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Thermomechanics and statistical mechanics of an adiabatically isolated body

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A statistical distribution for an adiabatically isolated body is proposed and its temperature is defined as a function of a given energy. It is obtained as a result of the generalization of the statistical distribution for an ensemble of oscillators, in which the probability is proportional to the time of motion on each small section of the oscillator trajectory in the phase space. This distribution makes it possible to explain the thermoelastic effect — the dependence of the body temperature on the deformation under its adiabatic mechanical loading. The proposed explanation is in clear agreement with the first law of thermodynamics.

Keywords: adiabatic, thermoelastic effect, statistical distribution, partition function, temperature.

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1. Introduction

Close interrelations can be found between two rather remote sections of thermal physics — experimental study of mechanical and thermal phenomena in an adiabatically isolated body and statistical mechanics in adiabatic isolation conditions. The key condition here is the adiabatic isolation condition which releases a body from „shaking“ by external fluctuations. The first experimental results which form the basis of thermomechanics were presented in classical papers [1,2]. They can be combined into a simple empirical formula which describes a relative change of temperature of an adiabatically isolated body under uniaxial mechanical deformation

$$\frac{\Delta T}{T} = -\frac{\alpha}{c\rho} \sigma, \quad (1)$$

where α is (linear) thermal expansion coefficient, c is specific heat capacity, ρ is body density, σ is mechanical stress. Note that temperature decreases ($\Delta T < 0$) for most bodies under tension ($\sigma > 0$). It should be also noted that the effect itself is, evidently, a manifestation of the nonlinearity (anharmonicity) of interatomic forces. A statistical distribution for small subsystems of an isolated body, which can also include its atoms, is only approximately described by the Gibbs distribution [3]:

$$f_B(p, q) = A \exp\left[-\frac{H(p, q)}{k_B T}\right], \quad (2)$$

since the body state equation in this case reduces to a simple equality

$$H(p, q) = E. \quad (3)$$

Here H is the Hamiltonian function, p and q — generalized momentums and coordinates, k_B — the Boltzmann constant, A — normalization constant, E — system energy. Thus, it is of current interest to find a proper substitute of distribution (2) for an adiabatically isolated body.

While noting the long-time history of the thermomechanics of an adiabatically isolated body [4], we would like to point out the non-decreasing interest in it and the new experimental results obtained recently [5,6]. The thermoelastic effect can also be a ground for advanced technologies of solid-state cooling in cooling units [7]. Thereat, the effect itself is still explained somewhat vaguely. This applies, in particular, to the energy balance in the adiabatic deformation process [8].

A relation between thermomechanics and statistical mechanics is established in the present paper on the basis of a simple mechanical explanation [9] of the thermoelastic effect, where an adiabatic invariant is used [10]:

$$I = \frac{E}{\omega} \quad (4)$$

in the dynamics of a parametrically perturbed harmonic oscillator (ω is oscillator frequency). This mechanical approach is somewhat modified and generalized. The generalization consists in the transition to an ensemble of harmonic (anharmonic) oscillators which demands that the appropriate statistics be introduced. Special attention is paid to the energy balance in the thermomechanics of an isolated body which, of course, reduces to the first law of thermodynamics

$$dQ = 0 = dE - dA, \quad (5)$$

where dQ is the transferred heat energy, dE is the change of system energy, dA is the work of external forces.

