Does Equipartition of Energy Occur in Nonlinear Continuous Systems?

The celebrated work of Fermi, Pasta, and Ulam was the first of numerous attempts to study the distribution of energy in nonlinear continuous media. These attempts have all been indirect in that the systems are simulated by lattices of particles interacting through nonlinear potentials. The results have consistently failed to support the classical point of view regarding equipartition of energy—and yet they have stirred little excitement in the physics community. Perhaps this is so for two reasons: (i) the systems analyzed may be subject to an infinite number of conservation laws (and thus may be effectively linear), so that the individual degrees of freedom are not coupled and equipartition of energy cannot occur; (ii) the results may simply be artifacts of the lattice simulations.

Here I present some results from two of my own studies, the first of a one-dimensional model of the blackbody problem (Adrian Patrascioiu, *Physical Review Letters 50(1983): 1879)* and the second of a three-dimensional system that may give insight into the specific heats of systems with two species of degrees of freedom, such as the rotations and vibrations of diatomic molecules (K. R. S. Devi and A. Patrascioiu, *Physica D 11(1984): 359).*

In the case of blackbody radiation, the continuous medium (the electromagnetic field) is linear. Nonlinearity is introduced into the problem through the interaction of the field with the atoms in the walls of the cavity. Let us investigate a one-dimensional version of this problem, two nonlinear oscillators (particles and nonlinear springs) interacting through a linear string (Fig. 1). The string represents the electromagnetic field, and the oscillators represent the atoms. This model has the advantage that the string can be treated exactly so that no spatial lattice is needed.

The string and the particles move in the z direction only. The equation of motion for the string is

$$\frac{\partial^2 z(x,t)}{\partial t^2} - \frac{\partial^2 z(x,t)}{\partial x^2} = 0, \quad \text{for } x \neq \pm 1, \tag{1}$$

and the equations of motion for the particles on the left and right, respectively, are

$$m\frac{\partial^2 z(x,t)}{\partial t^2}\bigg|_{x=-1} = \mu \frac{\partial z(x,t)}{\partial x}\bigg|_{x=-1} + F\big(z(-1,t)\big) \tag{2}$$

and

$$m\frac{\partial^2 z(x,t)}{\partial t^2}\bigg|_{x=1} = -\mu \frac{\partial z(x,t)}{\partial x}\bigg|_{x=1} + F\big(z(1,t)\big). \tag{3}$$

Here m is the mass of each particle, μ is the string tension, and the nonlinear spring force F'(z) is defined by

$$F(z) = -\frac{dV}{dz},$$

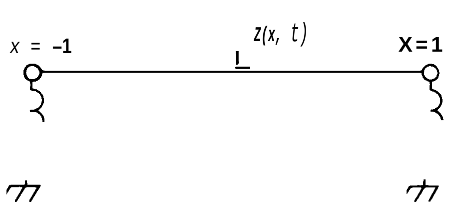
where

$$V = k\frac{z^2}{2} + \lambda\frac{z^4}{4} + c\,|z|.$$

These equations are written in units such that the length of the string is 2 and the speed of sound is 1. The most general form for the solution of Eq. 1 is $z(x,t) = f(t+x) + g(t-x)$. Substituting this general solution into Eqs. 2 and 3 yields a system

A ONE-DIMENSIONAL MODEL OF THE BLACKBODY PROBLEM

Fig. 1. The blackbody problem was modeled as the interaction of a linear string (which represents the electromagnetic field) and two nonlinear oscillators (which represent atoms in the walls of the cavity). Motion of both the string and the oscillators is restricted to the z direction and is described by the function *z(x, t)*.



of two coupled ordinary differential equations for the functions f and g.

The excitation of the string at $t = 0$ was specified by setting $f(x) = a \sin(\omega x + \pi/2)$ and $g(x) = 0$. The differential equations were integrated numerically, and conservation of energy was used to verify the accuracy of the calculations.

