Thermodynamics of relativistic Newton–Wigner particle in external potential field

A S Larkin and V S Filinov
Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
E-mail: alexanderlarkin@rambler.ru

Abstract. Thermodynamic properties of relativistic spinless particle described by the Klein–Gordon equation have been studied using the Newton–Wigner theory of particle in external potential field. Concept of Wiener path integral was extended on relativistic case. A new path integral Monte-Carlo method was developed for relativistic particle in external potential field. The bounds of applicability of available analytical approaches and related results have been specified by comparison with Monte Carlo calculations. Developed path integral formalism can be directly extended on systems of many identical Newton–Wigner particles, which interact with external field and each other.

1. Introduction
The most fundamental approach to research relativistic quantum systems of many particles is currently a quantum field theory (QFT). It studies quantum fields, i.e. systems with an infinity number of degrees of freedom. Wherein particles are usually considered as elementary excitations of corresponding field. Such approach automatically takes into account a production and annihilation of particles and considers interactions as exchange of virtual particles.

The main working tool in QFT is technique of Feynmann diagrams [1]. The diagrams represent graphically a series of perturbation theory, in which coupling constants are usually small parameters. Feynmann diagrams are applicable to a large number of different cases, however it is useless for strongly non-ideal systems when coupling can not be guessed as weak. For example, such systems are non-ideal quark-gluon plasma or bounded states of particles.

One of the most straightforward approach to calculate properties of non-ideal systems is making use of the lattice models. Lattice QFTs are based on path integral formalism, which was introduced in quantum mechanics by Feynmann [2]. For example, in works [3] equation of state of quark-gluon plasma has been studied by using the lattice QCD. Calculations on lattice are very costly and require powerful supercomputers.

The alternative approach to study the relativistic systems is to use the path integral model of the a system with variable number of particles described by the relativistic kinetic energy operator \[ \sqrt{\vec{p}^2 c^2 + m^2 c^4} \] and interacting by some effective pair potential. This method was used to calculate thermodynamic and transport properties of quark-gluon plasma [4]. It requires less computer resources and could be applied to system with large chemical potentials. Furthermore this method has been used in applications to plasma [5] and solid bodies [6].
In this work we calculate the thermodynamic properties of relativistic spinless particle described by the Klein-Gordon equation. For this purpose we use the path integral approach derived from one-particle relativistic theory proposed by Wigner and Newton in [7]. Such approach turns out to be equivalent to direct solution of relativistic wave equations, such as Klein-Gordon equation.

2. Klein-Gordon equation

Let’s begin with consideration of free spinless particle of mass \(m\) in 3-dimensional space. Then the well-known relativistic expression for energy looks like: \(E = p^2c^2 + m^2c^4\). One can obtain Klein-Gordon equation (KGE) for free particle through formal substitution for \(E \rightarrow i\hbar \frac{\partial}{\partial t}\), \(p \rightarrow -i\hbar \nabla\). So in coordinate representation [1]:

\[
\left[ \frac{\hbar^2}{c^4} \frac{\partial^2}{\partial t^2} - \frac{\hbar^2}{c^2} \nabla^2 - m^2 \right] \phi(x, t) = 0. \tag{1}
\]

The solutions of this equations are plane waves \(\phi(x, t) = e^{-i(Et - px)/\hbar}\) with positive and negative energies \(E = \pm \sqrt{p^2c^2 + m^2c^4}\). One can easy show, that these functions are also solutions of the differential equations

\[
\frac{i\hbar}{\partial t} \phi(x, t) = \pm \sqrt{m^2c^4 + c^2(-i\hbar \nabla - e/c A(x))^2} \phi(x, t); \tag{2}
\]

the sign “plus” corresponds to plane waves with \(E \geq 0\), while the “minus” one relates to \(E \leq 0\) respectively. The scalar product of quantum states \(|\Phi\rangle\) and \(|\Psi\rangle\) at time moment \(t\) is defined in coordinate representation as [1]

\[
\langle \Phi | \Psi \rangle = i\hbar \int d^3x \left( \phi^* \frac{\partial}{\partial t} \psi - \psi \frac{\partial}{\partial t} \phi^* \right), \tag{3}
\]

and for states with positive and negative energy separately satisfies all attributes of scalar product, including positive definiteness.

