Toward a relativistic microscopic substantiation of thermodynamics: classical relativistic many-particle dynamics

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Abstract. An exact closed relativistic kinetic equation is derived for a system of identical classical particles interacting with each other through a scalar field. The law of variation of the energy of a system of particles in terms of the microscopic distribution function is obtained.

1. Introduction
In the late 19th and early 20th centuries, there were two main concepts regarding the microscopic origin of the laws of thermodynamics. The first of these was developed in the classic works of Maxwell, Boltzmann, Gibbs and Poincaré and was based on molecular kinetic concepts. At that time, classical Newtonian mechanics was the only theory that allowed the description of the microscopic dynamics of many-particle systems. However, the reversibility of the equations of classical dynamics and the irreversible behavior of real systems are in a certain contradiction with each other. This contradiction was one of the reasons for the popularity of the works of Ostwald, Mach, Duhem and Helm based on the concept of energetism. Within the framework of this concept, the fundamental principle of all phenomena in the world is energy – a kind of indestructible hidden substance. In particular, matter is just one of the manifestations of energy. Within the framework of the energetism concept, the molecular-kinetic theory was interpreted as a primitive mechanistic picture, and the existence of atoms was actively questioned.

The fierce fight between the representatives of these concepts [1] almost stopped after the experimental proof of the existence of atoms and the main method of theoretical study of the equilibrium properties of matter became Gibbs’ statistical mechanics, which is an integration of Newtonian classical mechanics in the Hamiltonian form and the concepts of the theory of probability in the form of probabilistic measures in the phase spaces of the systems under study. According to statistical mechanics, the relationship between the Hamiltonian of a system and its thermodynamic properties is realized through these probabilistic measures. The implementation of this connection for the purpose of calculating and analyzing thermodynamic functions is a problem of huge mathematical complexity. But the main problems of statistical mechanics are of a much more fundamental nature and are not at all reduced to computational problems.

First of all, this is the problem of explaining and substantiating the zero principle of thermodynamics, according to which any isolated many-particle system, regardless of the initial state, irreversibly passes over time to a state with steady-state macroscopic parameters. The zero law of thermodynamics is postulated in both phenomenological thermodynamics and statistical mechanics. Note that the irreversibility of the dynamics of many-particle systems is only a necessary, but not a sufficient condition for the fulfillment of the zero principle of thermodynamics. From this it follows...
that the possibility of microscopic substantiation of the zero principle of thermodynamics in the framework of classical Newtonian mechanics is at least doubtful, because it is required to deduce macroscopic irreversibility from microscopic reversibility. In essence, both the concept of energetism and the concept of probability are not entirely correct attempts to go beyond the limits of classical mechanics. The doubtfulness of the first of them is due to the introduction of some fantastic hidden substance, and the second is due to the internal inconsistency between deterministic classical mechanics and probabilistic assumptions.

The problem of internal consistency of the statistical approach to problems of classical mechanics. The fact of the matter is not only in the long-known paradoxes (in fact, internal contradictions) of Loschmidt and Zermelo that have not yet been rationally resolved. As shown in the works of Kac [2], the use of probabilistic assumptions such as the molecular chaos hypothesis in the framework of the Kac dynamic ring model leads to a result that contradicts the exact dynamic solution of this model. This counterexample to statistical mechanics raises strong doubts about the internal consistency of statistical mechanics.

In the post-Gibbsian time, the development of classical (i.e., non-quantum) statistical mechanics was mainly focused on the following directions.

1. Investigation of the mathematical structure of Gibbs' statistical mechanics (reduction of the problem of the partition functions calculating to systems of BBGKY-type equations for distribution functions [3-5], conditions for the existence of the thermodynamic limit [6-7], exactly solvable models [8, 9], ergodic theory [10], etc.).
2. Non-equilibrium statistical mechanics (kinetic equations of BBGKY type [3-5, 11], method of non-equilibrium statistical operator [12], methods of the theory of random processes [13]).
3. Relativistic generalization of the classical kinetic theory of gases [14-17], statistical mechanics [18-22].

