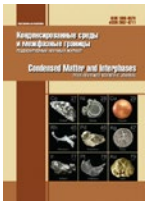

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Relativistic model of interatomic interactions in condensed systems

A. Yu. Zakharov[1]✉, **M. A. Zakharov**[1]

[1]*Yaroslav-the-Wise Novgorod State University,*
41, ul. Bolshaya Saint Petersburgskaya, Veliky Novgorod 173003, Russian Federation

Abstract

A method was proposed to describe the dynamics of systems of interacting atoms in terms of an auxiliary field. The field is equivalent to the specified interatomic potentials at rest, and represents the classical relativistic field under dynamic conditions. It was determined that for central interatomic potentials, allowing for the Fourier transform, the auxiliary field is a superposition of elementary fields satisfying the Klein-Gordon-Fock equation with complex mass parameters.

Keywords: Interatomic potentials, Classical relativistic dynamics, Retarded interactions, Irreversibility phenomenon, Klein-Gordon-Fock equation

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✉ Anatoly Yu. Zakharov, e-mail: anatoly.zakharov@novsu.ru

1. Introduction

Nowadays, the modeling of both thermodynamic and kinetic properties of condensed systems is performed mainly in terms of nonrelativistic approximation. The smallness of the velocities of atomic particles compared to the speed of light serves as some basis for neglecting the relativistic effect of interactions retardation. In this framework, the system of interacting atoms is characterized by a Hamiltonian, which gives a principal (but still far from real) possibility to calculate the partition function or the generating functional of the system in terms of the Gibbs approach, or to solve the hierarchy of equations for equilibrium or nonequilibrium distribution functions in terms of the BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) approach. However, the exact solutions in each of these options for any "realistic" interatomic potentials are still unknown. There are no a priori estimates of the errors of the approximations used.

However, the issue of modeling condensed systems is not limited to solving problems within the framework of statistical mechanics. This is because the microscopic foundation of thermodynamics within the framework of statistical mechanics, which combines Newtonian classical mechanics (in Hamiltonian form) with the concept of probability, is not a comprehensive and flawless option, and is not the only possible solution. Besides, there are no solutions of many fundamental issues within the framework of statistical mechanics.

1. The zeroth law of thermodynamics (stating the existence of a state of thermodynamic equilibrium in macroscopic systems) has not been explained within the framework of statistical mechanics, but is a postulate in the same way as in phenomenological thermodynamics [1].

2. Classical mechanics itself is in clear contradiction with thermodynamics, so a microscopic foundation of thermodynamics requires going beyond Newtonian classical mechanics. In the late 19th – early 20th century, the concept of probability was expected to solve this issue (Maxwell, Boltzmann, Gibbs, Einstein, Smoluchowski, P. and T. Ehrenfest, …). However, in 1909, a discussion paper by Ritz and Einstein was published [2], in which Ritz argued that the cause of irreversibility was due to the (relativistic) effect of retarded interactions, and Einstein argued that probability was the only cause of irreversibility. Finally, in 1956, Kac proposed an exactly solvable mechanical model, the Kac ring model [3]. He found an exact solution of this model, which is deterministic, reversible, and does not show any features of thermodynamic behavior. The same study showed that introducing a very plausible probabilistic adjustment into the model leads to the thermodynamic behavior of the system and to the phenomenon of irreversibility. Thus, the reason for the thermodynamic behavior of the ring model is not only beyond classical mechanics, but also contradicts it. Therefore, combining mutually exclusive Newtonian deterministic mechanics and the concept of probability does not seem convincing.

3. In the following years, many papers have been published, providing substantial arguments in favor of Ritz's hypothesis [2]. Papers [4–7] studied two-body problems with retarded interactions between the bodies and determined that the systems irreversibly transfer to the state of rest within $t \to \infty$. In paper [8], the dynamics of a two-particle harmonic oscillator with retarded interaction between particles was studied. It was determined that there always are nonstationary (both growing and damped) free oscillations in this system. Paper [9] studied the dynamics of a one-dimensional chain of atoms with retarded interactions. It was determined that stationary free oscillations in this system are impossible, i.e., the irremovable relativistic retardation of interactions between atoms completely destroys the classical non-relativistic dynamical picture of Born. Besides, the paper described a microscopic dynamical (i.e. free from probability) mechanism of reaching thermodynamic equilibrium in crystals.

