

Fermi-Pasta-Ulam β lattice: Peierls equation and anomalous heat conductivity

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The Peierls equation is considered for the Fermi-Pasta-Ulam β lattice. Explicit form of the linearized collision operator is obtained. Using this form the decay rate of the normal-mode energy as a function of wave vector k is estimated to be proportional to $k^{5/3}$. This leads to the $t^{-3/5}$ long-time behavior of the current correlation function, and, therefore, to the divergent coefficient of heat conductivity. These results are in good agreement with the results of recent computer simulations. Compared to the results obtained through the mode coupling theory our estimations give the same k dependence of the decay rate but a different temperature dependence. Using our estimations we argue that adding a harmonic on-site potential to the Fermi-Pasta-Ulam β lattice may lead to finite heat conductivity in this model.

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I. INTRODUCTION

The Peierls equation has played an important role in understanding properties of solids since its original derivation by Peierls [1,2]. It was successfully used for qualitative explanation of heat conduction in dielectrics and for prediction of such phenomena as second sound and Poiseuille flow [3]. In spite of these successes quantitative predictions are hard to make due to the enormous complexity of the equation even for solids with simple dispersion laws. It is well known that approximating the solid by isotropic continuum leads to divergent heat conductivity even in three dimensions if only three-phonon collisions are considered [2,4]. This divergence can be eliminated if more careful analysis of the dispersion relations is performed [5]. In this paper we would like to consider the collision operator of the linearized Peierls equation for a simple one-dimensional model: linear chain with quartic interaction also known as Fermi-Pasta-Ulam (FPU) β lattice.

One-dimensional lattices have drawn considerable attention since the original work of Fermi, Pasta, and Ulam [6] and originated a vast area of research [7]. It is now well established by computer simulations that the heat conductivity in FPU lattices diverges when the size of the lattice goes to infinity [8–12]. The simulations give a power law dependence of the heat conductivity on the number of particles N as approximately $N^{2/5}$. This form of N dependence is related to the $t^{-3/5}$ long-time behavior of the current correlation function. Theoretical work in this area [9,10] was based on the application of the mode coupling theory [13,14]. Application of Peierls equation to the analysis of heat conduction in FPU lattices was limited to qualitative estimations [1,10,15]. It is therefore of interest to check if more careful analysis of the Peierls equation can explain some of the anomalous properties of the FPU chains.

To this end we will consider the explicit form of the Peierls equation for the FPU lattice in Sec. II. In Sec. III we apply this equation to estimate the long-time behavior of the

current correlation function as well as the wave-vector dependence of the decay rate for mode energies. Concluding remarks are given in Sec. IV.

II. THE PEIERLS EQUATION

The Hamiltonian for the FPU β lattice is

$$H = \sum_r \frac{p_r^2}{2m} + \sum_r \frac{C}{2} (u_{r+1} - u_r)^2 + \sum_r \frac{\lambda}{4} (u_{r+1} - u_r)^4. \quad (1)$$

Here u_r is the displacement of the particle at site r , p_r is the momentum conjugate to u_r , and m is the mass of the particle. We also use λ as a coupling constant. Cyclic boundary conditions are imposed, i.e., $u_{r+N} = u_r$, where N is the number of particles. We can introduce action variables J_k and angle variables α_k related to u_r and p_r through

$$\sum_r u_r e^{-ikr} = \sqrt{\frac{N}{2m}} \left(\sqrt{\frac{J_k}{\omega_k}} e^{i\alpha_k} + \sqrt{\frac{J_{-k}}{\omega_{-k}}} e^{-i\alpha_{-k}} \right),$$

$$\sum_r p_r e^{ikr} = i \sqrt{\frac{mN}{2}} \left(\sqrt{J_k \omega_k} e^{-i\alpha_k} - \sqrt{J_{-k} \omega_{-k}} e^{i\alpha_{-k}} \right). \quad (2)$$