Despite the outstanding achievements in theoretical studies of condensed matter in the framework of statistical mechanics, the fundamental problem of a consistent microscopic foundation of the laws of thermodynamics remains unsolved. Because of the fundamental contradiction between classical Newtonian mechanics and the undoubted laws of thermodynamics, the microscopic substantiation of thermodynamics should be sought outside of classical mechanics.

In this regard, we note the works [23-26], in which the dynamics of two-particle systems with retarded interactions between particles is investigated and it is established that the retardation of interactions leads to a radical rearrangement of the dynamics of the systems. A possible connection between the rearrangement of dynamics and thermodynamic effects was not indicated in these works.

In the works [27, 28] it is shown that the retardation of interactions leads to the irreversibility of the dynamics of both many-particle and few-particle systems, and it is also hypothesized that the retardation of interactions between particles is a microscopic probability-free mechanism leading to thermodynamic behavior of the systems.

It is essential that the retarded interaction of particles cannot be described in terms of the potential energy, which depends on the simultaneous values of the coordinates of these particles. Therefore, the Hamiltonian of such a system as a function of instantaneous coordinates and momenta of particles also does not exist. This is in full agreement with the well-known result on the absence of a relativistically invariant Hamiltonian for a system of interacting particles [29-30] and at the same time indicates the need to search for an alternative concept of microscopic substantiation of thermodynamics.

Thus, the dynamics of a system of particles with retarded interactions should be described within the framework of field theory. The complete system of equations for the dynamics of the closed system "particles + field" consists of equations for the dynamics of particles and equations for the evolution of the field generated by these particles. In the absence of external fields, the field variables can be eliminated from this complete system of equations and a closed system of functional differential equations describing the particle dynamics can be obtained. As applied to a system consisting of point charged particles, this program was implemented in [31, 32].
Note that the evolution of a system of particles with instantaneous interactions between them can also be described in the framework of the field theory with an infinite velocity of propagation of interactions and with the subsequent elimination of field variables. However, there is a fundamental difference between systems with instant and retarded interactions, which manifests itself after the elimination of field variables. It is as follows.

• The system with instantaneous interactions is Hamiltonian one and, as a consequence, it contains Poincaré integral invariants (including the invariance of the Liouville phase volume), the Poincaré recurrence theorem holds, invariance with respect to the time reversal $t \rightarrow -t$, as well as existence and uniqueness theorems for the Cauchy problem.

• The system with retarded interactions between particles, on the contrary, is not Hamiltonian and therefore Poincaré’s invariants do not exist in it, Liouville’s theorem and equation do not hold, the dynamics equations are not invariant with respect to time reversal. However, it is these properties of a system with retarded interactions that are consistent with the laws of thermodynamics and therefore can be used for a consistent microscopic substantiation of thermodynamics.

In recent works [27, 28, 33-35], the description of the dynamics of systems with retarded interactions was carried out in terms of microscopic (i.e. not-averaged) distribution functions

$$f(r, v, t) = \sum \delta(r - R_s(t))\delta(v - v_s(t)),$$

where $R_s(t)$ is the radius vector of the $s$-th particle depending on the time $t$. It is shown that the retardation of interactions leads to the irreversibility of the dynamics of the system, and this property is equally valid both for many-body and for few-body systems.

In order to find sufficient conditions for equilibration, in [36, 37] the dynamics of a one-dimensional chain of atoms with retarded interactions between them was investigated.

It is shown in [36] that all free vibrations of a chain of atoms with retarded interactions are damped and at $t \rightarrow \infty$ the system goes into a state of rest. All the kinetic energy of atoms is irreversibly completely transferred into the energy of the field, through which the interaction between the particles takes place.

In [37], the dynamics of forced (under the action of an alternating external field) vibrations of a one-dimensional chain of atoms with retarded interactions is investigated. It is shown that stationary oscillations are established in the system as $t \rightarrow \infty$. This transition is interpreted as the process of dynamical equilibration between a system of particles and an alternating external field.