4. The Kolmogorov probability theory is based on the theory of measure and is not a unique model, but only one of many non-equivalent probability models [10]. Probability measures in phase space (microcanonical, canonical, and grand canonical ensembles), axiomatically introduced by Gibbs, are also non-unique. In particular, even the Gibbs principle of equal a priori probabilities in the microcanonical distribution is a postulate. Its application does

not lead to an unambiguous result due to the peculiarities of the measures distribution in multidimensional (infinite-dimensional at the limit) spaces [11, 12] (in this case it refers to measures in the phase space of the system).

Thus, nonrelativistic statistical mechanics is based on two not quite consistent concepts: Newtonian classical mechanics (in Hamiltonian form) and the concept of probability. These concepts can be coordinated only when there is an external stochasticization mechanism. The hypothesis of molecular chaos of Boltzmann, the principle of weakening of correlations of Bogoliubov, separate consideration of long-range and short-range parts of interparticle potentials (Boltzmann–Vlasov, Vlasov–Maxwell equations, etc.) can be used to simulate such a mechanism in terms of kinetic theory, but there is no direct evidence for choosing any of these options.

At the same time, in the framework of relativistic dynamics there are indications of thermodynamic behavior even in few-body systems without the application of the concept of probability. Therefore, the modeling of relativistic dynamics of particle systems is a promising direction.

The aim of this study was to develop a classical relativistic kinetic theory of systems of interacting particles (atoms).

It solved the following specific tasks.

1. The field form of relativistic dynamics of the system of interacting atoms was developed.

2. It was determined that the interatomic central potentials of general form admit a decomposition by Klein-Gordon-Fock static potentials with complex mass parameters.

3. We developed an unambiguous procedure for the transition from the classical nonrelativistic model of interatomic interactions to the relativistic auxiliary field providing the interaction between atoms.

4. The qualitative properties of solutions of the relativistic auxiliary field dynamics equations were analyzed.

2. Field form of interatomic interactions and substantiation of the auxiliary field concept

Let us consider a model of a condensed system consisting of neutral particles (atoms), which in the nonrelativistic approximation is characterized by a scalar two-particle central interatomic potential of a general form $v(r)$, which can be represented by a Fourier integral:

$$v(r) = \int \frac{d\mathbf{k}}{(2\pi)^3} \tilde{v}(k^2) e^{i\mathbf{kr}}, \quad (1)$$

where

$$\tilde{v}(k^2) = \int d\mathbf{r} v(r) e^{-i\mathbf{kr}}. \quad (2)$$

This potential is a starting point for the transition from static interatomic potentials to an auxiliary relativistic dynamical field, which is equivalent to interatomic potentials only under static conditions.

Currently, quite a lot of model interatomic potentials are known [13–15], but only a small part of them is used in studies based on the molecular dynamics method [16–18].

Under the nonrelativistic approximation, interactions between atoms are instantaneous. Therefore, an atom and the instantaneous field created by it are a single entity with a finite number of degrees of freedom. In the relativistic theory, every motion of an atom (the source of the field) leads to the evolution of its field, the propagation velocity of which does not exceed the speed of light. Therefore, the evolution of the system of interacting atoms includes both the dynamics of particles and the dynamics of the relativistic field created by the atoms.

Thus, the nonrelativistic approximation in the dynamics of interacting atoms is characterized by taking into account a finite number of degrees of freedom of the atoms and neglecting an infinite set of degrees of freedom of the accompanying field.

2.1. Relativization in physics

The long and complicated process of "relativization" of all branches of physics from classical mechanics to thermodynamics began soon after the introduction of the theory of relativity. The first works on the relativistic generalization of the kinetic theory of ideal gases were published by Planck [19] and Jüttner [20, 21]. Synge [22] constructed the relativistic gas dynamics for an ideal gas. Later, numerous vigorous attempts have been made to formulate relativistic thermodynamics [23–25], relativistic statistical mechanics, and kinetics [26–34].