Now let’s proceed to a spinless particle with electric charge \(e\) in external electromagnetic field, which is set by four-dimensional potential \(A^\mu = (A^0, A)\) without time dependence. In this case KGE has the form [1]:

\[
\left[ \frac{i\hbar}{\partial t} - eA^0(x) \right]^2 - c^2 \left( -i\hbar \nabla - \frac{e}{c} A(x) \right)^2 \phi(x, t) = m^2c^4 \phi(x, t) = 0. \tag{4}
\]

Solutions with positive and negative energies satisfy differential equations, which are obtained from (2) through generalization on electromagnetic field:

\[
\left( \frac{i\hbar}{\partial t} - eA^0(x) \right) \phi(x, t) = \pm \sqrt{m^2c^4 + c^2 \left( -i\hbar \nabla - \frac{e}{c} A(x) \right)^2} \phi(x, t). \tag{5}
\]

These equations are relativistic analogue of Schrodinger equation for particle in external electromagnetic field in coordinate representation.

In quantum field theory the positive-energy wave functions are interpreted as states of particles, while the states with negative energy are considered as antiparticles. Full solution of KGE (4) is the superposition of wave functions for both particles and antiparticles, which satisfy system of these two differential equations (5). The product of wave functions introduced
by (3) does not meet requirements for scalar product, as it leads to negative quantum probability. This as well as some other difficulties were the reason for developing the quantum field theory [1].

If we consider only the positive-energy solutions of KGE, then there would not be such problems. In fact, this will be the one-particle relativistic theory suggested by Newton and Wigner in 1940’s [7]. Although in such theory pair production is not taken into account, such approach can be used for temperatures of the order of 0.1mc², because of pair generation will be negligible. At the same time the relativistic corrections to quantum effects and dynamics may be important.

### 3. Newton–Wigner theory

Let’s briefly consider the basic ideas of the original work [7]. Our main interest is so-called the Newton–Wigner (pseudo)particle in external potential field described by the hamiltonian $\hat{H} = \omega(p) + V(\hat{x})$, where $\omega(p) = \sqrt{p^2c^2 + m^2c^4}$ is the relativistic kinetic energy while $\hat{p}$, $\hat{x}$ are momentum and position operators. Eigenvectors of the momentum operator $|p>$ have the Lorentz-invariant normalization and form a full system [9]:

$$<p|p'> = (2\pi\hbar)^3 \frac{\omega(p)}{mc^2} \delta^{(3)} (p - p'), \quad 1 = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{mc^2}{\omega(p)} |p><p|.$$  

(6)

One can define the wave function for state $|p>$ in momentum representation as $\Psi(p) = <p|\Psi>$, where we don’t indicate dependence on time for brevity. Scalar product $<\Phi|\Psi>$ in momentum representation has form

$$<\Phi|\Psi> = \int \frac{d^3p}{(2\pi\hbar)^3} \frac{mc^2}{\omega(p)} \Phi^*(p)\Psi(p).$$  

(7)

Squared module of the $|<\Phi|\Psi>|^2$ is proportional to the probability of transition from $|\Psi>$ to $|\Phi>$ and is Lorentz-invariant [9].

Action of arbitrary quantum operator $\hat{A}$ on wave functions is defined as $\hat{A}\Psi(p) = <p|\hat{A}|\Psi>$. In particular, action of the momentum operator $\hat{p}$ in the momentum representation is simple multiplication on $p$, while the coordinate operator $\hat{x}$ looks like [7]:

$$\hat{x} \Phi(p) = \left[ \frac{i\hbar}{\partial p} - i\hbar \frac{pc^2}{2\omega^2(p)} \right] \Phi(p).$$  

(8)

Quantum averages for arbitrary observable value $\hat{A} = \hat{A}(\hat{p},\hat{x})$ in state $|\Psi>$ can be calculated as

$$<\Psi|\hat{A}|\Psi> = \int \frac{dp}{2\pi\hbar} \frac{mc^2}{\omega(p)} \Psi^*(p)\hat{A}(p,\hat{x})\Psi(p).$$  