Here $k = 2\pi n/N$ is a dimensionless wave vector and n is an integer. The wave vector is usually restricted to the interval $-\pi < k \leq \pi$ but any other interval of length 2π can be chosen. The frequencies ω_k are given by

$$\omega_k = 2 \sqrt{\frac{C}{m}} \left| \sin \frac{k}{2} \right|. \quad (3)$$

In the action and angle variables Hamiltonian (1) has the form

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$$H = \sum_k \omega_k J_k + \lambda \sum_{\substack{kk'k''k''' \\ \epsilon\epsilon'\epsilon''\epsilon''' = \pm 1}} V_{\epsilon k \epsilon' k' \epsilon'' k'' \epsilon''' k'''} \times \sqrt{\frac{J_k J_{k'} J_{k''} J_{k'''}}{\omega_k \omega_{k'} \omega_{k''} \omega_{k'''}}} e^{i(\epsilon\alpha_k + \epsilon'\alpha_{k'} + \epsilon''\alpha_{k''} + \epsilon'''\alpha_{k'''})}. \quad (4)$$

Coefficient $V_{\epsilon k \epsilon' k' \epsilon'' k'' \epsilon''' k'''}$ is given by

$$V_{\epsilon k \epsilon' k' \epsilon'' k'' \epsilon''' k'''} = \frac{1}{Nm^2} \sin \frac{\epsilon k}{2} \sin \frac{\epsilon' k'}{2} \sin \frac{\epsilon'' k''}{2} \sin \frac{\epsilon''' k'''}{2} \times \cos \frac{\epsilon k + \epsilon' k' + \epsilon'' k'' + \epsilon''' k'''}{2} \times \Delta_{\epsilon k + \epsilon' k' + \epsilon'' k'' + \epsilon''' k'''}. \quad (5)$$

Here Δ_l is given in terms of Kronecker δ 's as

$$\Delta_l = \sum_m \delta_{2\pi m, l} \quad (6)$$

with m being an integer. Note that only terms with $m=0$ and $m=\pm 1$ have to be considered in Eq. (5). Indeed, the maximum length for the sum of four wave vectors is 4π but coefficient (5) vanishes in this case.

In the problem of heat conduction the quantities of interest are the mode energy $E_k = \omega_k J_k$ and the total heat current given by

$$j_h = \sum_k v_k \omega_k J_k = \sum_k v_k E_k, \quad (7)$$

where v_k is the group velocity. Note that E_k and j_h represent only the harmonic parts of the corresponding quantities, it is assumed that the contributions from the anharmonic corrections are small for weak coupling. The approximate time evolution of the average energy of the normal mode for weak coupling and for the lattice with no temperature gradient and close to the thermal equilibrium is given by the homogeneous linearized Peierls equation [1,2,4]. The equation is usually considered in the context of quantum mechanics for lattices with cubic anharmonicity. Derivation of this equation for the lattice with classical Hamiltonian (4) is straightforward. Note that in this case the following conditions on wave vectors and frequencies have to be satisfied simultaneously:

$$\begin{aligned} \pm k \pm k' \pm k'' \pm k''' &= 0, \text{ or } \pm 2\pi, \\ \pm \omega \pm \omega' \pm \omega'' \pm \omega''' &= 0 \end{aligned} \quad (8)$$

with the same ordering of signs for both relations. With the k dependence of frequencies (3) the relations can be satisfied only when two plus signs and two minus signs appear in Eq. (8), i.e., in quantum-mechanical terms, only the processes conserving the number of phonons contribute. In addition, although normal processes exist for this number conserving case, they only result in exchange of quasimomenta between two colliding phonons, and, therefore, cannot change the

phonon distribution. Thus, only umklapp number conserving processes contribute in the collision integral of the Peierls equation. We can write the linearized Peierls equation for the average energy \bar{E}_k of mode k , where overlining denotes averaging over a distribution function. The equation has the form

$$\begin{aligned} \frac{\partial \bar{E}_k}{\partial t} &= - \frac{(24\lambda k_B T)^2 \pi}{N^2 m^4} \\ &\times \sum_{k' k'' k'''} \left[\frac{|V_{kk' - k'' - k'''}|^2 \delta(\omega_k + \omega_{k'} - \omega_{k''} - \omega_{k'''})}{\omega_k \omega_{k'}^2 \omega_{k''}^2 \omega_{k'''}^2} \right. \\ &\left. \times (\omega_k \bar{E}_k + \omega_{k'} \bar{E}_{k'} - \omega_{k''} \bar{E}_{k''} - \omega_{k'''} \bar{E}_{k'''}) \right]. \end{aligned} \quad (9)$$