The exact results of works [36, 37] demonstrate a deterministic dynamic microscopic mechanism of thermodynamic equilibration for a simple particular model — in a one-dimensional chain of atoms.

The purpose of this work is to create of the classical relativistic dynamical theory of a system of identical particles interacting with each other through a scalar field of general form.

2. Relativistic kinetic equation

As it is known [38], the relativistic equation of motion of a particle has the form

$$\frac{d\gamma_a}{d\tau_a} = F_a(\gamma_a, p_a).$$

Here $d\tau_a$ is proper time along the world line of a $a$-th particle, $x^\mu = (x^0, r) = (ct, r)$ is the spacetime four-vector, $p_a^\mu = \gamma_a m_a(c, v_a)$ is the energy-momentum four-vector for $a$-th particle, $F_a^\mu = (F_a^0, F_a) = \gamma_a \left(\frac{v_a F_a}{c}, F_a\right)$ is the four-vector of force, acting on $a$-th particle, $\gamma_a = \frac{1}{\sqrt{1-(v_a/c)^2}}$ is the Lorentz factor.

After multiplying equation (2) by the delta-functions in the four-dimensional Minkowski spacetime $\delta^4(x - x_a(\tau_a))\delta^4(p - p_a(\tau_a))$, integrating over the proper time $\tau_a$ and summing over $a$, we get
Consider the microscopic distribution function for particles of type $A$ (as indicated in [39], the idea of introducing such an invariant construction belongs to R.L. Stratonovich):

$$\mathcal{F}_A(x,p) = \sum_a \int d\tau_{aA} \delta^4(x - x_{aA}(\tau_{aA})) \delta^4(p - p_{aA}(\tau_{aA})).$$

Using the formula

$$\frac{d}{d\tau_a} \left[ \delta^4(x - x_{aA}(\tau_{aA})) \delta^4(p - p_{aA}(\tau_{aA})) \right]$$

and integrating by parts on left-hand side of (3) leads to the relativistic kinetic equation in the covariant form:

$$\frac{p^\nu}{m_A} \frac{\partial}{\partial x^\nu} + F^\nu(x,p) \frac{\partial}{\partial p^\nu} + \frac{\partial F^\nu(x,p)}{\partial p^\nu} \mathcal{F}_A(x,p) = 0.$$  

The classical Klimontovich microscopic phase density [39,40,17,19]

$$f_A(r,p,t) = \sum_a \delta^3(r - r_{aA}(t)) \delta^3(p - p_{aA}(t))$$

can be obtained from (4) by integrating over the variable $p^0$:

$$\int d^4p_0 \mathcal{F}_A(x,p)$$

$$= \int d^4p_0 \sum_a \delta^3(r - r_{aA}(t)) \delta^3(p - p_{aA}(t)) \delta(p^0 - p^0_{aA}) \frac{m_A}{p^0_{aA}}$$

$$= m_A \sum_a \delta^3(r - r_{aA}(t)) \delta^3(p - p_{aA}(t)) = m_A f_A(r,p,t).$$

It means that

$$\mathcal{F}_A(x,p) = \frac{1}{m_A p^0} \delta \left( p^0 - \sqrt{p^2 + m_A^2 c^2} \right) f_A(r,p,t).$$

In classical statistical mechanics, the interaction between particles is taken into account by introducing scalar functions — potential energies. However, potential energy is an attribute of non-relativistic physics only. At the same time, at each point in space, we can determine the value of the scalar field $\phi(r,t)$. A smooth embedding of the Newtonian force $-\nabla \phi(r,t)$ in a pseudo-Euclidean space leads to the following 4-force [38]:

$$F^\mu(x,p) = \left( g^{\mu\nu} - \frac{p^{\mu} p^{\nu}}{m^2 c^2} \right) \frac{\partial \phi(x)}{\partial x^\nu},$$

