13,14

Period, oscillation energy, and temperature of an adiabatically isolated body

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For the previously proposed definition of the (inverse) temperature of an adiabatically isolated body in the form of a derivative of the logarithm of the density of states of the canonical energy distribution of the system, a relationship between temperature and the minimum period of a certain oscillatory motion of atoms in the stationary regime is found. At the same time, it is shown that the temperature is determined by the oscillation energy equal to the difference between the total energy of the body and the potential energy of deformation. The deformation, taking into account anharmonicity, is equal to the sum of mechanical deformation in an external force field and thermal expansion. In the presence of dissipation or adiabatic deformation of a body, its temperature is determined approximately by the period „almost" of oscillatory motion in the configuration space.

Keywords: thermomechanics, isolated mechanical system, anharmonicity, adiabatic deformation.

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1. Introduction

The question of the concept of temperature and its relation to mechanics arises when analyzing the thermoelastic effect, in which a slight change in body temperature is observed during its adiabatic mechanical deformation [1,2]. At the same time, the use of statistical mechanics in the form of the canonical Gibbs distribution is questionable, since it predicts nonzero energy fluctuations, whereas in an isolated system the energy is constant [3]. A purely mechanical explanation of the thermoelastic effect based on the theorem on the adiabatic invariant [4] in the case of a single oscillator is proposed in Ref. [5]. Here, parametric excitation is considered in the harmonic approximation, and the role of anharmonicity is reduced to the influence of mechanical load on the parameters of harmonic oscillations. In the first approximation of the theory of perturbation by the constants of anharmonicity, such an explanation of the thermoelastic effect is sufficient. However, in the following order, the effect of thermal expansion will be significant in the same parametric excitation. The purpose of this study is to consistently account for the effects of anharmonicity in thermomechanical phenomena.

For a complex mechanical system with nonlinear internal forces, it is necessary to use statistical methods with a suitable statistical distribution. For an isolated body, we need to find a replacement for the canonical distribution [3]. We will leave aside deviations from the canonical distribution caused by other reasons. For example, in the case when the „thermostat" has finite dimensions [6], or the system is non-ergodic [7]. There are also opportunities for mathematical generalizations [8]. The microcanonical Gibbs distribution will be used for an isolated system in this paper. The transition from the canonical distribution to the microcanonical distribution is carried out as follows. The statistical sum of the canonical Gibbs ensemble can be represented as [9]:

$$Z(\beta) = \int_0^\infty M(W)\exp(-\beta W)dW, \tag{1}$$

where $M(W)$ is the density of system states, $\beta = 1/k_{\mathrm{B}}T$. The integral in (1) has the form of the Laplace transform [10]. Then the inverse Laplace transform defines the density function of states [11]:

$$M(W) = \frac{1}{2\pi i}\int_{-i\infty}^{+i\infty} Z(\beta)\exp(\beta W)d\beta. \tag{2}$$

The temperature of an isolated body is defined here in terms of the average value of β for the microcanonical distribution:

$$\frac{1}{k_{\mathrm{B}}T} = \frac{\partial \ln M(W)}{\partial W}. \tag{3}$$

Obviously, $M(W)$ coincides with the statistical sum for an isolated system, defined similarly as in Ref. [9], but within the framework of covariant quantum mechanics [12]. Finally, we find the statistical sum of the canonical Gibbs ensemble as the trace of the statistical operator,

$$Z(\beta) = \mathrm{Tr}\,\hat\rho\,(\beta) \tag{4}$$

where the statistical operator, in turn, is the solution of the parabolic equation [9]

$$-\hbar\frac{\partial\hat\rho}{\partial\beta} = \hat H\hat\rho \tag{5}$$

with the initial condition $\hat{\rho}(0) = \hat{1}$, where $\hat{1}$ is the unit operator, $\hat{H}$ is the Hamilton operator of the system under consideration.

A question arises when determining the temperature of an isolated body using the formula (3). According to (3), this temperature depends on the total energy of the body W. However, under mechanical loading, the body acquires static energy of elastic deformation, which, obviously, is not directly related to internal heat and body temperature. If we take into account the nonlinearity of the forces of interatomic interaction (anharmonicity), thermal deformation is added to the mechanical deformation of the body [13,14]. It was suggested in Ref. [15] that the total elastic energy of all types of stationary deformation of a body should be subtracted from its total energy W, and we call the remainder the oscillation energy and directly relate it to body temperature. A justification of this assumption is obtained in the most general form in this paper.

