmetries) that define the possible universality classes; (ii) on a practical ground, to estimate heat conductivity in finite systems, a crucial issue to compare with experimental data on, say, carbon nanotubes. In spite of several efforts, the theoretical scenario is still controversial. In $d=1$, arguments based on mode-coupling theory (MCT) [7,8], a well-known approach to estimate long-time tails of fluids [9] and to describe the glass transition [10], yield $\alpha=2/5$. This estimate was criticized as inconsistent in Ref. [6], where renormalization group arguments were instead shown to give $\alpha=1/3$. Nevertheless, the 2/5 value was later derived both from a kinetic-theory calculation for the quartic (β) Fermi-Pasta-Ulam (FPU) model [11] and from a solution of the MCT by means of an *ad hoc* ansatz [12]. It was thereby conjectured [12] that 2/5 is found for a purely longitudinal dynamics, while a crossover toward 1/3 can be observed only in the presence of a coupling to transversal motion. Unfortunately, the accuracy of numerical simulations is generally insufficient to disentangle the whole picture. The only two convincing studies concern the hard point gas, which has been recently found to be characterized by $\alpha=1/3$ [13], and the purely quartic FPU model, where instead α is definitely larger than 1/3 (and possibly closer to 2/5) [14]. The situation is even more controversial in $d=2$ where logarithmic divergence is expected [15].

The exact self-consistent solution of the MCT equations presented in this Rapid Communication demonstrates that the overall scenario is different from that one proposed in [12], namely, that $\alpha=1/3$ in the presence of cubic nonlinearities. This prediction is confirmed by our numerical simulations of the FPU model with cubic potential, which yields sizably different α values with respect to the quartic case. Altogether, theoretical and numerical results indicate that the asymptotic scaling behavior is determined by the order of the leading nonlinearity in the interaction potential.

Let us consider the simplest one-dimensional version of the self-consistent MCT for the normalized correlator of the Fourier transform of the displacement field $G(q,t)=\langle Q^{*}(q,t)Q(q,0)\rangle/\langle|Q(q)|^{2}\rangle$. In dimensionless units in which the particle mass, the lattice spacing, and the bare sound velocity are set to unity, they read [8,16]

$$\ddot{G}(q,t)+\varepsilon\int_0^t\Gamma(q,t-s)\dot{G}(q,s)ds+\omega^2(q)G(q,t)=0,$$

$$\Gamma(q,t)=\omega^2(q)\frac{2\pi}{N}\sum_{p+p'-q=0,\pm\pi}G(p,t)G(p',t). \qquad (1)$$

We consider periodic boundaries so that the wave numbers are $q=2\pi k/N$ with $-N/2+1\leq k\leq N/2$. Notice that $G(q,t)=G(-q,t)$. Equations (1) must be solved with the initial conditions $G(q,0)=1$ and $\dot{G}(q,0)=0$.

The first of Eqs. (1) is exact and is derived within the well-known Mori-Zwanzig projection approach [17]. In the small-wave-number limit, it describes the response of an elastic string at finite temperature. The above mode-coupling

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approximation of the memory function Γ has been derived for a chain of atoms interacting through a nearest-neighbor anharmonic potential $V(x)$ [8,16] whose expansion around its minimum at $x=0$ is of the form $x^2/2+g_3x^3/3+\cdots$ (see, e.g., the Lennard-Jones potential). Both the coupling constant ε and the dispersion relation $\omega(q)$ are temperature-dependent input parameters that must be computed independently by simulation or approximate analytical approaches [8,16]. For the aims of the present Rapid Communication, we may restrict ourselves to considering their bare values, obtained in the harmonic approximation that, in our units, read $\varepsilon=3g_3^2k_BT/2\pi$ and $\omega(q)=2|\sin\frac{q}{2}|$. Of course, the actual renormalized values are needed when a quantitative comparison with a specific model is looked for. Moreover, since the anomalies we are interested in stem from the nonlinear interaction of long-wavelength modes, we let $\omega(q)=|q|$, in the analytic treatment presented below.