where $g^{\mu\nu}$ is the inverse of the metric tensor in the Minkowski space. The kinetic equation (6) will take the form

$$\left( \frac{p^\mu}{m_A} \frac{\partial}{\partial x^\mu} + \left( g^{\mu\nu} - \frac{p^{\mu} p^{\nu}}{m_A^2 c^2} \right) \frac{\partial \phi(x)}{\partial x^\nu} \right) \mathcal{F}_A(x,p) = \frac{5p^\mu}{m_A^2 c^2} \frac{\partial \phi(x)}{\partial x^\mu} \mathcal{F}_A(x,p).$$
It should be emphasized that the equation (11) for particles of type $A$ contains not averaged distribution functions (4) and therefore this equation describes the dynamics of the system, not the dynamics of the probability density.

In the following, we will assume that there are no external forces. In this case, the 4-force (10) can be represented by the functional of the microscopic distribution function (4):

$$F^\mu(x, p) = F^\mu(x, p, \{\mathcal{F}_A\}).$$  

(12)

The equations (11)-(12) form a closed system with respect to the distribution function (4). It is important to note that the value of the force (12) at the point $(x, p)$ (that is, at some moment in time $t$) is determined by all distribution functions $\mathcal{F}_A(x', p')$, defined at the previous points $(x', p')$ of the Hilbert causality cone (that is, at the previous times $t' < t$). This natural from a physical point of view causality principle from a mathematical point of view means that among all possible solutions of the equation of motion for the field through which the particles interact, we must exclude non-physical advanced solutions and keep the retarded solutions. The non-invariance of the kinetic equation with respect to time reversal is due to the retardation of the potentials:

$$t \to -t, \quad r \to r, \quad p \to -p.$$  

(13)

To clarify the meaning of this statement, we write down the kinetic equation (11) in terms of the Klimontovich distribution function (7). For this, we integrate the equation (11) over $p^0$ taking into account the relation (9). As a result, we get:

$$\left(\frac{\partial}{\partial t} + \frac{cp}{\sqrt{p^2 + m^2_A c^2}} \frac{\partial}{\partial r} + F(r, p, t) \frac{\partial}{\partial p}\right) f_A(r, p, t)$$

$$= \frac{3}{m_A c^4} \left(\frac{\partial \phi(r, t)}{\partial t} + \frac{cp}{\sqrt{p^2 + m^2_A c^2}} \frac{\partial \phi(r, t)}{\partial r}\right) f_A(r, p, t).$$  

(14)

The formula for the force $F(r, p, t)$ follows from (10) and the expression

$$F^\mu = \frac{p^\mu}{mc} \left(\frac{\mathbf{r}}{c}, \mathbf{F}\right).$$  

(15)

Thus, we have

$$F(r, p, t) = -\frac{m_A c}{\sqrt{p^2 + m^2_A c^2}} \left[\frac{\partial}{\partial r} + \frac{p}{m_A c^2} \left(\frac{\partial}{\partial r} + \sqrt{p^2 + m^2_A c^2} \frac{\partial}{\partial ct}\right)\right] \phi(r, t).$$  

(16)

In the instantaneously comoving frame of reference we get classical expression for the Newtonian force:

$$F(r, t) = -\frac{\partial \phi(r, t)}{\partial t}.$$  

(17)

Note that by virtue of (12) the scalar field $\phi(x)$ is a linear functional of $\mathcal{F}_A(x, p)$ and, therefore, of $f_A(r, p, t)$. According to the Riesz theorem on the representation of a linear continuous functional, the field $\phi(x)$ can be written as follows:

$$\phi(r, t) = \int \ dx' \ dp' \ K(x, p; x', p') \mathcal{F}_A(x', p').$$  

(18)

Let us show that the kernel $K$ of the integral representation (18) is determined by a given interatomic potential. Indeed, the potential at point $r$, taking into account the retardation of interaction $\tau_a$, can be written as
where \( \phi(\mathbf{r}, t) \) is the potential energy determined for the particles at rest, \( c \) is the speed of transmission of the interaction (speed of light). Note that the resulting expression (19) is an analog of the Liénard–Wiechert potentials.