(9)

Time evolution of the Newton–Wigner particle is controlled by the differential equation

$$i\hbar \frac{\partial}{\partial t} \Psi(p,t) = \hat{H}\Psi(p,t),$$  

(10)

being the Schrödinger equation with relativistic kinetic energy. Note that this equation can be obtained from KGE (2) with $V(x) = eA_0(x)$ and $A_0(x) = 0$ after the transition to the momentum representation for positive-energy wave function $\phi(x,t)$ [1]:

$$\phi(x,t) = \frac{2\pi\hbar}{c\sqrt{2mc^2}} \int \frac{d^4k}{(2\pi\hbar)^4} \delta([k^0 - eA_0(x)]^2 - \omega^2(p)/c^2)\theta(k^0)e^{ikx/c}\Phi(k,t).$$  

(11)

It turns out that scalar product of coordinate wave functions (3) transforms into expression (7) of Newton–Wigner theory.
4. Partition function of the Newton–Wigner particle

Thermodynamic properties of quantum system are defined by the partition function $Z = S \rho \left[ e^{-\beta H} \right]$, where $\beta = 1/kT$ is the inverse temperature [10]. One can write a partition function for Newton–Wigner particle, using eigenvectors of momentum, the completeness relation, normalization (6) and integral representation for delta function:

$$Z = \int dx \int dp_N \int dp_0 \frac{mc^2}{2\pi \hbar} \omega(p_0) < p_N | e^{-\beta H} | p_0 > e^{-i(p_0 - p_N)x/\hbar}. \quad (12)$$

Here integral is taken over the large finite one-dimensional volume $L$. Thereby partition function $Z$ is function of variables $\beta$ and $L$. Note that generalization to higher dimensions is straightforward.

For obtaining an expression for $Z$ in form of path integral, we use usual manipulation for Feynmann integrals (see, for example, [11]). We divide the interval from 0 to $\beta$ into large number $N$ of small parts with length $\epsilon = \beta/N$ and apply the completeness relation (6) $N - 1$ times. When $\epsilon \to 0$ matrix elements have form

$$< p_{n+1} | e^{-\beta H} | p_n > = \left( \frac{\omega(p_n)}{mc} \right)^{1/2} \left( \frac{\omega(p_n)}{mc^2} \right)^{1/2} \int dx_n e^{-i(p_{n+1} - p_n)x_n/\hbar - \epsilon\omega(p_n) - \epsilon V(x_n)}. \quad (13)$$

Substituting the matrix elements into formula for $Z$ we obtain multi-dimensional integral of the form

$$Z = \int dx \prod_{k=1}^{N-1} \int dx_k \prod_{n=1}^{N} \int dp_n \frac{mc^2}{2\pi \hbar} \exp \left[ \frac{i}{\hbar} p_n (x_n - x_{n-1}) - \epsilon\omega(p_n) - \epsilon V(x_n) \right]. \quad (14)$$

This result can be simplified through integration over momentums ( [12]). Finally we have expression for partition function in the form of path integral as limit at $N \to \infty$:

$$Z = \int dx \prod_{k=1}^{N-1} \int dx_k \prod_{n=1}^{N} \left[ \frac{mc}{\pi \hbar} K_1 \left( \frac{\beta mc^2}{\hbar} \sqrt{1 + \frac{N^2}{\beta^2 \hbar^2 \epsilon^2} (x_n - x_{n-1})^2} \right) \right] \epsilon^2 V(x_n), \quad (15)$$

where $x_0 = x$, $x_N = x$; $K_1(x)$ is the MacDonald function of the first order. One can write this path integral in the symbolic form, which is similar to Wiener integrals [13]:

$$Z = \int dx \int d_{RW}[0,x;x_{\beta h},x] x(\tau) \exp \left\{ -\frac{1}{\hbar} \int_0^{\beta h} d\tau V(x(\tau)) \right\}. \quad (16)$$

Here the measure $d_{RW}$ is a relativistic expansion of the usual Wiener measure $d_W$.