Direct numerical simulations [8] indicate that nonlinear and nonlocal losses in Eq. (1) are small compared to the oscillatory terms. This suggests splitting the G dynamics into phase and amplitude evolution,

$$G(q,t)=C(q,t)e^{i\omega(q)t}+\text{c . c.} \tag{2}$$

Upon substituting this equation into Eq. (1), one obtains, in the slowly varying envelope approximation, $qC\gg\dot{C}$,

$$2\frac{\partial}{\partial t}C(q,t)+\varepsilon\int_0^t dt'M(q,t-t')C(q,t')=0 \tag{3}$$

plus a similar expression for C^*, while the new kernel M turns out to be

$$M(q,t)=q^2\int_{-\infty}^{\infty}dpC^*(p-q,t)C(p,t), \tag{4}$$

where the sum in Eq. (1) has been replaced by a suitable integral, since we consider the thermodynamic limit $N=\infty$ and small q values, which are, by the way, responsible for the asymptotic behavior.

Notice that Eqs. (3) and (4) have been obtained after discarding the second order time derivative of $C(q,t)$ as well as the integral term proportional to $\dot{C}$, besides all rapidly rotating terms. The validity of this approximation is related to the separation between the decay rate of $C(q,t)$ and $\omega(q)$; its correctness will be checked *a posteriori*, after discussing the scaling behavior of $C(q,t)$. Notice also that in this approximation, Umklapp processes do not contribute: it is in fact well known that they are negligible for long-wavelength phonons in 1D [5].

Having transformed the second order differential equation for G into a first order one for C, we can introduce a simple scaling argument yielding the dependence of C on q and t as follows (see also [18], where a similar equation was investigated):

$$C(q,t)=g(\sqrt{\varepsilon}tq^{3/2}),\quad M(q,t)=q^3f(\sqrt{\varepsilon}tq^{3/2}). \tag{5}$$

This shows that the decay rate for the evolution of $C(q,t)$ is of the order $q^{3/2}\sqrt{\varepsilon}$, which has to be compared with the scale q of the corresponding phase factor. Accordingly, amplitude and phase dynamics become increasingly separated for $q\to 0$. High q values ($q\approx 1$) are those for which the slowly varying envelope approximation is less accurate. However, if ε is small enough, such modes are correctly described, too. This has been checked in the numerical solution of Eqs. (1) (see Figs. 1 and 2 below).

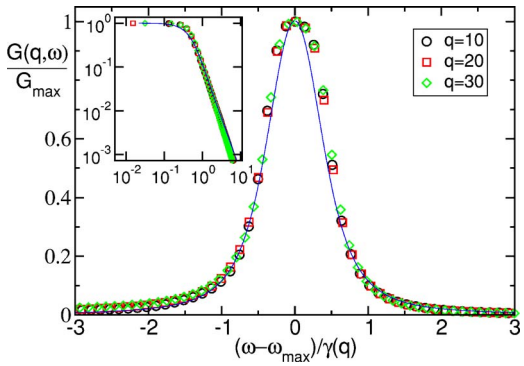

FIG. 1. (Color online) Fourier transform $G(q,\omega)$ of the correlation functions for three different wave numbers $\varepsilon=1$, $N=2000$. The solid line is the line shape computed by the approximate analytic theory, i.e., by Fourier transforming the function $C(q,t)$ defined in Eqs. (5) and (8). The same curves are plotted in the inset on a log-log scale, where only positive frequencies are shown.

The functions f and g can be determined by substituting expression (5) into Eqs. (3) and (4). Upon setting $x=\sqrt{\varepsilon}tq^{3/2}$, one obtains the equation

$$g'(x)=-\int_0^x dy\,f(x-y)g(y), \tag{6}$$

$$f(x)=x^{-2/3}\int_{-\infty}^{+\infty}dy\,g^*(|x^{2/3}-y|^{3/2})g(y^{3/2}). \tag{7}$$

The small-x behavior can be determined analytically,

$$g(x)=\frac{1}{2}\exp\left(-\frac{ax^{4/3}}{4}\right),\quad f(x)=\frac{a}{x^{2/3}}, \tag{8}$$

where a is a suitable constant that is determined self-consistently from Eq. (6). To assess the validity of the above