Integrating over time and introducing the dependence on the momentum, we get:

\[
\phi(\mathbf{r}, t) = \int U(\mathbf{r} - \mathbf{r}')(t) \sum_a \delta \left( \mathbf{r}' - \mathbf{r}_a \left( t - \frac{\mathbf{r}' - \mathbf{r}_a}{c} \right) \right) \, d^3\mathbf{r}'
\]

\[
= \iint U(\mathbf{r} - \mathbf{r}') \sum_a \delta \left( \mathbf{r}' - \mathbf{r}_a \left( t - \frac{\mathbf{r}' - \mathbf{r}_a}{c} \right) \right) \, d^3\mathbf{r}' \times \delta \left( \mathbf{p}' - \mathbf{p}_a \left( t - \frac{\mathbf{r}' - \mathbf{r}_a}{c} \right) \right) \, d^3\mathbf{p}'.
\]  

As a result, we can write the potential (20) in terms of the distribution function (7):

\[
\phi(\mathbf{r}, t) = \iint U(\mathbf{r} - \mathbf{r}') f_a(\mathbf{r}', \mathbf{p}', t - \frac{\mathbf{r}' - \mathbf{r}_a}{c}) \, d^3\mathbf{r}' \, d^3\mathbf{p}'.
\]  

Comparing (21) with (18), we conclude that the kernel of the linear operator has the form:

\[
K(\mathbf{x}, \mathbf{p}; \mathbf{x}', \mathbf{p}') = \frac{m_a p^0_a}{c} U(\mathbf{r} - \mathbf{r}') \delta \left( t - t' - \frac{\mathbf{r}' - \mathbf{r}_a}{c} \right).
\]  

For a qualitative analysis of the causes of irreversibility within the framework of the obtained kinetic equation (14), we expand the distribution function in powers of the retardation time:

\[
f_a(\mathbf{r}', \mathbf{p}', t - \frac{\mathbf{r}' - \mathbf{r}_a}{c}) = f_a(\mathbf{r}', \mathbf{p}', t) + \sum_{s=1}^{\infty} \frac{(-1)^s}{s!} \left( \frac{\mathbf{r}' - \mathbf{r}_a}{c} \right)^s \frac{\partial^s f_a(\mathbf{r}', \mathbf{p}', t)}{\partial t^s}.
\]

The time reversal operation (13) leads to a sign change only for members with odd values of \( s \). Since the equations (14), (16) and (21) contain terms that do not change sign under time inversion, the resulting kinetic equation is not invariant under the time inversion.

Thus, the resulting kinetic equation (14) describes the irreversible evolution of a system of particles interacting via the scalar field \( \phi(\mathbf{r}, t) \). Irreversibility is a consequence of the retardation of the interaction, which is expressed by the corresponding functional dependence of the potential on time.

### 3. The law of energy change of a system of particles

Let us multiply the equation of motion (2) by the delta function \( \delta^4(\mathbf{x} - \mathbf{x}_a(\tau_a)) \), integrate over time \( \tau_a \) and summate over \( a \):

\[
\sum_a \int d\tau_a \frac{dp_a^\mu}{d\tau_a} \delta^4(\mathbf{x} - \mathbf{x}_a(\tau_a)) = \sum_a \int d\tau_a F_a^\mu(\mathbf{x}_a, p_a) \delta^4(\mathbf{x} - \mathbf{x}_a(\tau_a)).
\]

Taking the integral on the left-hand side by parts, we get:

\[
\frac{d\mathbf{T}_a}{d\tau_a} = c \sum_a \int d\tau_a F_a^\mu(\mathbf{x}_a, p_a) \delta^4(\mathbf{x} - \mathbf{x}_a(\tau_a)).
\]