However, so far it has not been possible to develop a unified approach to the development of relativistic thermodynamics, relativistic statistical mechanics, and relativistic kinetic theory of systems consisting of interacting particles [35]. The main difficulty is to find a covariant form of accounting interactions between particles, since the relativistic theory does not include the concept of potential energy of interparticle interactions [36–38]. Therefore, only the model of contact interaction between particles was developed for the relativistic kinetic theory: the interaction occurs only at the points of intersection of their world lines [39–41]. The scope of applicability of this model is limited to the case of extremely short-range interactions between particles, which is obviously insufficient for applications in terms of the theory of condensed systems.

In the relativistic theory, atoms interact via the field, so the system of interacting particles actually consists of two subsystems: the particles and the field. The interaction between atoms is of electromagnetic origin, but the model (1) is sufficient to describe the dynamics of the system of interacting atoms, without detailing the origin of interatomic interactions.

2.2. Equations for static fields

We assumed that the Fourier transform (2) of the interatomic potential (1) had no singularities on the semi-axis $k^2 > 0$ of the complex plane k^2. Following [42], the equation for the static potential $v(r)$, generated by a particle located at the origin $\boldsymbol{r} = 0$, was:

$$f(\Delta)\{v(\mathbf{r})\} = \int \frac{d\mathbf{k}}{(2\pi)^3} f(-k^2)\tilde{v}(k^2)e^{-i\mathbf{kr}} = -4\pi\delta(\mathbf{r}), \quad (3)$$

where $f(\Delta)$ is the required function of the Laplace operator Δ.

Using the Fourier transform, we found:

$$f(-k^2) = -\frac{4\pi}{\tilde{v}(k^2)}. \quad (4)$$

This relation connects the Fourier transform of the static potential $\tilde{v}(k^2)$ with the differential equation (3) describing the corresponding static field.

In particular:

• The Fourier-transform of the Coulomb potential $\tilde{v}_1(k^2) = \frac{4\pi}{k^2}$ corresponds to the Poisson equation:

$$\Delta\varphi(\mathbf{r}) = -4\pi\delta(\mathbf{r}), \quad (5)$$

• The Fourier transform of the Yukawa potential $\tilde{v}_1(k^2) = \frac{4\pi}{k^2}$ corresponds to the static Klein–Gordon–Fock equation (or the Debye–Hьckel equation [43]):

$$(\Delta - \mu^2)\varphi(\mathbf{r}) = -4\pi\delta(\mathbf{r}). \quad (6)$$

Thus, the static interatomic potential $v(r)$, which can be represented as a Fourier integral (1), corresponds to the static field $\varphi(\mathbf{r})$, which satisfies the linear equation:

$$\left(\tilde{v}(-\Delta)\right)^{-1}\varphi(\mathbf{r}) = \rho(\mathbf{r}), \quad (7)$$

where $\rho(\boldsymbol{r})$ is the field source density.

The general solution of this equation is the sum of the general solution of the corresponding homogeneous equation:

$$\left(\tilde{v}(-\Delta)\right)^{-1}\varphi(\mathbf{r}) = 0 \quad (8)$$

and any particular solution of equation (7).

2.3. Qualitative analysis of solutions of the homogeneous static field equation

According to equation (8), the eigenvalue of the operator $\left(\tilde{v}(-\Delta)\right)^{-1}$ is zero. Taking into account the relation (4), this means that the function $\left(\tilde{v}(k^2)\right)^{-1}$ equals zero at the corresponding value of k^2:

$$\frac{1}{\tilde{v}(k^2)} = 0. \quad (9)$$

We will consider this condition as an equation with respect to k.

Since the function $\tilde{v}(k^2)$ at all real values of k is real and has no singularities, the imaginary parts of all roots of equation (9) must not equal zero:

$$k_s = \alpha_s + i\beta_s \Rightarrow k_s^2 = (\alpha_s^2 - \beta_s^2) + 2i\alpha_s\beta_s, \beta_s \neq 0. \quad (10)$$

In particular, k_s can be purely imaginary (at $\alpha_s = 0$), as it takes place for the Yukawa potential.