5. Average energy and heat capacity of the Newton–Wigner particle

Thermodynamic quantities can be derived from partition function $Z$. In particular, average energy $E$ and heat capacity at constant volume are obtained through calculation of derivations of $Z$ of $\beta = 1/kT$ [10]:

$$E = -\frac{1}{Z} \left( \frac{\partial Z}{\partial \beta} \right)_L, \quad C_L = k\beta^2 \left[ \frac{1}{2} \left( \frac{\partial^2 Z}{\partial \beta^2} \right)_V - \left( \frac{1}{2} \frac{\partial Z}{\partial \beta} \right)_V \right]. \quad (17)$$

However direct differentiation of path integral (15) leads to numerically unstable expression [15]. Therefore, one should transform path integral similar to Wiener integrals [16] to exclude
derivatives of measure. We make the change of variables \( x = \eta L, x_k = \lambda \xi_k + \eta L \), where \( \lambda = \lambda(\beta) \) is function we will choose below; it has measured in lengths. After such change path integrals for partition function and its derivatives can be written in form of

\[
Z = (\lambda^{-1}L) \int_1^L d\eta \left[ \prod_{k=1}^{N-1} \int d\xi_k \right] \rho_K \rho_V;
\]

\[
\frac{1}{Z} \left( \frac{\partial Z}{\partial \beta} \right)_L = -\lambda^{-1} \frac{\partial \lambda}{\partial \beta} + \frac{1}{Z} (\lambda^{-1} L) \int_1^L d\eta \left[ \prod_{k=1}^{N-1} \int d\xi_k \right] \rho_K \rho_V (\phi_K + \phi_V);
\]

\[
\frac{1}{Z} \left( \frac{\partial^2 Z}{\partial \beta^2} \right)_V = \left( \lambda^{-1} \frac{\partial \lambda}{\partial \beta} \right)^2 - \frac{\partial}{\partial \beta} \left( \lambda^{-1} \frac{\partial \lambda}{\partial \beta} \right) + \frac{1}{Z} (\lambda^{-1} L) \int_1^L d\eta \left[ \prod_{k=1}^{N-1} \int d\xi_k \right] \rho_K \rho_V \times
\]

\[
\left[ (\sigma_K + \sigma_V) + (\phi_K + \phi_V)^2 + (\phi_K + \phi_V) \left( 2\lambda^{-1} \frac{\partial \lambda}{\partial \beta} - mc^2 \right) \right].
\]

Here \( \rho_K \) is the factor which relates to relativistic measure \( d_{RW} \), and \( \rho_V \) relates to the potential part of the partition function:

\[
\rho_K = \prod_{n=1}^{N} \frac{mc}{\pi \hbar} \frac{K_1(\beta mc^2)}{\sqrt{1 + \frac{\beta^2 N^2}{m^2}(\xi_n - \xi_{n-1})^2}}
\]

\[
\rho_V = \prod_{n=1}^{N} \exp \left\{ -\frac{\beta}{N} V(\eta L + \lambda \xi_n) \right\}.
\]

Functions \( \phi_K, \phi_V, \sigma_K, \sigma_V \) are the first and the second derivatives of (19) of \( \beta \) respectively:

\[
\phi_K = \frac{\partial \rho_K}{\partial \beta}, \phi_V = \frac{\partial \rho_V}{\partial \beta}, \sigma_K = \frac{\partial^2 \rho_K}{\partial \beta^2}, \sigma_V = \frac{\partial^2 \rho_V}{\partial \beta^2}.
\]

Explicit expressions for these functions are derived by simple differentiation. However they are cumbersome so we haven’t written them here.

Let’s turn now to a choice of the function \( \lambda(\beta) \). In case of non-relativistic Wiener integrals one uses so-called heat wave length \( \lambda_{\text{term}} = \sqrt{2\pi \hbar^2 \beta/m} \), so in formula (18) the term \( \lambda^{-1} \frac{\partial \lambda}{\partial \beta} \) has to be equal to average kinetic energy of free particle \( \frac{1}{2} kT \) [13]. Therefore it is natural to select function \( \lambda(\beta) \), which meets two requirements:

(i) in non-relativistic limit \( (\beta mc^2 \to \infty) \) \( \lambda \) has to turn into a heat wave length \( \lambda_{\text{term}} \);

(ii) a quantity \( \lambda^{-1} \frac{\partial \lambda}{\partial \beta} \) has to be equal to average energy of free relativistic Newton–Wigner particle at a temperature \( T \).

