Towards non-statistical foundation of thermodynamics

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Abstract. It is shown that the irreversible behavior exists even in two-body system. It is due to the retardation of the interactions between the particles. It is established that a two-particle oscillator with a delayed interaction between particles has an infinite spectrum of both stationary and non-stationary oscillations, which depends on the equilibrium distance between the particles.

1. Introduction
It is well known that all the field theories have a property of delay of the interactions. Such are the electromagnetic interaction of charges in vacuum, the interaction of vibrational systems through a medium, the interactions between the particles in a plasma or colloidal systems, etc. The delay of the interactions leads to violation of Newton’s third law on the equality of action and reaction [1], and also it is one of the mechanisms for the irreversible behavior of many-body systems [2, 3].

Note that in papers [2, 3] neither probabilistic considerations nor the conditions $N \gg 1$ ($N$ is number of degrees of freedom in the system) were used. In this connection, it is of interest to study in detail the mechanisms of the manifestation of retardation in the irreversibility of systems with a small number of degrees of freedom.

We define a two-body oscillator as a system of two particles with identical masses $m$, the interaction between which at rest is described by the potential $W(R_1 - R_2)$ with the following properties.

1. The function $W(R_1 - R_2)$ has a minimum at $|R_1 - R_2| = L$.
2. Near the minimum point, this function can be approximated by quadratic function

$$W(R_1 - R_2) = W(L) + \frac{k(|R_1 - R_2| - L)^2}{2},$$

(1)

Let us consider the case of one-dimensional small oscillations of these particles along a straight line connecting these bodies. In the absence of retardation, the solution of this problem is trivial and describes the oscillations of the particles with circular frequency $\left(\frac{2k}{m}\right)^{1/2}$. The frequency of these oscillations does...
not depend on either $L$ or $W(L)$. The retardation in the interactions between these two particles leads to a qualitatively different result, including the irreversible behavior of the system as a whole.

2. Oscillator with retardation

We denote the deviations from the equilibrium positions of the particles in the rest state by $x_1(t)$ and $x_2(t)$. Equations of motion for the system in view of the interaction retardation $\tau$ have the form:

\[
\begin{align*}
\ddot{x}_1(t) + \omega_0^2 [x_1(t) - x_2(t - \tau)] &= 0; \\
\ddot{x}_2(t) + \omega_0^2 [x_2(t) - x_1(t - \tau)] &= 0,
\end{align*}
\]

where $\omega_0 = \left(\frac{k}{m}\right)^{1/2}$.

In general case, $\tau$ is not a constant, but a function of the position of the particles, that is, of the solution of the system of equations (2). The solution of such a problem in a general formulation goes far beyond the possibilities of modern mathematics. The condition of smallness of the oscillations is

\[
|x_i(t)| = L, \quad (k = 1, 2).
\]

It substantially simplifies the situation since in this case the principal term of the interaction retardation is reduced to the constant

\[
\tau = \frac{L}{v},
\]

where $v$ is the propagation velocity of the interaction. Thus, in the case of small oscillations, the system of equations (2) is linear.

The Euler substitution

\[
x_i(t) = C_i e^{i\Omega t}
\]

leads to the following characteristic equation with respect to dimensionless frequency $\Lambda$:

\[
\Lambda^4 - 2\Lambda^2 + \left[1 - e^{-2i\Omega \tau}\right] = 0.
\]

The roots of this transcendental equation depend on $\tau$ and in general case are complex:

\[
\Lambda = \alpha + i\gamma.
\]

The equation (6) with respect to the complex value $\Lambda$ is equivalent to a system of two equations for real quantities $\alpha$ and $\gamma$:

\[
\begin{align*}
\alpha^4 - 6\alpha^2 \gamma^2 + \gamma^4 - 2(\alpha^2 - \gamma^2) + \left[1 - e^{-2i\Omega \tau}\cos(2\omega_0 \alpha \tau)\right] &= 0; \\
4\alpha \gamma (\alpha^2 - \gamma^2 - 1) + e^{2i\Omega \tau} \sin(2\omega_0 \alpha \tau) &= 0.
\end{align*}
\]

Note that $\alpha$ determines the oscillation frequency, and $\gamma$ characterizes the rate of change in the amplitude of the oscillations. Therefore, the condition for stationarity of the oscillations is that $\gamma = 0$, whence we get
where \( n \) is an arbitrary integer.

Substituting \( \tau \) from (9) and \( \gamma = 0 \) into equation (8), we obtain the equation for \( \alpha \)

\[
\alpha^4 - 2\alpha^2 + 2\sin^2 \left( \frac{m}{2} \right) = 0.
\]

The roots of this equation are real if and only if \( n \) is an even number. Under this condition, the solutions are as follows:

\[
\alpha_1 = \alpha_2 = 0; \quad \alpha_{3,4} = \pm \sqrt{2}.
\]

Thus, stationary oscillations of a two-particle oscillator with retarded interactions occur only for a discrete set of equilibrium distances \( L \) between the particles, determined by the condition (9).