2. Oscillation period and temperature of the isolated mechanical system

We specify the type of the Hamilton function of the system in an external force field:

$$H = \frac{1}{2} m_{lk}^{-1} p_l p_k + V(q) - F_k q_k, \tag{6}$$

where m_{lk} is a positive definite, symmetric mass matrix. We assume that

$$\sum_k F_k = 0, \tag{7}$$

We also consider the center of mass to be at rest. For simplicity, we consider a uniaxial force field, otherwise additional equilibrium conditions are necessary. Let's represent the density matrix $\rho(q, q'; \beta)$ as a Feynman functional integral [9]:

$$\rho(q, q'; \beta) = \int Dq \exp\left\{ -\int_0^{\hbar\beta} d\beta \left[\frac{1}{2} m_{lk} \dot{q}_l \dot{q}_k + V - F_k q_k \right] \right\}. \tag{8}$$

Here, the action in the exponent is represented in Euclidean form. Assuming $q' = q$, we obtain the probability density $\rho(q, q; \beta)$ that the system will be detected in the vicinity of the point q of the configuration space, and

$$Z(\beta) = \int d^N q \rho(q, q; \beta) \tag{9}$$

is equal to the statistical sum of the canonical distribution. This expression should be substituted into the formula (2) for the density function of states.

Let us use the saddle-point method to find the density of states $M(W)$ [16]. At the same time, forming the general exponent under the integral sign (2), we will add the classical term — βW to the classical action. Three integrals are subject to evaluation at once: the integral over β in the formula (2), N is the multiple integral over matching coordinates (9) (N is the number of degrees of freedom of the system) and the functional integral (8). First, we evaluate the last two integrals. It is necessary to find the extremum of the Euclidean action in the exponent in (8) (with addition βW) under the additional conditions that the trajectories are closed, $q_k(0) = q_k(\beta)$, and also smooth: $\dot{q}_k(0) = \dot{q}_k(\beta)$. The latter follows from the extremum condition for the integral (9): the derivatives of the action on the coordinates of the coinciding boundary points $q_k(0) = q_k(\beta)$ are zero. The is the method for evaluating the last two integrals gives an exponential expression

$$Z(\beta) = \exp\{-\Psi\},$$

where

$$\Psi = \tilde{S} - \frac{1}{2} \ln \det \frac{\delta^2 \tilde{S}[\tilde{q}]}{\delta q_k(\beta) \delta q_l(\beta)} \tag{10}$$

— free energy of the system. Here $\tilde{q}_k(\beta)$ is the closed classical trajectory of the system in the configuration space,

$$\tilde{S} = \int_0^{\hbar\beta} d\beta \left[\frac{1}{2} m_{lk} \dot{\tilde{q}}_k \dot{\tilde{q}}_l + V - F_k \tilde{q}_k - W \right] \tag{11}$$

— is an action on a classical trajectory, and $\delta^2 \tilde{S}[\tilde{q}] / \delta q_k(\beta) \delta q_l(\beta)$ is the variational derivative of a second-order action calculated on a classical trajectory (one-loop approximation).

To understand what kind of closed classical trajectory we can talk about here, let us first limit ourselves to the quasi-classical approximation ($\hbar \to 0$), when the second term in (10) can be neglected. We emphasize that a closed classical trajectory should be nontrivial (different from the minimum potential point) for a given nonzero energy of the system. Then the saddle-point method provides an extremum condition for evaluating the integral (2) with respect to the parameter β:

$$H_E - W = 0, \tag{12}$$

where

$$H_E = -\frac{1}{2} m_{lk}^{-1} p_l p_k + V(q) - F_k q_k \tag{13}$$

— the Euclidean Hamilton function of the system, which, taking into account $p_k = m_{lk} \dot{q}_l$, gives the desired extreme value β:

$$\hbar\beta_0 = \oint \frac{\sqrt{m_{lk} dq_l dq_k}}{\sqrt{2(V - F_k q_k - W)}}, \tag{14}$$

where integration is carried out along an extreme closed trajectory of the system in the configuration space. But in the Euclidean representation of such a trajectory, apart from a trivial trajectory, there is no such thing. However, here we take into account [11] that the integration in (2) is based on imaginary values β, so that the value

$$i\hbar\beta_0 = \oint \frac{\sqrt{m_{lk} dq_l dq_k}}{\sqrt{2(W - V + F_k q_k)}}, \tag{15}$$