2. Statistical mechanics of an adiabatically isolated body

Statistical mechanics in the general sense [3,11] describes the evolution of small subsystems of a large system in its „equilibrium“ state, which in the considered case depends on the single initial parameter E in equation (3). Here we will reformulate the conventional mechanics of an isolated system in terms of statistical mechanics by introducing the corresponding distribution density in its phase space. We begin with the simplest mechanical system — a harmonic oscillator described by a Hamiltonian function

$$H(p, q) = \frac{p^2}{2m} + \frac{f_0 q^2}{2}, \tag{6}$$

where m is mass, f_0 is the elastic constant. Oscillations of an isolated oscillator with the given energy E have a half-period

$$\tau_0 = \int_{-a}^a \frac{dq}{\sqrt{\frac{2}{m} \left(E - \frac{f_0 q^2}{2} \right)}} = \pi \sqrt{\frac{m}{f_0}}, \tag{7}$$

which does not depend on energy E and oscillation amplitude a . The statistical mechanics considers, instead of a real motion trajectory, the probability of detection of a system in the small neighborhood of each point of a phase space

$$dP(p, q) = f(p, q) dp dq. \tag{8}$$

This probability in the given case is, evidently, proportional to the time interval

$$dt = \frac{dq}{\sqrt{\frac{2}{m} \left(E - \frac{f_0 q^2}{2} \right)}}, \tag{9}$$

which is occupied by mechanical movement in the region under consideration. Thereat, the canonical momentum

$$p = \sqrt{2m \left(E - \frac{f_0 p^2}{2} \right)} \tag{10}$$

is an associated parameter. It can be easily checked that the desired distribution density can be written as a delta function

$$f(p, q) = A \delta \left(\frac{p^2}{2m} + \frac{f_0 p^2}{2} - E \right), \tag{11}$$

while the statistical sum, which determines the normalization, is equal to the half-period of mechanical movement

$$Z = \tau_0. \tag{12}$$

The notion of temperature must be also defined for a complete transition to the terms of statistical mechanics in

this mechanical problem. In [9], oscillator „temperature“ is naturally identified with the total mechanical energy of its oscillations: $T = E$ ($k_B = 1$). Though this simplification does not belittle the physical justification of the approach suggested in [9], we need a proper definition of temperature for a large system. The only simple definition of temperature (reciprocal temperature $\beta = 1/T$) of an isolated body can be as follows [12]:

$$\langle \beta \rangle = \frac{\partial \ln Z}{\partial E}. \tag{13}$$

We get $\langle \beta \rangle = 0$ for one harmonic oscillator, so that its temperature is not defined. We may state that this simple mechanical system does not have full statistics, and the notion of temperature also has no sense.

In order to use formula (13), we pass on to an oscillator ensemble which will be considered as an isolated body model (Einstein model). Oscillators can also be anharmonic. It is easy to write down the distribution density for an ensemble of N independent oscillators

$$f_N(p, q) = A \delta(E_1 + E_2 + \dots - E) \delta \left(\frac{p_1^2}{2m} + V(q_1) - E_1 \right) \times \delta \left(\frac{p_2^2}{2m} + V(q_2) - E_2 \right) \dots, \tag{14}$$

where $i = 1, 2, \dots, N$ is oscillator number, $V(q)$ is potential energy, and its statistical sum

$$Z_N = \int_0^E dE_1 \int_0^{E-E_1} dE_2 \dots \tau(E_1) \tau(E_2) \dots \tag{15}$$

Here τ is the half-period of anharmonic oscillations. We obtain the following for an ensemble of harmonic oscillators in which the half-period τ_0 does not depend on energy

$$Z_N = \frac{E^{N-1}}{2^{N-2}} \tau_0^N. \tag{16}$$

Temperature in this case is defined and equal to

$$T = \frac{1}{\langle \beta \rangle} = \frac{E}{N-1}, \tag{17}$$

which agrees with [9] and seems to be quite reasonable.