However, there exists a set of values of the parameter \( L \) for which both stationary and non-stationary oscillations are possible, i.e. solution of the system of equations (8) with \( \gamma = 0 \) and \( \gamma \neq 0 \), respectively. From the immense set of solutions of this system of equations depending on the parameter \( L \), we consider a subset for which the condition (9) is satisfied:

\[
L = \frac{mv}{2\omega}.
\]

In this case, the system of equations (8) is greatly simplified:

\[
\begin{cases}
\alpha^4 - 6\alpha^2 \gamma^2 + \gamma^4 - 2(\alpha^2 - \gamma^2) + \left[1 - e^{2\alpha_0 \tau} (-1)^n \right] = 0; \\
4\alpha \gamma (\alpha^2 - \gamma^2 - 1) = 0.
\end{cases}
\]

For \( \gamma \neq 0 \) we have

\[
\gamma = \eta \sqrt{\alpha^2 - 1},
\]

where \( \eta = \pm 1 \).

Substituting this expression for \( \gamma \) into the first of the equations (13), we find

\[
(-1)^n e^{2\alpha_0 \tau} = 4\alpha^2 (1 - \alpha^2).
\]

As follows from the domain of definition of the expression (14) for \( \gamma \), the right-hand side of the equation (15) is non-positive, so \( n \) in this equation is an odd number (\( n = 2s + 1 \)), and the equation itself becomes

\[
(2s + 1)\eta = \frac{1}{\pi} \frac{\alpha \ln \left| 4(\alpha^4 - \alpha^2) \right|}{(\alpha^2 - 1)^{3/2}},
\]

where \( \alpha^2 > 1 \).

The right-hand side of this equation is a monotonically increasing function on the interval \((1, +\infty)\).
The range of this function fills the entire interval \((-\infty, +\infty)\). Therefore, for each value of \((2s + 1)\eta\), the equation (16) has an unique solution \(\alpha_s(\eta)\).

The graph of the function contained in the right-hand side of this equation is shown in Fig.1.

![Graph of the function](image)

**Figure 1.** The graph of the function \(y(\alpha) = \frac{1}{\pi} \frac{\alpha \ln|4(\alpha^4 - \alpha^2)|}{\left(\alpha^2 - 1\right)^{1/2}}\).

3. Discussion

The delay in the interaction between the constituents of a two-body oscillator leads to the following effects:

1. Stationary oscillations exist only for a discrete set of equilibrium distances between the particles, determined by the condition (9). The frequencies of all stationary oscillations \(\omega\) are the same:

   \[
   \omega = \sqrt{2} \omega_0. 
   \]

   Condition (9), with account for the relation (17), can be represented in an equivalent form

   \[
   L = \frac{n}{4} \lambda, \tag{18}
   \]

   where \(\lambda = \frac{2\pi}{\gamma} \left(\frac{m}{2k}\right)^{1/2}\) is the wavelength corresponding to the oscillation frequency (17).

2. If the equilibrium distance \(L\) between the particles does not satisfy the condition (9), then there are only non-stationary oscillations in the system. Depending on the sign of \(\gamma = \Im\lambda\), the corresponding oscillations either decay or increase. In both of these cases, the energies of the oscillations are not
conserved. For $\gamma > 0$, the corresponding oscillations are damped and the mechanical energy of these oscillations decreases. For $\gamma < 0$, the amplitude of the corresponding oscillations increases exponentially and the assumptions (3), (4) are no longer applicable. In particular, $\tau$ is no longer a constant (4), but a function that depends on the solution of the system of equations (2). Thus, the delay of interactions between the particles performs functions similar to those of a thermodynamic reservoir, which, however, is not something external, but is inextricably linked to the particles.

3. Especially it should be noted that even under the condition (9), in addition to stationary oscillations, the non-stationary oscillations with different frequencies corresponding to the complex roots of the characteristic equation may also exist (6):

$$
\omega(\eta) = \alpha(\eta)\omega_0, \quad \gamma(\eta) = \eta\omega_0 \left(\alpha^2(\eta) - 1\right)^{1/2}.
$$

(19)

Thus, taking into account the seemingly insignificant but always existing retardation in the interaction between the particles leads to a qualitative change in the dynamics of the mechanical system. In addition to the appearance of an infinite spectrum of oscillations, the phenomenon of the irreversibility of dynamics also takes place. Therefore, the classical theory of systems of particles with retarded interactions can be used for the microscopic probability-free foundation of thermodynamics. This approach has certain advantages over the Gibbsian probabilistic foundation of classical thermodynamics.

