Generation of dispersion in non-dispersive nonlinear waves in thermal equilibrium

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In this work, we examine the important theoretical question of whether dispersion relations can arise purely from nonlinear interactions among waves that possess no linear dispersive characteristics. Using two prototypical examples of non-dispersive waves, we demonstrate how nonlinear interactions can indeed give rise to effective dispersive-wave-like characteristics in thermal equilibrium. Physically, these example systems correspond to the strong nonlinear coupling limit in the theory of wave turbulence. We derive the form of the corresponding dispersion relation, which describes the effective dispersive structures, using the generalized Langevin equations obtained in the Zwanzig-Mori projection framework. We confirm the validity of this effective dispersion relation in our numerical study using the wavenumber-frequency spectral analysis. Our work may provide insight into an important connection between highly nonlinear turbulent wave systems, possibly with no discernible dispersive properties, and the dispersive nature of the corresponding renormalized waves.

Turbulent dynamics typically exhibit chaotic motions with a cascade-like transfer of excitations across a wide range of spatial scales. This transfer characterizes the behavior of fully-developed turbulence in fluids [1–3] as well as weakly-nonlinear, dispersive-wave turbulence [4–14]. For the latter, the energy transfer is mediated by resonant interactions among groups of three or more waves. The resonance conditions of these interacting waves are determined primarily by the associated linear dispersion relation [14]. The wavenumber-frequency spectral (WFS) analysis is often used to identify the dispersion relation of these waves; for example, this method was used recently to study the dispersion relations of Kelvin and Rossby waves [15–18].

Traditionally, one begins the analysis of wave turbulence by assuming that the wave system under investigation possesses a linear dispersion relation [14]. However, an important theoretical question remains whether dispersive characteristics of certain types of wave turbulence may arise as a consequence of nonlinear wave interactions, that is, the dispersive structure of the waves is not inherited from their linear dispersive behavior [19]. In this article, we describe the emergence of dispersive wave characteristics in nonlinear dynamical systems in thermal equilibrium, whose governing laws reveal no a priori associated linear dispersive-wave-like properties at all. We use the WFS analysis to show that an effective dispersion relation can indeed be measured from the turbulent motions of these waves in thermal equilibrium. The systems we consider are generalized versions of the Fermi-Pasta-Ulam (FPU) chain [20] and the Majda-McLaughlin-Tabak (MMT) model [21, 22] in which all traces of a linear dispersion relation have been removed. We present a theoretical analysis to understand how their effective dispersion relations are induced, and we further show that our theoretical predictions of these relations are in good agreement with those measured by the WFS method. These effective dispersion relations are somewhat unexpected generalizations of the analogous relations in the explicitly dispersive-wave-like regimes of the two models [23–26].

As will be seen below, the effective dispersion relations are generated by nonlinear interactions among waves, and their forms are strongly related to the equilibrium measures of the respective systems. However, we believe that the scenario for inducing effective dispersive characteristics is general, not limited to thermal equilibrium, and similar dispersive structures may be induced by nonlinear interactions under a driven-damped, nonequilibrium setting. These structures may play an important role in controlling long-time dynamics—just as in our MMT case below in which nonlinearity-induced resonances are shown to control the long-time dynamics in thermal equilibrium. Furthermore, this scenario also raises a possibility that the dispersion relation measured by the WFS method for some physical systems may be renormalized in the sense discussed here.

Fermi-Pasta-Ulam Chain

We first investigate the emergence of the effective dispersion relation in an extension of this one-dimensional model chain of particles with nearest-neighbor interactions. If we denote the position and momentum of the j-th particle by $q_j$ and $p_j$, the Hamiltonian of the system is given by

$$\mathcal{H} = \sum_{j=1}^{N} \frac{1}{2} p_j^2 + \frac{\alpha'}{2} (q_j - q_{j+1})^2 + \frac{\beta'}{4} (q_j - q_{j+1})^4$$

$$= \sum_{k=1}^{N} \frac{1}{2} |P_k|^2 + \frac{\alpha'}{2} \bar{\omega}_k^2 |Q_k|^2 + V(Q), \quad [1]$$

where $\bar{\omega}_k = 2 \sin(\pi k/N). \quad [2]$

and $P_k, Q_k$ and $V(Q)$ are the Fourier transforms of $p_j, q_j$ and the quartic term, respectively, and $N$ is the number of particles in the chain. The parameters $\alpha'$ and $\beta'$ ($> 0$) determine

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Also, as a result, the FPU chain with \( \alpha' \) and \( \beta' \) the strength of the nonlinearity.

The case of \( \alpha' = 1 > 0 \) (taken with no loss of generality) corresponds to a single-well potential, and equation [1] becomes the original FPU chain. Since its introduction with the goal to numerically study the route to thermal equilibrium [20], the FPU chain has played an important role in the theory of crystals, soliton physics, and wave dynamics [27,28].