Here we have introduced the energy-momentum tensor for particles:

\[
\mathbf{T}_a^\mu = \sum_a c m_a \int d\tau_a u_a^\mu u_a^\nu \delta^4(\mathbf{x} - \mathbf{x}_a(\tau_a)).
\]

Integration over proper time brings the expression (25) to the form
Note that

\[ \tau_{\text{part}} = \sum_a c m_a \int d\tau_a u_a^0 u_a^0 \delta^4(x - x_a(\tau_a)) \]

\[ = \sum_a m_a u_a^0 u_a^0 \delta^3(r - r_a(t)) \frac{dr_a}{dt} \]

\[ = \sum_a \delta^3(r - r_a) \gamma_a m_a c^2. \]

is the energy density of the particles system.

Let us integrate (27) over the volume occupied by the particle system

\[ \int d^3 r \frac{\partial}{\partial y} T_{\mu}^{\nu} = \int \sum_a \gamma_a^{-1} F_{\mu}^{\nu} (x_a, p_a) \delta^3(r - r_a(t)) d^3 r. \]

According to the Gauss theorem, the terms on the left-hand side of the equality containing divergence can be reduced to the flow of the energy-momentum tensor through the infinitely distant surface. Such integrals are equal to zero, since there are no charges and currents at infinity. As a result, taking into account \( y c m = p^0 \) we get

\[ \frac{d}{dt} \sum_a m_a u_a^\mu = \int \sum_a \frac{m_a}{p^0} F_{\mu}^{\nu} (x_a, p_a) \delta^3(r - r_a(t)) d^3 r. \]

Assuming that the index \( \mu \) runs over the spatial values, we obtain the law of change in the total energy of the system of particles (28):

\[ \frac{d}{dt} \sum_a \frac{m_a c^2}{\sqrt{1 - \gamma_a^2}} = c^2 \int \sum_a m_a \frac{F_0^0(x_a, p_a)}{p^0} \delta^3(r - r_a(t)) d^3 r. \]

Since

\[ F^0 = \gamma \frac{v F}{c} = \frac{p^0}{mc\sqrt{p^0 + m^2 c^2}}, \]

the equation (31) takes the form

\[ \frac{d}{dt} \sum_a \frac{m_a c^2}{\sqrt{1 - \gamma_a^2}} = c \int \sum_a \frac{p_a F_0 (r_a, p_a)}{p_a^2 + m_a^2 c^2} \delta^3(r - r_a(t)) d^3 r. \]

Let us express the integral on the right-hand side in terms of the microscopic distribution function (7):

\[ \int \sum_a \frac{p_a F_0 (r_a, p_a, t)}{p_a^2 + m_a^2 c^2} \delta^3(r - r_a(t)) \delta^3(p - p_a(t)) d^3 r d^3 p \]

\[ = \int \frac{f_A (r, p, t)}{p^2 + m^2 c^2} \delta^3 (r - r_a(t)) \delta^3 (p - p_a(t)) d^3 r d^3 p \]

Then, taking into account the expression (16) for the force, we obtain the final expression for the rate of change of the total energy of the particles:
From this, as well as from the equation (14) taking into account the expansion (23), it follows that the total energy of the system of particles changes irreversibly.

4. Conclusions
The main results of this work are as follows.

1. The dynamics of a system of particles is described by the kinetic equation (11) in terms of the relativistically invariant microscopic distribution function (4).

2. The dynamic scalar field through which the particles interact is expressed through the interatomic potentials of the particles at rest and the microscopic distribution functions (18), (21).

3. The causality principle and the relativistic effect of delayed interactions are sufficient for the existence of a state of thermodynamic equilibrium in both many-particle and few-particle isolated classical systems.

Thus, the relativity theory and the principle of causality lead to the following conclusions.

a. The non-existence of instantaneous interactions between particles is the reason that generates the thermodynamic behavior of systems.

b. A consistent microscopic explanation and substantiation of the zero principle of thermodynamics within the framework of classical nonrelativistic mechanics is impossible.

c. The energy excess of the initial state over the final state of the system is carried away by the field through which the particles interact.

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