The collision operator on the right-hand side of Eq. (9) is a Hermitian operator in the Hilbert space with the inner product given by

$$\langle g | f \rangle = \int_{-\pi}^{\pi} dk g^* f_k. \quad (10)$$

It can be shown that the collision operator has a continuous spectrum that is bounded from below by zero [16,17]. We wrote Eq. (9) in the form that makes it easy to see that $\bar{E}_k = \text{const}$ and $\bar{E}_k = \text{const}/\omega_k$ are eigenstates of the collision operator with zero eigenvalues. The first eigenstate corresponds to the conservation of the total energy. The second one corresponds to the conservation of the sum of action variables for all modes (or, in quantum-mechanical language, to the conservation of the number of phonons). Note that the second eigenstate has an infinite norm.

We can write the average energy as

$$\bar{E}_k = k_B T + \delta \bar{E}_k, \quad (11)$$

where $k_B T$ is the equilibrium value of \bar{E}_k and $\delta \bar{E}_k$ is a deviation from that value. If we want the average energies to approach their equilibrium value of $k_B T$ for long times then $\delta \bar{E}_k$ should be orthogonal to both of the zero eigenvalue eigenstates of the collision operator [4], i.e., we must have

$$\int_{-\pi}^{\pi} dk \delta \bar{E}_k = 0, \quad \int_{-\pi}^{\pi} dk \frac{\delta \bar{E}_k}{\omega_k} = 0. \quad (12)$$

The δ function appearing in Eq. (9) is meaningful only in the limit of $N \rightarrow \infty$. In this limit we replace the sums by integrals and Kronecker δ 's by δ function according to

$$\frac{2\pi}{N} \sum_k \rightarrow \int dk, \quad \frac{N}{2\pi} \delta_{k, k'} \rightarrow \delta(k - k'). \quad (13)$$

After the limit is taken we will have terms containing products of two δ functions in the integrand. Therefore, two integrations can be rather easily performed. Integrations can be done much more easily and the resulting expressions have a

simpler form if the wave vector is restricted to the interval from 0 to 2π rather than from $-\pi$ to π . Using explicit expressions for $V_{kk'-k''-k''}$ and ω_k we obtain after tedious but straightforward calculations

$$\frac{\partial \bar{E}_k}{\partial t} = -\frac{(3\lambda k_B T)^2 \sin \frac{k}{2}}{4\pi C^{7/2} m^{1/2}} \left(\int_{int} dk' \frac{\sin \frac{k'}{2} \bar{E}_{k'}}{\sqrt{\frac{1}{4} \left(\cos \frac{k}{2} + \cos \frac{k'}{2} \right)^2 - \sin \frac{k}{2} \sin \frac{k'}{2}}} - \int_0^{2\pi} dk' \frac{\sin \frac{k'}{2} \bar{E}_{k'} - \frac{1}{2} \sin \frac{k}{2} \bar{E}_k}{\sqrt{\frac{1}{4} \left(\cos \frac{k}{2} + \cos \frac{k'}{2} \right)^2 + \sin \frac{k}{2} \sin \frac{k'}{2}}} \right). \quad (14)$$

Subscript *int* in the first integral in Eq. (14) means that the integral is taken over the interval where the integrand is real. This interval consists of two segments: from 0 to $l_1(k)$ and from $l_2(k)$ to 2π , where $l_1(k)$ and $l_2(k)$ are the two solutions of the transcendental equation for k' :

$$\frac{1}{4} \left(\cos \frac{k}{2} + \cos \frac{k'}{2} \right)^2 - \sin \frac{k}{2} \sin \frac{k'}{2} = 0. \quad (15)$$

The solutions, which depend on k as a parameter, satisfy $l_1(k) \leq l_2(k)$. In the following section we will use Eq. (14) to estimate the long-time behavior of the heat current correlation function and the N dependence of the coefficient of thermal conductivity.