When \( \beta mc^2 \gg 1 \), a partition function of Newton–Wigner particle is reduced into non-relativistic partition function \( Z_{\text{nrel}} \), and its average energy turns into energy of non-relativistic particle \( E_{\text{nrel}} \). So taking into account rest energy \( mc^2 \) we have:

\[
Z \rightarrow Z_{\text{nrel}} e^{-\beta mc^2}, \ E \rightarrow E_{\text{nrel}} + mc^2.
\]

Partition function of free Newton–Wigner particle in a volume \( L \) can be founded from the definition \( Z_0 = Sp \left[ e^{-\beta \omega(p)} \right] \). One should obtain it, using completeness relation for momentum eigenvectors (6):

\[
Z_0 = \frac{L}{2\pi \hbar} \int \frac{dp}{2\pi \hbar \omega(p)} e^{-\beta \sqrt{p^2 c^2 + mc^2}}.
\]
The integral can be expressed with MacDonald function [12]. Thus partition function and average energy of free relativistic particle are equal to

$$Z_0 = \frac{mcL}{2\pi^2\hbar^2}K_1(\beta mc^2), \quad E_0 = \frac{1}{\beta} + mc^2\frac{K_0(\beta mc^2)}{K_1(\beta mc^2)}.$$ (23)

It is easy to check that $\lambda(\beta)$ is of the form

$$\lambda = \frac{\pi\hbar}{mc} e^{-\beta mc^2},$$ (24)

and satisfies requirements (i) (ii), thus and so it is relativistic expansion of heat wave length.

Note an important detail of expression (18). In case of free particle, i.e. $V(x) = 0$, functions $\phi_V$ and $\sigma_V$ have to be equal to zero. But functions $\phi_K$ and $\sigma_K$, appearing from derivatives of the measure of path integrals $d\mathcal{H}_V$ look non-trivial. At the same time outer summands in (18) are already equal to thermodynamic quantities for free Newton–Wigner particle (ii). Therefore integrals of $\phi_K$ and $\sigma_K$ have to equal to zero. Of course, if external field is applied, equality to zero of these integrals is not obvious. However straight numerical calculations for different potentials $V(x)$ show that integrals of $\phi_K$ $\sigma_K$ are negligible. Thereby one can keep only “potential” summands $\phi_V$, $\sigma_V$ in (18), and measure of path integral should not be differentiated.

6. Path integral Monte-Carlo

Path integrals for thermodynamic quantities (18) can be calculated numerically using Monte-Carlo method, which is similar to approach for Wiener integrals [13]. Representation of the partition function in form of path integral shows that arbitrary thermodynamic quantity $\Theta$ can be written as multidimensional integral (with large $N$):

$$\Theta = \int d\eta d\xi_1 ... d\xi_{N-1} \rho(\eta, \xi_1, ..., \xi_{N-1})\theta(\eta, \xi_1, ..., \xi_{N-1}),$$ (25)

where positive function $\rho(\eta, \xi_1, ..., \xi_{N-1})$ is interpretable as probability density in space of $(\eta, \xi_1, ..., \xi_{N-1})$, and $\theta(\eta, \xi_1, ..., \xi_{N-1})$ as function to average.