We introduced the notation:

$$\mu_s^2 = -k_s^2 \quad (11)$$

and transformed equation (9) into:

$$\frac{1}{\tilde{v}(k^2)} = \left(\prod_s \left[k^2 + \mu_s^2 \right]^{\gamma_s} \right) F(k^2) = 0, \quad (12)$$

where $F(k^2)$ is a certain function with no zeros, γ_s is the multiplicity of the root μ_s^2.

As $k^2 = -\Delta$ and all the operators:

$$\hat{L}_s = \left[\Delta - \mu_s^2 \right]^{\gamma_s}, \quad \hat{L} = \prod_s \left[\Delta - \mu_s^2 \right]^{\gamma_s}, \quad F(-\Delta) \quad (13)$$

commute, equation (8) is equivalent to the family of equations:

$$\left(\Delta - \mu_s^2 \right)^{\gamma_s} \varphi_s(\mathbf{r}) = 0. \quad (14)$$

To avoid unnecessary complexity, we restrict ourselves to considering the case when the multiplicity of all the roots of equation (9) is equal to 1, $\gamma_s = 1$:

$$\left(\Delta - \mu_s^2 \right) \varphi_s(\mathbf{r}) = 0. \quad (15)$$

The form of this equation resembles the problem of mathematical physics on the eigenvalues μ_s^2 of the Laplace operator, which can be obtained from the boundary conditions imposed on the function $\varphi_s(\mathbf{r})$. However, this similarity is only apparent. In this case, μ_s^2 are not derived from the boundary conditions for the functions $\varphi_s(\mathbf{r})$, but are solutions of equation (9).

In the particular case when $\tilde{v}(k^2)$ is a rational algebraic function, the set of operators $\hat{L}_s$ is finite ($s = 1, 2, \ldots, M$). Otherwise, this set may be infinite.

It should be noted that each of the functions $\varphi_s(\mathbf{r})$ satisfying equation (14), as well as all linear combinations of these functions equal zero upon the application of the operator $\hat{L}$. The general solution of equation (8) is a linear combination of the general solutions of equations (14) with arbitrary coefficients:

$$\varphi(\mathbf{r}) = \sum_s C_s \varphi_s(\mathbf{r}). \quad (16)$$

Thus, the free auxiliary static field $\varphi(r)$, equivalent to the instantaneous central interatomic potential, can be represented as a superposition of **elementary fields** $\varphi_s(r)$ satisfying equation (14).

As an example, let us briefly analyze possible variants of **static elementary potentials** depending on the complex parameter μ_s and satisfying equation (14). In this case we will not omit the solutions to this equation, which at first glance may seem "non-physical".

In the case of central (i.e., spherically symmetric) potentials, the general solution of equation (14) is as follows:

$$\varphi_s(r) = \frac{1}{r} \left(A_s e^{\mu_s r} + B_s e^{-\mu_s r} \right), \quad (17)$$

where

$$\mu_s = ik_s = -\beta_s + i\alpha_s, \quad r = |\mathbf{r}|, \quad (18)$$

and α_s and β_s are determined by formula (10).

At $\alpha_s = 0$, the potential $\varphi_s(\mathbf{r})$ is a linear combination of two terms, $\frac{e^{-\beta_s r}}{r}$ and $\frac{e^{\beta_s r}}{r}$. One of them tends to zero at $r \to \infty$ (Yukawa potential), and the second increases infinitely in absolute value and may seem "unphysical". However, there is a precedent for an interparticle potential that does not tend to zero at $r \to \infty$ and provides quark confinement in terms of quantum chromodynamics [44, 45].

In a more general case $\alpha_s \neq 0$, the elementary potentials $\varphi_s(r)$ are complex-valued functions of the coordinate r, depending on the complex parameters μ_s. In this case, the total potential (16), a linear combination of elementary potentials, is a real-valued function. In particular, if the number of complex elementary potentials is two, then the parameters μ_1, μ_2 are mutually conjugate:

$$\mu_2 = \mu_1^*, \quad (19)$$

and the total real static potential is as follows:

$$\varphi(r) = \frac{1}{r} \begin{Bmatrix} e^{-ar} \left[A\cos(br) + B\sin(br) \right] + \\ + e^{ar} \left[C\cos(br) + D\sin(br) \right] \end{Bmatrix}, \quad (20)$$

where $a = \mathrm{Re}\,\mu_1$, $b = \mathrm{Im}\,\mu_1$, and A, B, C, D are arbitrary real constants. This potential is a linear combination of sinusoidal functions of r. Their amplitudes change exponentially.