III. THE LONG-TIME BEHAVIOR OF THE CORRELATION FUNCTION

The coefficient of thermal conductivity can be calculated by using the current correlation function. The correlation function is defined as

$$D_N(t) = \frac{1}{N} \int d\{J_k\} d\{\alpha_k\} j(t) j(0) \frac{e^{-H/k_B T}}{Z}. \quad (16)$$

Here $\{J_k\}$ and $\{\alpha_k\}$ denote the set of action and angle variables for all the modes, Z is the partition function for the equilibrium ensemble, and j is the total-energy current. The coefficient of heat conductivity is given by

$$\kappa = \frac{1}{k_B T^2} \lim_{t \rightarrow \infty} \int_0^t d\tau \lim_{N \rightarrow \infty} D_N(\tau). \quad (17)$$

We can rewrite $D_N(t)$ as [18]

$$D_N(t) = \frac{1}{N} \int d\{J_k\} d\{\alpha_k\} \xi_j(0) \tilde{\rho}(t) \quad (18)$$

with

$$\tilde{\rho}(t) = e^{-iLt} \left(\frac{j(0)}{\xi} \frac{e^{-H/k_B T}}{Z} + \frac{e^{-H/k_B T}}{Z} \right), \quad (19)$$

where L is the Liouville operator corresponding to Hamiltonian (4) and ξ is an auxiliary parameter ensuring the correct dimensions for $\tilde{\rho}(t)$. The parameter does not appear in

the final expressions. In going from Eq. (17) to Eq. (18) we also used the fact that the average current over the equilibrium distribution is zero. Equation (18) shows that the correlation function can be expressed through the average current per particle with the averaging performed over the nonequilibrium distribution function (19). If we approximate the total heat current by its harmonic part (7) we can see that it depends only on the action variables and, therefore, the time evolution of the correlation function can be reduced to the time evolution of the average mode energies which is governed by Eq. (14). Note that if only harmonic terms are kept in distribution function (19) at $t=0$ then the initial average energy for mode k is

$$\bar{E}_k(0) = k_B T + \frac{2v_k k_B^2 T^2}{\xi}. \quad (20)$$

This has the form given in Eq. (11) with the deviation from $k_B T$ orthogonal to both of the zero eigenvalue eigenstates of the collision operator. Therefore, we expect the average mode energies to approach $k_B T$ for long times. To estimate the time behavior of \bar{E}_k based on (14) we will use the relaxation-time approximation [3]. We assume that the energy of each mode approaches zero with a characteristic time τ_k which depends on the wave vector, i.e.,

$$\frac{\partial \bar{E}_k}{\partial t} \approx -\frac{1}{\tau_k} (\bar{E}_k - k_B T). \quad (21)$$

Some plausibility arguments in support of this approximation were given in Refs. [5,19]. In this approximation and for $N \rightarrow \infty$ the correlation function (for which we now drop the subscript N) is given by

$$D(t) = \frac{2k_B^2 T^2}{\pi} \int_0^\pi dk e^{-t/\tau_k v_k^2}. \quad (22)$$

Since the decay rate for energy of the normal mode with $k=0$ is zero (due to the conservation of the total momentum)

we can expect $1/\tau_k$ to behave as some positive power of k for small k . The long-time behavior of $D(t)$ in Eq. (22) will be determined by the small- k behavior of $1/\tau_k$. Following Ref. [5] we will further assume that the k dependence of $1/\tau_k$ for small k is the same as in the multiplicative part of the collision operator in Eq. (14).