To calculate an integral(25) Metropolis algorithm [18] with two kinds of steps is used in this work. Steps of the first kind consist of random change in the variable $\eta$, $\delta\eta \leq \Delta\eta$ and correspond to shift particle’s position in volume. Steps of the second kind consist of random change of variables $\xi_n$, $\delta\xi_n \leq \Delta\xi$ and can be interpreted as deformation of the trajectory representing the particle [19]. Initially, one makes a random choose of step kind: first or second. Then one calculates ratio $a$ of the function $\rho$ value on new configuration to its value on old configuration. If $a \geq 1$ then new configuration $(\eta, \xi_1, ..., \xi_{N-1})$ is accepted. If $a$ is less then 1, than acceptance probability equals to $a$. After that the algorithm makes a new step. After each step function $\theta(\eta, \xi_1, ..., \xi_{N-1})$ is calculated, and finally it will be averaged over all $M$ accepted configurations. According to (25), such procedure gives average value $\Theta$.

The algorithm described above contains technical parameters $\Delta\eta$, $\Delta\xi$. Choice of this parameters doesn’t affect on final result of calculation; only speed of convergence of the Monte-Carlo is depended on them. The configuration $\eta = \xi_1 = ... = \xi_{N-1} = 0$ is used as initial. It turns into equilibrium in some number of steps, and for faster convergence one should drop out $M$ initial configurations in averaging of $\theta(\eta, \xi_1, ..., \xi_{N-1})$. On practice for one particle $M$ was taken to be of order of $10^6 - 10^7$ steps. Discretization $N$ of path integrals was taken 50 for temperatures $kT \geq 0.1mc^2$. 


Thermodynamic behavior of relativistic harmonic oscillator

The Newton–Wigner particle in quadratic potential is referred to as relativistic harmonic oscillator [14]. Its Hamiltonian is \( \hat{H} = \omega(p) + \frac{mc^2}{2} \hat{x} \), where a position operator is defined by the formula (8), and \( \omega \) is a parameter of oscillator (don’t confuse it with kinetic energy \( \omega(p) \)). Thermodynamic properties of oscillator are set by two parameters: temperature \( T \) and “frequency” \( \omega \) (volume \( L \) could be considered infinite due to finite motion of particle). Let’s explore domains of applicability of available analytical approaches to the oscillator. It is of interest to consider wide area of temperatures and “frequencies” neglecting at a first approximation by pair creation and annihilation at high energies.

At high temperature, when \( kT \gg mc^2 \) and \( kT \gg \hbar \omega \) at once, oscillator is relativistic system, but it’s quantum nature is insignificant. So it can be described in terms of classical statistics, and kinetic and potential contribution in average quantities can be isolated [8]. Particularly, average energy and heat capacity are

\[
E_{cl} = \frac{3}{2} \beta^{-1} + mc^2 \frac{K_0(\beta mc^2)}{K_1(\beta mc^2)},
\]

\[
C_{Lcl} = k \left[ 1 + (\beta mc^2)^2 - (\beta mc^2) \frac{K_0(\beta mc^2)}{K_1(\beta mc^2)} - \left( \frac{K_0(\beta mc^2)}{K_1(\beta mc^2)} \right)^2 \right], \quad (26)
\]

where kinetic contribution is obtained from (23) and potential one equals to \( \frac{1}{2}kT \). Note that in the high temperature limit \( E_{cl} \rightarrow \frac{3}{2}kT \) \( C_{Lcl} \rightarrow 2k \).

On the contrary, when temperature is relatively low \( (kT << mc^2) \), relativistic effects are negligible, so oscillator can be studied with non-relativistic mechanics, classical or quantum (depends on ratio between \( kT \) and \( \hbar \omega \)). Thereby, harmonic oscillator behaves as it is depicted on figure 1, where non-relativistic area is colored in blue, and classical relativistic mechanics is applicable in orange area. In the rest area one has to use quantum relativistic theory.

Above the conformity between Newton–Wigner theory and KGE was shown. Therefore one could expect equality between states of the relativistic harmonic oscillator and stationary
Figure 3. Dependencies of average energy on inverse temperature for harmonic oscillator for different values of $\hbar \omega$: top left—$\hbar \omega = 0.2mc^2$, top right—$\hbar \omega = mc^2$, bottom left—$\hbar \omega = 2mc^2$, bottom right—$\hbar \omega = 5mc^2$. 1—Monte-Carlo (this work), 2—classical relativistic behavior (26), 3—theory based on approximate KGE solution (28).