Note that the statistical thermodynamics of systems involving model potentials as in (20) and decreasing oscillation amplitudes was studied in [46, 47]. However, statistical thermodynamics of systems with model potentials, the oscillation amplitudes of which increase at $r \to \infty$, does not exist due to the divergence of configuration integrals. But this circumstance is not an obstacle

to studying the dynamics of systems with such model potentials.

2.4. Equations for dynamical fields

In terms of the nonrelativistic theory, the static field is closely related to the particles generating it and does not constitute separate degrees of freedom. The situation changes radically in terms of the theory of relativity: the dynamical field, generated by the particles and described by the relativistic equations of motion, comes into play.

The transition from static field equations to dynamic equations for electromagnetism was carried out by L. Lorenz and Riemann [48,49] in 1867 long before the theory of relativity appeared. The result was to replace the Laplace operator Δ in the Laplace and Poisson equations by the D'Alembert operator $\Box$:

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \Rightarrow$$
$$\Rightarrow \Box = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}. \quad (21)$$

Thus, after the Lorenz-Riemann transformation (21), the field becomes a component of the system of interacting particles. The consequences of this transformation are as follows.

1. The system consists of two subsystems, one of which is the particles and the other is the dynamic field produced by these particles.

2. Neither the direct action of atoms on each other nor the direct action of the field on itself (self-action) exist.

3. The only type of interactions that exists in a system is the interaction between atoms and the field. A well-known example of such type of theories is classical electrodynamics.

4. The set of degrees of freedom of the system of "particles + field which provides interaction between particles" is infinite even when the number of particles is finite. As a result, the system of interacting particles is no longer a dynamical system with a finite number of degrees of freedom. Setting initial conditions only for particles is not sufficient for the unique solvability of the Cauchy problem for particles.

5. The dynamics of a system of interacting particles within the field framework depends not only on the equations of particle motion and field evolution, but also on the boundary conditions for the field.

6. In the microscopic foundation of thermodynamics on the basis of the nonrelativistic theory with instantaneous interatomic interactions within the framework of Gibbs statistical mechanics, a finite number of degrees of freedom is taken into account. An infinite (continual) set of field degrees of freedom of the system as a whole is ignored.

7. The existence of a field, as a mediator of interactions between particles, leads to both a radical change in the physical picture of the dynamics of a system of particles and to the development of an appropriate mathematical apparatus. In relativistic field dynamics, there are no Liouville equation, Poincaré recurrence theorem, and integral invariants. These theorems of analytical mechanics play a key role in the microscopic justification of thermodynamics in Gibbs statistical mechanics but have no place in relativistic field dynamics.

3. Green's functions of elementary fields and multiplicity of interaction retardations

The Green function of the Klein-Gordon operator $\hat{L}_s = \Box - \mu_s^2$ defined by the equation:

$$\left(\Box - \mu_s^2\right) G_s\left(\mathbf{r}-\mathbf{r}', t-t'\right) = -\delta\left(\mathbf{r}-\mathbf{r}'\right)\delta\left(t-t'\right) \quad (22)$$

and has the known form [50]:

$$G_s\left(\mathbf{r}-\mathbf{r}', t-t'\right) = \frac{\delta\left(t-t'-\frac{|\mathbf{r}-\mathbf{r}'|}{c}\right)}{4\pi|\mathbf{r}-\mathbf{r}'|}$$
$$-\theta\left(t-t'-\frac{|\mathbf{r}-\mathbf{r}'|}{c}\right) c\mu_s \frac{J_1\left(\mu_s\sqrt{c^2\left(t-t'\right)^2-|\mathbf{r}-\mathbf{r}'|^2}\right)}{4\pi\sqrt{c^2\left(t-t'\right)^2-|\mathbf{r}-\mathbf{r}'|^2}}, \quad (23)$$

where $\theta(t)$ is the Heaviside step function and $J_1(x)$ is the Bessel function.