Both the relaxation-time approximation and the assumption that the k dependence of the relaxation rate for small k is the same as in the multiplicative part of the collision operator has been widely used in the theory of heat conduction in insulators [3,5]. A convincing justification of both assumptions, however, is lacking. Reference [5] tries to justify both assumptions at least for wave vectors with small k by the following reasoning. If only the multiplicative part was kept in the collision operator the resulting equation would describe a physical situation when all modes except mode k are in equilibrium. In general this is not the case. However, for any initial nonequilibrium distribution of energy all modes except those with very small k quickly relax to equilibrium. As a result as far as the small- k modes are concerned after a short time the physical situation is similar to the one just described and the integral part of the collision operator becomes negligible compared to the multiplicative part.

If we accept both approximations for Eq. (14) then we expect $1/\tau_k \propto \sin^2(k/2)I(k)$ with

$$I(k) = \int_0^{2\pi} dk' \frac{1}{\sqrt{\frac{1}{4} \left(\cos \frac{k}{2} + \cos \frac{k'}{2} \right)^2 + \sin \frac{k}{2} \sin \frac{k'}{2}}}. \quad (23)$$

This integral can be reduced to an elliptic integral of the first kind through the substitution $x = \tan(k'/4)$:

$$I(k) \propto \int_0^\infty dx \frac{1}{\sqrt{P_k(x)}}, \quad (24)$$

where

$$P_k(x) = \left(1 - \cos \frac{k}{2} \right)^2 x^4 + 8 \left(\sin \frac{k}{2} \right) x^3 - 2 \left(\sin^2 \frac{k}{2} \right) x^2 + 8 \left(\sin \frac{k}{2} \right) x + \left(1 + \cos \frac{k}{2} \right)^2. \quad (25)$$

Integral (24) can be reduced to the Legendre normal form and its k dependence can be expressed in terms of the k dependence for the roots of the fourth-order polynomial (25) [20]. Since the calculations are rather involved and we are interested only in the small- k behavior of $I(k)$ we give here a less rigorous but simpler estimation that gives the same result for small k . We expand the coefficients in the polynomial in powers of k and keep the lowest-order terms in front of each monomial to get

$$I(k) \propto \int_0^\infty dx \frac{1}{\sqrt{\frac{k^4}{64} x^4 + 4kx^3 - \frac{k^2}{2} x^2 + 4kx + 2}}. \quad (26)$$

Note that for positive k the denominator remains positive in the integration range since

$$\frac{k^4}{64} x^4 - \frac{k^2}{2} x^2 + 2 > 0, \quad (27)$$

as can be checked by solving the corresponding quadratic equation for x^2 . Introducing the new variable $y = k^{1/3}x$ we obtain

$$I(k) \propto \frac{1}{k^{1/3}} \int_0^\infty dy \frac{1}{\sqrt{\frac{k^{8/3}}{64} y^4 + 4y^3 - \frac{k^{4/3}}{2} y^2 + 4k^{2/3}y + 2}}. \quad (28)$$

The integral appearing in Eq. (28) is finite and remains finite for $k=0$. As a result, for small k we have $I(k) \propto k^{-1/3}$ and, therefore,

$$\frac{1}{\tau_k} \propto k^{5/3}. \quad (29)$$

With this k dependence for the relaxation rate the time dependence of the correlation function is determined by the following integral:

$$D(t) \propto \int_0^\pi dk e^{-k^{5/3} \kappa t} v_k^2. \quad (30)$$

Here K is a positive constant. Keeping in mind that v_k is a constant for small k the long-time behavior of $D(t)$ is estimated to be

$$D(t) \propto \frac{1}{t^{3/5}}. \quad (31)$$

This implies that the heat conductivity coefficient κ diverges. Indeed, we have

$$\kappa \propto \lim_{t \rightarrow \infty} \int_0^t d\tau \frac{1}{\tau^{3/5}} \propto \lim_{t \rightarrow \infty} t^{2/5}. \quad (32)$$

Clearly the divergence of κ does not mean that the energy propagates through the lattice instantaneously. It just implies that the Fourier heat law is not valid in the infinite FPU β lattice. We can also estimate the dependence of κ on the size of the lattice. Following Ref. [8] we restrict the integral in Eq. (17) to times smaller than the characteristic time for the energy propagation N/v_k . This leads to the following N dependence for κ :

$$\kappa \propto N^{2/5}. \quad (33)$$

Thus we can see that κ diverges in the thermodynamic limit which is consistent with Eq. (32).