positive-energy solutions of equation

$$\left[ \left( i\hbar \frac{\partial}{\partial t} - \frac{m\omega^2}{2} x^2 \right)^2 - (-i\hbar \nabla)^2 - m^2 c^4 \right] \phi(x, t) = 0. \quad (27)$$

An explicit solution of this equation is unknown, however one can use the next approximations for energy levels, when temperatures are not very high ($kT \leq mc^2$) [17]:

$$E_n = \pm mc^2 \sqrt{1 + 2 \left( n + \frac{1}{2} \right) \frac{\hbar \omega}{mc^2}}. \quad (28)$$

Here one can calculate a partition function through direct summation over positive energies $Z(\beta) = \sum_n e^{-\beta E_n}$ then the average energy and heat capacity can be obtained from derivatives of $Z$. Corresponding series converges fast, so practically it can be can taken the sum over $n$ from 0 to $10^5$ with accuracy of 0.01%.

In this work we calculated average energy and heat capacity of the oscillator in a wide range of $\omega$ and $T$. As result boarders of applicability of non-relativistic and classical theories were
corrected and have been shown on figure 2. Also domain of applicability of the approximate KGE’s solutions (28) has been analysed. Corresponding areas are marked with different colors on the figure. No one analytical approach could be used in the uncoloured area, where oscillator’s thermodynamics can be studied only with numerical calculations.

8. Energy and heat capacity of the oscillator

Let’s consider thermodynamic properties of relativistic harmonic oscillator closer. The Monte-Carlo calculations were carried out for temperatures $kT$ from $0.1mc^2$ to $10mc^2$ for some values of “vibrational quantum” $\hbar\omega$. Now we have to discuss obtained result and compare them with predictions of classical mechanics (26) and approximate quantum theory (28). Particularly, it will become clear how we have plotted bounds of applicability in figure 2.

Firstly we look at average energy of the oscillator and it’s dependence on temperature. It is represented on figure 3 for different values of “vibrational quantum” parameter $\hbar\omega$: $0.2mc^2$, $mc^2$, $2mc^2$ and $5mc^2$. Results of numerical calculations obtained in this work are compared with predictions of analytical approaches (26), (28). It is clear that oscillator can be considered as classical when temperature is higher then $0.25mc^2$, $0.5mc^2$, $mc^2$ and $5mc^2$ for each value of $\hbar\omega$ respectively. Low-temperature theory based on approximate solution of KGE is rightful for $kT$
lower then \(0.2mc^2\), \(0.25mc^2\), \(0.5mc^2\) and \(0.5mc^2\) as it was shown in figure 2.

Now we turn to heat capacity of relativistic oscillator. Note that the Nernst theorem demands that heat capacity equals to zero when \(T \to 0\). However one can not avoid a statistical error in Monte-Carlo calculations of derivatives of partition function, which are multiplied by \(\beta^2 = 1/(kT)^2\) accordingly by (17). Therefore when temperature is low a relative error becomes significant. This is the reason of presenting the dependence of \(C_L/\beta^2 = Ck^2T^2\) rather than \(C_L\) versus \(\beta = 1/kT\). Results are shown in figure 4, where they are compared with analytical approximations (26) and (28). Behavior of oscillator is classical on high temperatures and can be described by approximate KGE solution on relatively low temperatures again. Note that \(C_L \to 0\) when \(T \to 0\) correspondingly with Nernst theorem.

9. Conclusion
Thermodynamic properties of relativistic spinless particle described by the Klein-Gordon equation have been studied using the Newton–Wigner theory of particle in external potential field. Concept of Wiener path integral was expanded on relativistic case. A new path integral Monte-Carlo method was developed for relativistic particle in external potential field. This method was tested on one-dimensional model of relativistic harmonic oscillator. Average energy and heat capacity of the oscillator have been calculated in a wide region of temperature and “frequency”. The bounds of applicability of available analytical approaches and results have been specified by comparison with Monte Carlo calculations. In regions of applicability of these analytical approaches, the predicted results agree very well with Monte Carlo calculations. Developed path integral formalism can be directly extended on systems of many identic Newton–Wigner particles, which interact with external field and each other.

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