I would like to emphasize what outcome one would predict by following the same line of thought used to derive the Rayleigh-Jeans formula. The system, being nonlinear and (probably?) sufficiently complicated, will wander with equal probability throughout its phase space of given total energy. Let us choose initial conditions such that the total energy is finite. If ensemble averages and time averages are equal for this microcanonical ensemble, that is, if

$$\langle A\rangle_\mu = \lim_{T\to\infty} \frac{1}{T} \int dt\, A(t),$$

then the time-average kinetic energy of either particle should tend to zero for any initial conditions since the number of degrees of freedom is infinite. Over my times of observation, this did not seem to be the case! Under the assumption that the times of observation were sufficiently long, this result indicates that the microcanonial measure (Eq. 7 in the main text) is not applicable. We are left with two possibilities: (i) the motion of the system is quasiperiodic, or (ii) the phase space is broken into an infinite number of ergodic cells of finite size.

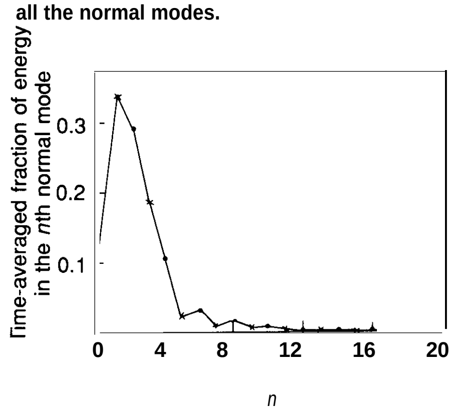
I also investigated the distribution of energy among the normal modes of the string. Figure 2 shows typical results for the time-average values of the fraction of the string energy in the *nth* normal mode. In all the runs performed the distribution of energy of the string among its normal modes is highly peaked (like the Planck distribution) and shows no tendency to become flat. Its shape does depend on the values of the various parameters in the problem and on the initial conditions. If all the parameters are kept fixed and the total energy is increased, the peak broadens. The shape of the distribution also varies with the frequency chosen for the initial excitation of the string, remaining constant over some range of ω and then jumping to a new shape.

The results of this study raised naturally several questions: (i) Was the observed unequal partition of energy among the normal modes of the string (the continuous medium) related to the one-dimensional nature of the medium? (ii) The unequal partition of energy reflected in the specific heats of diatomic gases results from motions of particles (rather than motions of a field, as in the case of blackbody radiation). Can this phenomenon be reproduced in a classical dynamical system?

To help answer these questions, Devi and I performed a study of a three-dimensional version of the system shown in Fig. 1. This system included four particles and six strings (Fig. 3). Our results exhibited several notable features over the times of observation: (i) time averages of, for example, total energies of particles and strings seemed to reach their asymptotic values; (ii) unequal partition of energy among the normal modes of the strings persisted, and the distributions obtained were reminiscent of that given by Planck's law; and (iii) for a variety of initial conditions, the four particles did not achieve the same average kinetic energy, a situation similar to the unequal partition of energy between the vibrational and the rotational degrees of freedom of diatomic gases. The fact that we obtained these types of results using several nonlinear (spring) potentials suggests their generality. ■

UNEQUAL PARTITION OF ENERGY

Fig. 2. Typical results for the distribution of energy among the normal modes of the string in the one-dimensional model of the blackbody problem (see Fig. 1). The exact shape of the energy distribution depends on the values assigned to various parameters, but in all cases the distribution was similar to a Planck distribution (see Fig. 2 of the main text) and was never flat, as it would be if the energy were partitioned equally among all the normal modes.



A THREE-DIMENSIONAL LATTICE

Fig. 3. The lattice below was used to investigate the dynamical behavior of a three-dimensional nonlinear system of particles and fields. Each of the four particles at the vertices of the regular tetrahedron is coupled to a nonlinear spring, and the particles are coupled to each other through linear strings.