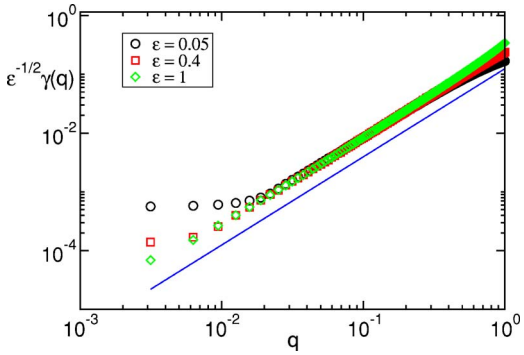

FIG. 2. (Color online) Scaling of the linewidth $\gamma(q)$ of $G(q,\omega)$ with q for three different values of the coupling constant ε and $N=2000$. The solid line corresponding to the power law $q^{3/2}$ is plotted for reference.

calculation, we have numerically integrated Eqs. (1) by the Euler method for the original dispersion relation $\omega(q)$ and different ε values. We have verified that a time step $\Delta t = 0.01$ guarantees a good numerical accuracy over the explored time range. The Fourier transform $G(q,\omega)$ is plotted in Fig. 1 for three different q values versus $\omega - \omega_{max}(q)$, where $\omega_{max}(q)$ is the frequency corresponding to the maximal value G_{max} of the spectrum [this is equivalent to removing the oscillating component from $G(q,t)$]. Furthermore, in order to test relation (5), the vertical axis is scaled to the maximum G value, while the frequencies are divided by the half-width $\gamma(q)$ at half of the maximum height. This latter quantity can be interpreted as the inverse lifetime of fluctuations of wave number q. The good data collapse confirms the existence of a scaling regime. The approximate analytical expression is in excellent agreement with the data. As expected, some deviations are present for small ω where Eq. (8) is not strictly applicable. Moreover, in the inset of Fig. 1, where the same curves are plotted using doubly logarithmic scales, one sees that the line shapes follow the predicted power law $\omega^{-7/3}$ over a wide range of frequencies. In Fig. 2 we show that $\gamma(q)$ is indeed proportional to $\sqrt{\varepsilon} q^{3/2}$. It is particularly instructive to notice that the agreement is very good also for a relatively large value of the coupling constant ($\varepsilon \simeq 1$), although the slowly varying envelope approximation is not correct for large q values. The deviations observed at small q values for small couplings are due to the very slow convergence in time. Better performances could be obtained by increasing both N and the integration time (10^4, in our units) well beyond our current capabilities.

It is crucial to compare these result with previous work. Making use of Eqs. (5) and (8), it can be shown that the memory function Γ contains terms of the form $q^2 e^{\pm iqt}/t^{2/3}$, i.e., it oscillates with a power-law envelope. Accordingly, its Laplace transform has branch-cut singularities of the form $q^2/(z \pm q)^{1/3}$. This finding is not consistent with the heuristic assumption of Refs. [7,8] and the result of [12], where MCT equations were solved with the ansatz $\Gamma(q,z) = q^2 \mathcal{V}(z)$. In addition, the numerical solution does not show any signature of the $q^2/z^{1/3}$ dependence found in [12]. For instance, it would imply a peak at $\omega = 0$ in the spectrum of Γ which is, instead, absent in numerical solutions.

To estimate the long-time decay of the energy-current autocorrelation, it is customary to consider the approximate expression [12],

$$\langle J(t)J(0)\rangle \propto \sum_q \left(\frac{d\omega}{dq}\right)^2 G^2(q,t). \tag{9}$$

This amounts to disregarding higher-order terms which are believed not to alter the leading behavior. As the sum in the above equation is dominated by the small-q terms, recalling that $d\omega/dq \simeq 1$, one then finds, by using Eq. (5),

$$\langle J(t)J(0)\rangle \propto \int dq\, g^2(\sqrt{\varepsilon} t q^{3/2}) \propto \frac{1}{t^{2/3}}, \tag{10}$$

i.e., $\alpha = 1/3$. Note that this result is independent of the actual form of g (provided convergence of the integral is ensured).