This implies the retarded potential of the Klein–Gordon field [50]:

$$\varphi_s\left(\mathbf{r},t\right) = \int d\mathbf{r}' \left[\frac{\rho\left(\mathbf{r}', t-\frac{|\mathbf{r}-\mathbf{r}'|}{c}\right)}{4\pi|\mathbf{r}-\mathbf{r}'|}\right.$$
$$\left. -\mu_s \int_0^\infty \rho\left(\mathbf{r}', t-\frac{1}{c}\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}\right) \frac{J_1\left(\mu_s\xi\right)}{4\pi\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}} d\xi\right], \quad (24)$$

where

$$\rho(\mathbf{r},t)=\sum_a \delta\left(\mathbf{r}-\mathbf{r}_a(t)\right) \quad (25)$$

is the instantaneous microscopic density of the number of particles (atoms).

1. The first summand in the right part of formula (24) contains the uniquely defined retardation τ_1 between the points $\mathbf{r}$ and $\mathbf{r}'$, corresponding to the waves travels at the speed of light c:

$$\tau_1=\frac{|\mathbf{r}-\mathbf{r}'|}{c}. \quad (26)$$

2. The second summand of the same formula contains an infinite set of retardations $\tau_2(\xi)$ between the same points $\mathbf{r}$ and $\mathbf{r}'$, depending not only on the distance between the points but also on the parameter ξ:

$$\tau_2(\xi)=\frac{\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}}{c}\geq\tau_1,\quad (0\leq\xi<\infty), \quad (27)$$

depending on the continuous parameter ξ and corresponding to Klein–Gordon waves travels propagating at speeds between 0 and c. Note that the retardation $\tau_2(\xi)$ can take arbitrarily large values. This means that no matter how distant the past of the system has a direct impact on its evolution at the current moment in time.

Note that the value $\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}$ can be formally mathematically interpreted as a distance in four-dimensional space x,y,z,ξ with a metric $d_2=\sqrt{x^2+y^2+z^2+\xi^2}$, where the propagation velocity of the Klein–Gordon field is equal to the speed of light c. Consequently, the projection of the velocity from the four-dimensional space x,y,z,ξ to the three-dimensional subspace x,y,z can take any values from 0 to c.

Thus, the relation between the evolution of the relativistic auxiliary field $\varphi(r,t)$ and the dynamics of the system of particles generating this field is non-local both in spatial variables and over time. Therefore, the interaction between the particles carried by the auxiliary field is also non-local.

We considered the contribution of one particle from the group of particles (25) moving according to the law $\mathbf{r}=\mathbf{r}_a(t)$, to the retarded Klein–Gordon potential (24). The microscopic density corresponding to one particle is defined by the expression:

$$\rho_a\left(\mathbf{r}',t-\frac{|\mathbf{r}-\mathbf{r}'|}{c}\right)=\delta\left(\mathbf{r}'-\mathbf{r}_a\left(t-\frac{|\mathbf{r}-\mathbf{r}'|}{c}\right)\right). \quad (28)$$

The contributed includes two components.

1.

$$\varphi_s^{(1)}(\mathbf{r},t)=\int d\mathbf{r}'\frac{\rho\left(\mathbf{r}',t-\frac{|\mathbf{r}-\mathbf{r}'|}{c}\right)}{4\pi|\mathbf{r}-\mathbf{r}'|}=$$
$$=\frac{1}{4\pi\left(|\mathbf{r}-\mathbf{r}_a(\tau)|-\frac{\left((\mathbf{r}-\mathbf{r}_a(\tau))\cdot\dot{\mathbf{r}}_a(\tau)\right)}{c}\right)}, \quad (29)$$

where τ is the variable related to t by a relationship:

$$\tau+\frac{|\mathbf{r}-\mathbf{r}_a(\tau)|}{c}=t. \quad (30)$$

2.

$$\varphi_s^{(2)}(\mathbf{r},t)=$$
$$=-\mu_s\int d\mathbf{r}'\int_0^\infty\frac{\rho\left(\mathbf{r}',t-\frac{1}{c}\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}\right)}{4\pi\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}}J_1(\mu_s\xi)d\xi. \quad (31)$$

Expression (29) for $\varphi_s^{(1)}(\mathbf{r},t)$ is a Lienard–Wiechert retarded potential [50, 51], depending on the position $\mathbf{r}_a(\tau)$ of the a-th particle and its velocity $\dot{\mathbf{r}}_a(\tau)$ at a single moment of time τ, determined by relation (30).