For a statistical explanation of the thermoelastic effect, let us consider an ensemble of anharmonic oscillators with potential energy

$$V(q) = \frac{f_0 q^2}{2} - \frac{g q^3}{3}, \tag{18}$$

where g is the anharmonicity constant. Now the oscillation half-period τ depends on oscillator excitation energy. Let us find this dependence approximately using a harmonic approximation of potential (18) in the neighborhood of the average value of its minimum point

$$q_E = \frac{g \langle q^2 \rangle}{f_0} = \frac{g E}{f_0^2}. \tag{19}$$

Mean displacement of the equilibrium point of anharmonic oscillations defines the linear expansion of an anharmonic body [13]. The half-period of oscillator oscillations is found using formula (7) where f_0 should be substituted by

$$f = V''(q_E) = f_0 - \frac{2g^2E}{f_0^2}. \quad (20)$$

Then we get

$$\tau(E) = \frac{\tau_0}{\sqrt{1 - \frac{2g^2E}{f_0^2}}} \cong \tau_0 \left(1 + \frac{g^2E}{f_0^3}\right). \quad (21)$$

The statistical sum of an ensemble of anharmonic oscillators is also found accurate to the second order according to the anharmonicity constant g :

$$Z_N \approx \frac{E^{N-1}}{2^N} \tau_0^N \left(1 + \frac{g^2E}{f_0^3}\right). \quad (22)$$

Then we determine the ensemble temperature in the specified approximation

$$T = \frac{E}{N-1} - \frac{g^2}{f_0^3} \left(\frac{E}{N-1}\right)^2. \quad (23)$$

It means that the average energy of an anharmonic oscillator in the ensemble $E/(N-1)$ should not be identified with average oscillation energy which defines ensemble temperature T . The disparity in the considered approximation is equal to the energy of oscillator oscillations with an amplitude equal to the average value of thermal expansion q_E .

The disparity in (23) confirms the rightfulness of the first law of thermodynamics (5) in the thermomechanics of an adiabatically isolated body. Indeed, the work of an external force, let us say, under tension ($F > 0$) of an anharmonic oscillator increases its internal energy

$$\frac{E}{N-1} = T + \frac{g^2}{f_0^3} \left(\frac{E}{N-1}\right)^2 + \frac{F^2}{2f_0}. \quad (24)$$

Let us regroup the terms in the right member of this equality, by separating the elastic energy of total deformation $q_E + F/f_0$:

$$\frac{E}{N-1} = (T - q_E F) + \frac{f_0 q_E^2}{2} + \frac{f_0}{2} \left(q_E + \frac{F}{f_0}\right)^2. \quad (25)$$

Separation of the elastic energy of total deformation is required for consistency with the first law of thermodynamics [14]. Thus, the suggested statistical description of the dynamics of an isolated ensemble of anharmonic oscillators makes it possible to explain the thermoelastic effect described by empirical formula (1) (the first term in (25)), as well as to justify the energy balance in the process of deformation of an adiabatically isolated body.

To conclude the present paper, let us formulate a generalization of statistical distribution (14) for an Einstein model for the general case of an adiabatically isolated body:

$$f(p, q) = A \delta(H(p, q) - E), \quad (26)$$

where

$$H(p, q) = \frac{1}{2} m_{ik}^{-1} p_i p_k + V(q) \quad (27)$$

— Hamiltonian function, m_{ik} — symmetric matrix of mass constants in the quadratic form of kinetic energy, arising after exclusion of the system center of mass coordinates. It is assumed here that the body center of mass coordinates are excluded, since they are cyclic variables with zero potential energy. The half-period τ for such variables is infinite.

3. Conclusion

We have approached the determination of distribution density (26) for an adiabatically isolated body based on the empirical regularities observed during its mechanical deformation. A new approach to statistical mechanics provides a corresponding definition of temperature of an isolated body entirely in internal terms

$$\left\langle \frac{1}{T} \right\rangle = \frac{\partial \ln Z}{\partial E}, \quad (28)$$

$$Z = \int \prod dq dp \delta(H(p, q) - E). \quad (29)$$

Of course, the new statistics with distribution density (26), in addition to the suggested empirical justification, needs a theoretical justification as well. Such a justification can be a formulation of the quantum theory and the associated statistical mechanics in the covariant form suggested in [15].

Conflict of interest

The authors declare that they have no conflict of interest.

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