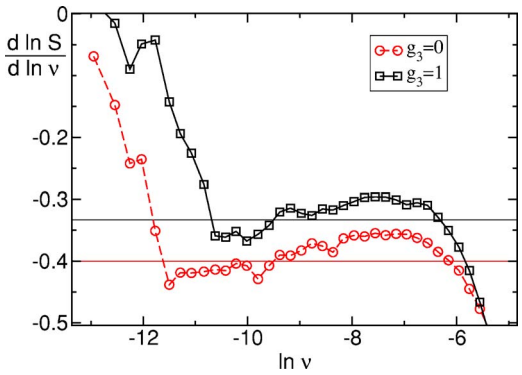

FIG. 3. (Color online) The logarithmic derivative of the energy-flux spectrum $S(\nu)$ versus the frequency ν for the FPU potential with energy density set equal to 10. The two horizontal lines correspond to the theoretical predictions $-1/3$ and $-2/5$. The statistical error is on the order of the observed irregular fluctuations.

This scaling has also been checked to hold by directly evaluating the sum (9) with the numerically computed correlations G.

As already mentioned at the beginning, several numerical simulations have been performed to estimate the exponent α. Since the most accurate data [14] differ significantly from 1/3, we decided to run a new set of simulations. We considered the FPU model with interparticle potential $V(x) = x^2/2 + g_3 x^3/3 + x^4/4$ and periodic boundary conditions. We performed microcanonical simulations to compute the average power spectrum $S(\nu)$ of J (see Refs. [5,14] for details). The long-time tail manifests itself as a power-law divergence $\nu^{-\alpha}$ at low frequencies, $\nu \to 0$. In order to provide a reliable estimate of α, it is convenient to evaluate the logarithmic derivative $d \ln S / d \ln \nu$. As shown in Fig. 3, for $g_3 = 1$ this quantity does display a plateau around $-1/3$ (the growth towards zero at very small ν values is due to the cutoff introduced by the finite size of the lattice). On the other hand, the data obtained for $g_3 = 0$ (FPU-β model) indicate a noticeably different scaling exponent, which is much closer to $-2/5$ and in agreement with previous works [11,14].

We have thus reached the important conclusion that the memory kernel decays algebraically in the prescribed regime and, accordingly, the relaxation is not exponential $\ln C \simeq -q^2 t^{4/3}$ (i.e., non-Lorenzian line shapes). The further striking feature is that conventional hydrodynamics breaks down, since the peak widths scale as $q^{3/2}$ rather than q^2, as expected in the standard case. In addition, the linewidths are connected to transport coefficients being proportional to Λq^2, where Λ is the sound attenuation constant. The anomalous scaling can be recast in terms of a diverging $\Lambda(q) \sim q^{-1/2}$. Altogether, one may think of this as a superdiffusive process, intermediate between standard diffusive and ballistic propagation. Our result thus strengthen the picture emerging in Ref. [13] from the analysis of the hard point gas, where it has been shown that energy perturbations perform a Lévy walk. One merit of our approach is that it allows for a direct connection with anomalous diffusion problems [19]. As it is known, these can be modeled by generalized Langevin equations with power-law kernels. If we now assume that expression (8) for f holds for every x, we can solve Eqs. (3) by

Laplace transforming Eq. (4) to obtain $C(q,z)=iz^{1/3}/(iz^{4/3}+aq^2)$. This expression is precisely the Laplace transform of the Mittag-Leffler function $E_\mu(-(\lambda t)^\mu)$ [19,20] for $\mu=4/3$ and $\lambda(aq^2)^{3/4}$ [21]. This observation suggests that the effective evolution of fluctuations should be modeled by the fractional differential equation

$$\frac{\partial^\mu}{\partial t^\mu}C(q,t)+\lambda^\mu C(q,t)=0. \tag{11}$$

The case of interest here $(1<\mu\leq 2)$ corresponds to the so-called fractional oscillations [20]. It should be emphasized that in the present context, memory arises as a genuine many-body effect and need not be postulated *a priori*.

In conclusion, we have shown that MCT with the cubic nonlinearity (1) predicts a $t^{-2/3}$ decay of the heat current autocorrelation, i.e., $\alpha=1/3$. Our analysis reconciles this approach with the renormalization group calculation [6] and supports the idea that the mechanisms yielding anomalous transport in 1D are largely universal. The sizable deviations observed for quartic potentials suggest the existence of a different universality class that should be described by different mode-coupling equations with a quartic nonlinearity. A preliminary analysis confirms that this scenario is indeed correct [22]. Finally, we have analytically shown that memory effects emerging from the nonlinear interaction of long-wavelength modes can be described by a generalized Langevin equation with power-law memory. This provides a sound basis establishing a connection between anomalous transport and superdiffusive processes.

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