Omitting the discussion of the enormous mathematical difficulties associated with the use of Gibbs and related approaches to the practical implementation of statistical mechanics, we will discuss more fundamental problems in the theory of many-body systems.

The microscopic foundation of thermodynamics within the framework of statistical mechanics without establishing of the source of system stochastization is not satisfactory because of the numerous paradoxes generated by the use of probabilistic concepts in combination with deterministic classical mechanics. A certain clarity in the origin of these paradoxes was achieved by Kac [4]. He proposed a dynamic model – namely, a ring model, for which he obtained two solutions. The first solution is an exact dynamic solution that is reversible in time and also periodic in time. The second solution was obtained using the probabilistic assumptions; it has the property of irreversibility. In short time intervals, both solutions are almost identical, and for large time scales, they differ dramatically. Therefore, the probability approach to foundation of thermodynamics is not satisfactory. Exact theorems of classical mechanics are at variance not only with the probabilistic description of macroscopic systems, but also with the thermodynamic behavior of systems. Therefore, the physical cause of irreversibility is beyond the Newtonian classical mechanics.

In this regard, it is appropriate to note two essential points.

• The first point is the amazing work by Synge [5]. He solved “the electromagnetic two-body problem, based on the hypotheses (i) that the bodies are particles, (ii) that the fields are given by the retarded potential, (iii) that the force acting on a particle is the Lorentz ponderomotive force without a radiation term. It is found that energy disappears from the motion, so that the orbital particle slowly spirals in”.

• The second point is connected with the outstanding result of Wheeler and Feynman [6, 7]. They proved that classical electrodynamics is equivalent to the theory of direct non-instantaneous interaction between particles. This means that the field concept is not necessary for describing interactions between the particles. This result makes it possible to exclude from consideration the field through which the interaction between the particles occurs. An infinite number of degrees of freedom of the excluded field is manifested in the functional-differential equations of motion of the particles through retardations the interactions.

Thus, there are two ways of describing the evolution of a system of interacting particles.
The first way is to use a complete system of equations of motion for both particles and the fields. These equations of motion with the corresponding initial conditions for both particles and fields determine the evolution of both particles and the fields. At present, this is the main way in the theory of many-particle problems.

The second way is to use the motion equations of the particles on the basis of the concept of direct retarded interaction between the particles. One of the advantages of this approach is the possibility of describing the evolution of a system of particles interacting via potentials of a general type. In this case, setting the initial conditions only for particles is insufficient to uniquely determine the evolution. The solution of functional-differential equations depends not only on the initial state of the system, but also on its prehistory. This means that under the same initial conditions of a Cauchy-type problem for a particle system, different versions of its history lead to different versions of the evolution of this system. Therefore, the solution of the classical Cauchy problem for a system of particles with retarded interactions is not unique.

Probably for the first time the idea of the non-uniqueness of the Cauchy problem for many-body systems as the cause of irreversibility was proposed in the paper [8]. It is assumed that the non-uniqueness of the Cauchy problem solution is due to certain features of the interatomic potentials. In particular, potentials such as the top of a hill are considered as examples. In this case, there are infinitely many variants to roll down from this hilltop. Hence it was concluded that the non-uniqueness of the solution of the Cauchy problem leads to an indeterministic behavior of the system.

But, as it can be seen from our solution of the two-body oscillator model with delayed interaction, the deterministic and at the same time irreversible behavior of the system is provided by a more complete setting of the initial conditions: it is necessary to take into account the state of the system not only at the initial moment of time. In other words, a dynamical system with retarded interactions has the property of heredity, because of which dynamics depends not only on the actual state of the system at the initial moment of time, but also on the preceding states [9, 10].

Numerous attempts to explain the irreversibility on the basis of the ergodic theory linking probability and thermodynamics have never led to a clear understanding of the nature of irreversibility, at least within the framework of classical mechanics. However, it should be noted the recent papers [11, 12], in which the mechanism of macroscopic irreversibility as a consequence of microscopic irreversibility was developed. In these papers, atoms and molecules are considered as open systems being in continuous interaction with photons flows from their surroundings.

**4. Conclusion**
The described simple example leads to the following conclusions.

1. The irreversible behavior of systems of interacting particles is a common property for both few-body and many-body classical system, having its origin in the interactions retardations.

2. The unavoidable retardation of interactions is sufficient for the irreversible behavior of the systems. The systems are irreversible in itself — there is no need to use any probabilistic hypotheses or other assumptions to explain the phenomenon of irreversibility in systems of interacting particles.

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