It has a meaningful meaning in dynamics with nonzero energy and with real time. This is true, since (15) is equal to the time of movement along a certain closed trajectory in the configuration space of the system. We will proceed from the fact that the isolated system under consideration is conservative and nonsingular, its trajectory in the configuration (and phase) space, at a given energy W, lies entirely in a limited region of the configuration space. This means that the trajectory will eventually fall into an arbitrarily small neighborhood of the starting point. If we use the theory of stability of solutions of ordinary differential Lyapunov equations [17], we can expect that a small variation in the initial data will lead to an intersection of the trajectory with the starting point. This means that periodic solutions exist in the mechanical problem under consideration. If so, the repetition of the specified movement has long periods $n\hbar\beta_0$. We are interested in the shortest oscillation period of the system at a given energy W. Having obtained a solution to the extremum problem in the field of mechanical motion of a system with real time, one should return to the Euclidean domain of statistical mechanics. It is necessary to replace $W \to -iW$ in the formula (1) for the statistical sum of the canonical distribution to make sense and be real (see [11]). We will make the same substitution in formulas (2) and (3). After that, we also get a mathematically meaningful expression for temperature:

$$\frac{1}{k_{\rm B}T} = i\beta_0 = \frac{1}{\hbar}\oint \frac{\sqrt{m_{lk}dq_l dq_k}}{\sqrt{2(W - V + F_k q_k)}}. \qquad (16)$$

However, we cannot accept T_0 as body temperature without taking into account the second term in (10). Its meaning is clarified in the harmonic approximation or, in other words, Einstein's model of a solid body as an ensemble of harmonic oscillators. In this approximation, the determinant reduces to the product of [9]:

$$\prod_{k=1}^{N}\left(\operatorname{sh}\frac{\hbar\omega_k\beta}{2}\right)^2, \qquad (17)$$

where ω_k is the frequency of the oscillators (phonons) in the ensemble, and is equal to $Z_N^{-2}(\beta)$, where $Z(N)(\beta)$ is the statistical sum of the canonical ensemble of oscillators. From here we can find the density of states $M(W)$ and the temperature of the ensemble using formulas (2) and (3), as it is done in Ref. [12]. It should be noted that, in the harmonic approximation, there is also a periodic motion with the shortest period — this is a collective oscillation corresponding to the optical phonon of the highest frequency ω_k. In this case, the potential energy of harmonic oscillations and, consequently, the phonon frequencies do not depend on the collective background motion. Therefore, all constructions in Ref. [12] remain valid, and we exclude the quasi-classical contribution to temperature (16) by choosing its starting point. Returning to the general expression for the free energy (10), we obtain the following extremum condition for estimating the integral (2):

$$\frac{d\Psi}{d\beta} = W, \qquad (18)$$

which is an ordinary differential equation with the main variable β. It is this equation that must be used to account for anharmonicity. Now, the collective vibrational motion of atoms modulates the potential energy and frequencies of phonons to the extent of anharmonicity. As we already know, the solution of equation (18) with respect to β should be sought in the form of β_0 (16) on the periodic trajectory of the system with a minimum period. However, for a physically meaningful determination of temperature, the temperature limit value at $W \to 0$ should be subtracted from the found solution $T_0 = 1/k_{\rm B}\beta_0$. Thus, with minimal energy, the temperature, as it should be, will be zero. At the final stage, in formulas (2) and (3), we replace $W \to -iW$ again. Thus, we will obtain a definition of the temperature of an isolated system, taking into account anharmonicity. The obtained result shows that the temperature is effectively determined by the oscillation energy

$$W - V\big(\langle q_k\rangle\big) + F_k\langle q_k\rangle,$$

where, taking into account anharmonicity, $\langle q_k\rangle$ is equal to the sum of mechanical and thermal deformations. At the same time, the potential energy of external forces $F_k\langle q_k\rangle$ is also included in the energy balance.

3. Conclusion

We have considered the idealized case of an isolated body. In real bodies, there is always dissipation associated with plastic deformation and loss of energy, for example, due to thermal radiation. In this case, we can talk about „almost“ periodic cycles in the atomic dynamics of a body, and, accordingly, about an approximate determination of temperature. To this should be added the adiabatic nature of mechanical deformation, which implies not only thermal isolation of the body but also a slow change in load over time, allowing the establishment of an almost periodic regime of internal atomic dynamics. The energy balance in adiabatic mechanical deformation is considered in Ref. [18].

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