After introducing the wave-like variable

\[
\bar{a}_k = \frac{P_k - i\omega_k Q_k}{\sqrt{2\omega_k}}
\]

the Hamiltonian in equation [1] with \( \alpha' = 1 \) becomes

\[
\mathcal{H} = \sum_{k=1}^{N} \omega_k |\bar{a}_k|^2 + V(\bar{a})
\]

which describes a wave system with the linear dispersion relation [2] for the wave \( \bar{a}_k \). The term \( V(\bar{a}) \) represents the wave-wave interactions.

We extend the FPU system by allowing the Hamiltonian \( \mathcal{H} \) in equation [1] to have a double-well potential, which occurs when \( \alpha' < 0 \). We note that there is no bare linear-wave dynamics in this case. Instead, the linear part of the FPU equations indicates that small-amplitude solutions should grow exponentially. Hence, one would not expect to see spectral peaks located around (a multiple of) the frequency \( \omega_k \) in equation [2], which has no direct relation to the linear dynamics. Also, as a result, the FPU chain with \( \alpha' < 0 \) cannot be transformed to a description by a wave-like variable such as the above \( \bar{a}_k \) in equation [3], whose form is related to the bare linear dispersion relation in the non-interacting system.

Applying the Zwanzig-Mori (ZM) formalism [29–32], we project the FPU dynamics in thermal equilibrium on the linear span of the variable pair \((Q_k(t), P_k(t))\) to obtain the exact linear Langevin equation (LLE):

\[
\begin{align*}
\partial_t Q_k(t) &= P_k(t) \\
\partial_t P_k(t) &= -(\omega_k')^2 Q_k(t) - \int_0^t \Gamma'_k(t-s) P_k(s) \, ds + F'_k(t),
\end{align*}
\]

where by invoking the equipartition theorem we can show that \( \omega_k' \) has the following form:

\[
\omega_k' = \omega_k \frac{(K)}{(U)} \equiv \omega_k \eta_L.
\]

Here,

\[
K = \frac{1}{2} \sum_{k=1}^{N} \langle |P_k|^2 \rangle \quad \text{and} \quad U = \frac{1}{2} \sum_{k=1}^{N} \omega_k' \langle |Q_k|^2 \rangle
\]

denote the kinetic and potential energy, respectively, \( \langle \cdot \rangle \) denotes thermal average, \( F'_k(t) \) is a random force, and the memory kernel \( \Gamma'_k \) is related to \( F'_k(t) \) via the fluctuation-dissipation theorem [33]. Note that the expression for \( \omega_k' \) in equation [5] is formally exact, and that the renormalization factor \( \eta_L \) is independent of the wavenumber \( k \). Note also that the LLE [4] is valid for both signs of \( \alpha' \).

For low wavenumbers \( k \), \( \omega_k' \) gives a relatively long time scale while the noise \( F'_k(t) \) contains the contribution of high wavenumber modes, leading to relatively short time correlations. Therefore, we can ignore the memory effects in the LLE [4], and thus reduce the system to driven-damped oscillators with the effective dispersion given by \( \omega = \omega_k' [20] \). The system [4] can also be written using more wave-like variables,

\[
a'_k(t) = \frac{P_k - i\omega_k Q_k}{\sqrt{2\omega_k'}},
\]

for which the above LLE [4] becomes

\[
\partial_t a'_k(t) = -i\omega_k a'_k(t) - \frac{1}{2} \int_0^t \Gamma'_k(t-s) [a'_k + (a'_{N-k})^*] \, ds + \frac{F'_k(t)}{\sqrt{2\omega_k'}}.
\]
Equation [5] gives the effective frequency $\omega'_k$ of the wave $a'_k$ for low wavenumbers $k$ in the strongly nonlinear FPU chains, regardless of the sign of $\alpha'$.