Expression (31) for $\varphi_s^{(2)}(\mathbf{r},t)$ has a noticeably more complicated structure. We changed the order of integration over the variables ξ and $\mathbf{r}'$ in formula (31) and considered the integral over $\mathbf{r}'$:

$$\Psi(\xi,\mathbf{r},t)=$$
$$=\int d\mathbf{r}'\delta\left(\mathbf{r}'-\mathbf{r}_a\left(t-\frac{1}{c}\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}\right)\right)\frac{1}{\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}}. \quad (32)$$

To integrate over $\boldsymbol{r}'$, we multiplied both sides of this relation by $\delta\left(\tau-t+\frac{1}{c}\sqrt{\xi^2+|\mathbf{r}-\mathbf{r}'|^2}\right)$ and integrated over the variable τ. As a result, the left part of this equality remained unchanged, and the right part was transformed to the following form:

$$\Psi(\xi,\mathbf{r},t)=\int d\tau\int d\mathbf{r}'\delta\left(\tau-t+\frac{1}{c}\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}'\right|^2}\right)\times$$
$$\times\frac{1}{\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}'\right|^2}}\delta\left(\mathbf{r}'-\mathbf{r}_a(\tau)\right)= \quad (33)$$
$$=\int d\tau\delta\left(\tau-t+\frac{1}{c}\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau)\right|^2}\right)\frac{1}{\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau)\right|^2}}.$$

The last integral has the form:

$$J(\xi,t,\mathbf{r})=\int d\tau\delta\left(F(\xi,t,\tau,\mathbf{r})\right)f(\xi,\mathbf{r},\tau), \quad (34)$$

where

$$F(\xi,t,\tau,\mathbf{r})=\tau-t+\frac{1}{c}\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau)\right|^2}, \quad (35)$$

and

$$f(\xi,\mathbf{r},\tau)=\frac{1}{\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau)\right|^2}}. \quad (36)$$

Integral (34) is calculated by the known formula:

$$J(\xi,t,\mathbf{r})=\sum_k\frac{f(\xi,\mathbf{r},\tau_k)}{\left|F_\tau'(\xi,t,\tau_k,\mathbf{r})\right|}, \quad (37)$$

where τ_k are the equation roots:

$$F(\xi,t,\tau,\mathbf{r})=\tau-t+\frac{1}{c}\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau)\right|^2}=0 \quad (38)$$

in relation to τ. To show that this equation has a single root depending on ξ and t, we obtained the partial derivative of the function $F(\xi,t,\tau,\mathbf{r})$ on the variable τ:

$$F_\tau'(\xi,t,\tau,\mathbf{r})=1-\frac{1}{c}\frac{\left(\mathbf{r}-\mathbf{r}_a(\tau)\right)\dot{\mathbf{r}}_a(\tau)}{\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau)\right|^2}}. \quad (39)$$

It follows from the inequality:

$$F_\tau'(\xi,t,\tau,\mathbf{r})>0 \quad (40)$$

and the asymptotic behavior of the function $F(\xi,t,\tau,\mathbf{r})$ at $\tau\to\pm\infty$ that the solution of equation (38) in relation to τ exists and is unique:

$$\tau=\tau(\xi,t). \quad (41)$$

Thus, for any values of ξ, there is an unambiguous correspondence between t and τ:

$$t=t(\xi,\tau),\quad \tau=\tau(\xi,t). \quad (42)$$

By substituting (41), (39), (37), and (36) into (33), we obtained:

$$\Psi(\xi,\mathbf{r},t)=$$
$$=\frac{1}{\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau(\xi,t))\right|^2}-\frac{\left(\mathbf{r}-\mathbf{r}_a(\tau(\xi,t))\right)\dot{\mathbf{r}}_a(\tau(\xi,t))}{c}}. \quad (43)$$