Apart from the k dependence of the decay rate for the mode energy, its temperature dependence is also of interest. It follows from Eq. (14) that as a function of temperature the decay rate is proportional to T^2 .

The estimations we have obtained are in rather good agreement with the results of computer simulations. The divergence of the heat conductivity coefficient as N^μ with $\mu \approx 0.37$ was observed in the numerical studies of the FPU β model [8,9,11,12]. This result is very close to estimation (33). Similarly, the $k^{5/3}$ dependence of the decay rate for mode energy was observed [9]. The temperature dependence of the decay rate reported in Ref. [9] is very close to T^2 for weak coupling.

In Ref. [9] the same types of t dependence for the correlation function and N dependence for κ were obtained by using the mode coupling theory. As a function of temperature the decay rate obtained through the mode coupling theory behaves as $T^{4/3}$ in the limit of weak coupling and as $T^{1/4}$ for strong coupling [9]. Thus, the temperature dependence in the weak coupling limit is different from our T^2 estimation. Note, however, that according to Ref. [9] the mode coupling results should be valid for strong coupling and on very long time scales. In general, the mode coupling theory as used in Ref. [9] allows one to make some general statements about the long-time behavior of the current correlation function for a class of one-dimensional lattices while Eq. (14) gives a more detailed picture of the energy equipartition between the normal modes for the special case of the β FPU lattice for the weak coupling case. If solved numerically, Eq. (14) will allow for the quantitative comparison of the energy equipartition given by the Peierls equation to the one observed in computer simulations. We will not attempt here to analyze the relation between our result and the mode coupling theory although this point clearly deserves attention.

In a recent publication [21] it is claimed that κ should diverge with system size L as $L^{1/3}$ for all momentum conserving one-dimensional systems. So far the most careful computer simulation [11] fails to confirm this claim. At present, therefore, this issue remains unsettled.

It is well known that for systems such as a gas of hard spheres or Lorentz gas it is impossible to obtain the correct long-time behavior for the correlation functions if one uses only the kinetic equation [13]. This is because for those systems the spectrum of the collision operator is discrete. As a result if only the kinetic equation is used the long-time be-

havior is determined by the smallest nonzero eigenvalue of the collision operator and has an exponential form. In contrast, in our case the collision operator has a continuous spectrum that is bounded from below by zero. This fact allows for the nontrivial time dependence of the correlation function to be obtained already in the framework of the kinetic equation.

IV. CONCLUDING REMARKS

Applying the Peierls equation to the FPU β lattice we estimated the wave vector and temperature dependence for the decay rate of the average mode energy, the long-time behavior of the current correlation function, and the dependence of the coefficient of heat conductivity on the size of the lattice. The obtained results are in good agreement with the results of the recent computer simulations. As we used a number of strong assumptions it can be of interest to solve Eq. (14) numerically in order to verify if the assumptions are correct and whether the time evolution of mode energies given by Eq. (14) is compatible with the results of computer simulations for the case of weak coupling.

Recently lattices with external substrate potentials drew considerable attention since some of them show finite heat conductivity for $N \rightarrow \infty$ [10,22–25]. We can apply our analysis of Sec. III to show that the FPU lattice with added harmonic on-site potential of the form $\sum_r u_r^2$ is likely to have finite heat conductivity for infinite lattice. It is easy to show that in this case for $k \rightarrow 0$ the harmonic frequency tends to a constant value while the group velocity becomes proportional to k . The energy of the normal mode with $k=0$ is still a constant of motion since coefficient (5) vanishes when at least one of the k 's is zero. Therefore, we can expect the decay rate of the mode energy to behave as k^ν for small k . This will lead to the $t^{-3/\nu}$ long-time behavior of the current correlation function and, therefore, finite heat conductivity for $\nu < 3$. Thus, if adding the harmonic on-site potential does not appreciably change the $k^{5/3}$ wave-vector dependence of the decay rate, we can expect to find finite heat conductivity in this case.

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