To examine the validity of the theoretical prediction found by the above LLE, we study the thermal equilibrium state of the FPU system by performing numerical simulations of the long-time dynamics of the canonical equations derived from the Hamiltonian [1]. We use time-averaging instead of ensemble-averaging to evaluate $\langle K \rangle$ and $\langle U \rangle$. The states over which we perform the averaging are the states that remain long after any transients disappear and whose statistics are consistent with the statistics in thermal equilibrium [23, 24]. In the left panel of Figure 1, we depict $\eta_k$ in equation [5] as a function of $\beta'$ for $\alpha' = -0.1 (<0)$ and $N = 256$. In the right panel of Figure 1, for $\beta' = 3$, we display the result of the WFS analysis as represented by the color-coding of the logarithmic modulus, $\ln|a_k(\omega)|^2$, of the temporal Fourier transform of the wave $a'_k(t)$. The peak locations $\omega'_k$ of this temporal spectrum of $a'_k$ can be viewed as the effective frequencies of $a'_k$. We compare $\omega'_k$ with $\Omega_k$ to show that the prediction $\omega'_k$ serves as an accurate approximation for the effective frequency of the renormalized wave $a'_k$ for all $k$. In other words, the variables $a'_k$, which are generalizations of the renormalized waves for the original FPU chain studied in [23, 24], retain their wave-like behavior, and the relation $\omega'_k$ as a function of the wavenumber $k$ serves as their effective dispersion relation even in the case of the double-well FPU potential, which has no bare linear dispersion relation and no nonlinearly stable dispersive waves. The existence of the clearly-pronounced frequencies $\omega'_k \approx \omega_k$ also enables us to conclude the existence of a sharp time-scale separation between that of the dispersive component and that of the noise in LLE [4], which is another generalization of the previous results in [23, 24].

**Majda-McLaughlin-Tabak Model**

We study its extension governed by the canonical equation of motion [21, 22]

$$i\partial_t a_k = \chi|k|^{\alpha} a_k + \int |k_1| k_2 k_3 k_4 |a_{k_1} a_{k_2} a_{k_3} a_{k_4}|^2 \delta(\Delta_{k_1 k_2} k_3 k_4) \, dk_{123},$$  

[6]

which is derived from a homogeneous, scale-invariant Hamiltonian. In Eq. (6), $\Delta_{k_1 k_2} k_3 k_4 = k_1 + k_2 - k_3 - k_4$, and $\delta(\cdot)$ denotes the Dirac delta function. Three parameters, $\alpha$, $\beta$ (>0), and $\chi$ (>0), characterize the dynamics: when $\chi = 1$, equation [6] reduces to the original MMT model introduced as a prototype to study numerically the validity of the weak turbulence theory [21]. If $\alpha = 2$ and $\beta = 0$, the MMT system corresponds to the nonlinear Schrödinger equation, while the case of $\alpha = 1/2$, $\beta = 3$ mimics the scaling present in water waves [34]. When $\chi = 0$, equation [6] is reminiscent of the Clebsch-variables formulation of the 3D Euler equations in fluid dynamics [19]. Note that for $\chi > 0$, the MMT equation [6] possesses the linear dispersion relation $\omega_k = \chi|k|^{\alpha}$, which is controlled by the parameter $\alpha$. For $\chi = 0$, no linear dispersion exists. Therefore, the extended MMT model [6] encapsulates a variety of dynamical systems, allowing us to compare its nonlinear-wave dynamics ranging from the usual weakly-interacting dispersive waves to the strongly-nonlinear limit.

In thermal equilibrium, for $\chi \neq 0$, the LLE obtained by ZM projection onto a single wave $a_k(t)$ of the MMT model yields an effective frequency

$$\Omega_k = \chi|k|^{\alpha} + \frac{1}{2} \int |k'|^2 \langle |a_k|^2 \rangle \, dk'$$  

[7]

of the long waves, i.e., for low wavenumbers $k$. The random-phase approximation (RPA) allows us to replace the four-point function in the integrand of equation [7] by a product of two two-point functions, and obtain the alternative approximate frequency

$$\Omega_k = \chi|k|^{\alpha} + \int |k'|^2 \langle |a_k|^2 \rangle \, dk'$$  

[8]

In view of equations [7] and [8], the bare linear dispersion relation $\omega_k = \chi|k|^{\alpha}$ is thus renormalized to an effective dispersion relation.

Numerical simulations performed in [25] reveal that both $\Omega_k$ and $\Omega_k$ are good approximations for the effective frequency of $a_k$ for not just small but all wavenumbers $k$ in the strongly nonlinear MMT system with $\chi > 0$. It is not obvious whether this result holds for the singular $\chi = 0$ case with no linear dispersion relation at all. Here, we investigate the system with $\chi = 0$ in thermal equilibrium numerically. Using the WFS method, we have obtained the effective frequency of $a_k$; we depict the comparison of $\Omega_k$ and $\Omega_k$ with this measured $\omega'_k$ in Figure 2. We thus see that the dispersive-wave-like character of the MMT dynamics again persists into the regime in which it is not immediately clear that it should. Equations [7] and [8] with $\chi = 0$, which are generalizations of the effective dispersion relation in the original MMT system [25], provide excellent approximations to this relation even when linear dispersion terms are entirely absent.