As a result, the expression for $\varphi_s^{(2)}(\mathbf{r},t)$ was transformed into:

$$\varphi_s^{(2)}(\mathbf{r},t)=$$
$$=-\frac{\mu_s}{4\pi}\int_0^\infty\frac{J_1(\mu_s\xi)}{\left(\begin{array}{c}\sqrt{\xi^2+\left|\mathbf{r}-\mathbf{r}_a(\tau(\xi,t))\right|^2}-\\-\frac{\left(\mathbf{r}-\mathbf{r}_a(\tau(\xi,t))\right)\dot{\mathbf{r}}_a(\tau(\xi,t))}{c}\end{array}\right)}d\xi. \quad (44)$$

Note that using this representation to quantitatively analyze the retarded Klein–Gordon field potential implies knowledge of the function $\tau(\xi,t)$, which is formally defined as a solution of equation (38) with respect to τ. This equation is transcendental, and it is hardly possible to find an exact analytical solution to it for the general case. However, under certain conditions, an approximate solution can be found, which only deviates from the exact solution by an arbitrarily small amount.

There is a fundamental difference between expressions (29) for $\varphi_s^{(1)}(\mathbf{r},t)$ and (44) for $\varphi_s^{(2)}(\mathbf{r},t)$.

1. The potential $\varphi_s^{(1)}(\mathbf{r},t)$ at the point $\mathbf{r}$ at the moment t depends on the instantaneous position $\mathbf{r}_a(\tau)$ and instantaneous velocity $\dot{\mathbf{r}}_a(\tau)$ of the generating particle at the single moment of time τ, determined by condition (30).

2. The potential $\varphi_s^{(2)}(\mathbf{r},t)$ at the point $\mathbf{r}$ at the moment t depends on an infinite series of positions $\mathbf{r}_a(\tau(\xi,t))$ and an infinite series of instantaneous velocities $\dot{\mathbf{r}}_a(\tau(\xi,t)\tau)$ of the generating particle at all moments of time, determined by condition (38) and parameterized by the variable $0\le\xi<\infty$.

In other words, an observer located at the point $\boldsymbol{r}$ at the moment t and using the field $\varphi_s^{(1)}(\mathbf{r},t)$ for observation, sees a point source of this field.

The same observer located at the point $\mathbf{r}$ at the moment t and using the field $\varphi_s^{(2)}(\mathbf{r},t)$ for observation, sees infinitely many sources instead of a point source of this field. These sources fill the whole trajectory of the source from the distant past to the point $\mathbf{r}=\mathbf{r}_a(t-\tau(\xi,t))\big|_{\xi=0}$.

4. Discussion and conclusions

The basic principles underlying this study are as follows.

1. Interatomic interactions have a field character. Therefore, any real system consists of particles and a field created by these particles, transmitting interactions between these particles.

2. In the case of atoms at rest, the interaction between them can be described by interatomic potentials. In the case of moving atoms, their interaction is described by an auxiliary scalar relativistic field.

3. The auxiliary scalar field is a superposition of elementary fields. Each of them is characterized by its own complex mass and satisfies the Klein-Gordon-Fock equation. The parameters of elementary fields are uniquely expressed through the characteristics of static interatomic potentials.

4. By virtue of finiteness of masses of elementary fields, the propagation velocity of Klein-Gordon-Fock fields can take any values smaller than the speed of light. This leads to the fact that the retardation of interactions between particles can reach any large values.

5. The retardation of interactions between particles is a real physical mechanism leading to irreversibility of the dynamics of both many-particle and few-particle systems.

Contribution of the authors

The authors contributed equally to this article.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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Information about the authors

Anatoly Yu. Zakharov, Dr. Sci. (Phys.-Math.), Full Professor, Professor at the Department of General and Experimental Physics, Yaroslav-the-Wise Novgorod State University (Veliky Novgorod, Russian Federation)
https://orcid.org/0000-0002-7850-0086
anatoly.zakharov@novsu.ru

Maxim A. Zakharov, Dr. Sci. (Phys.-Math.), Docent, Professor at the Department of Solid State Physics and Microelectronics, Yaroslav-the-Wise Novgorod State University (Veliky Novgorod, Russian Federation)
https://orcid.org/0000-0002-9144-340X
maxim.zakharov@novsu.ru

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