Having established that the wave profiles $a_k$ exhibit near-oscillatory behavior with the effective frequencies in thermal equilibrium well approximated by Eqs. [7] and [8], we ask the natural question whether the long term dynamics of this system is dominated by resonant interactions as is the case in the weakly-nonlinear limit of the MMT system [21]. For the strongly nonlinear original MMT system ($\chi = 1$ in equation [6]) in thermal equilibrium, depending on the values of

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**Fig. 2.** The color-coding of $\ln|a_k(\omega)|^2$ for $\chi = 0$, $\beta = 6$, and $N = 1024$ Fourier modes in the MMT model. Curves depicting the peak $\omega'_k$ of $\ln|a_k(\omega)|^2$, measured using the WFS method, and the predicted effective frequencies $\Omega_k$ in equation [7] and $\Omega_k$ in equation [8], are plotted.
thermal equilibrium even when computed from equation 6. The resonances outside the area bounded by the two dashed green lines are due to the periodicity of the finite system. Right: The modulus of the time average of $a_k^1 a_k^2 a_k^3 a_k^4$. In both cases, $\beta = 1$, $N = 512$, and $k_3 = 128$, with $k$ measured in units of $\pi/N$, where $N$ is the number of modes we used to approximate system 6 in our numerical simulation.

Fig. 3. Left: Resonance structure for the MMT model with $\chi = 0$ as visualized by projecting $|k_1|^{3/2} + |k_3|^{3/2} - |k_3|^{3/2} - |k_3|^{3/2}$ with fixed $k_3$, and $k$ computed from equation 9a. The resonances outside the area bounded by the two dashed green lines are due to the periodicity of the finite system. Right: The modulus of the time average of $a_k^1 a_k^2 a_k^3 a_k^4$. In both cases, $\beta = 1$, $N = 512$, and $k_3 = 128$, with $k$ measured in units of $\pi/N$, where $N$ is the number of modes we used to approximate system 6 in our numerical simulation.

Discussion

For the FPU chain, we point out that there is a possibility of using a nonlinear Langevin equation 35,36 to find an alternative effective frequency approximation

$$\tilde{\omega}_k = \tilde{\omega}_k \sqrt{\alpha' + \frac{6\beta'(U)}{N}} \equiv \tilde{\omega}_k \eta_N. \quad [10]$$

As shown in Figure 1, the results obtained via this approximation are also close to, and give a further confirmation of, those obtained via the approximation in equation 5. Note that $\tilde{\omega}_k$ can also be obtained using RPA 23,24. In our numerical simulation, when $\alpha' = -0.1$, $\eta_N$ remains positive no matter how small $\beta'$ is, as shown in the left panel of Figure 1, which further demonstrates that RPA is valid even in the regime without the linear dispersion relation, and that it may not be necessary to have linear dispersion to create random phases of the waves.

The MMT system was devised as a model to study dispersive wave turbulence, and a kinetic equation of weak turbulence theory was derived for its long-time dynamics in 21. For large nonlinearities, using the approach employed in the weak turbulence theory, we derived an effective kinetic equation based on the renormalized resonances, which possesses the renormalized Rayleigh-Jeans distribution as the thermal-equilibrium spectrum 25. This equation may, at least formally, be extended to the $\chi = 0$ case. The difficulty of ascertaining its true accuracy in this case lies in the possibility that the time-scale corresponding to the dispersion-generated effective frequencies may be comparable to the time-scale induced by the remaining nonlinear terms, thus violating the assumptions used in deriving this kinetic equation. The narrowness and height of the spectral peaks in Figure 2, which could be interpreted as an estimation of the effective ratio between these two time-scales, appear to indicate that the scale separation between them is still large. However, a precise quantification of this statement is not trivial, and will be relegated to future work. Nevertheless, we do believe that, in the future, studying this extension of the kinetic theory may provide insight into mechanisms underlying fluid turbulence away from equilibrium 19.

In contrast, the generalized FPU chain 1 allows for no sharp-resonance-based kinetic equation because the effective frequencies $\tilde{\omega}_k$ in equation 5 and $\tilde{\omega}'_k$ in equation 3 are constant multiples of the bare frequency $\tilde{\omega}_k = 2\sin(\pi k/N)$ in equation 2, whose functional form does not allow for nontrivial three-wave or four-wave resonances. However, perhaps the broadened-resonance approach of 37 might yield an appropriate kinetic equation.

The two non-dispersive wave systems we study here physically correspond to the strong nonlinear coupling limit of waves. In thermal equilibrium, strong interactions indeed give rise to dispersive-wave characteristics for these systems with induced dispersion relations. The realization that even for highly nonlinear systems with no priori expected dispersive-wave character, the dynamics can be dominated by relatively
weakened coupled-time harmonic waves oscillating fast with frequencies governed by an effective dispersion relation, hints at a potentially important link between highly nonlinear turbulent systems and weakly-coupled dispersive waves. This realization may provide new techniques for analyzing turbulent systems, thus leading to a better understanding of such systems.

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