On Statistical Distribution for Adiabatically Isolated Body

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The statistical distribution for the case of an adiabatically isolated body was obtained in the framework of covariant quantum theory and Wick’s rotation in the complex time plane. The covariant formulation of the mechanics of an isolated system lies in the rejection of absolute time and the introduction of proper time as an independent dynamic variable. The equation of motion of proper time is the law of conservation of energy. In this case, the energy of an isolated system is an external parameter for the modified distribution instead of temperature.

I. INTRODUCTION

Statistical Boltzmann distribution with density

\[ f(q, p) = A \exp \left[ -\frac{H(q, p)}{k_B T} \right] \]  

for an adiabatically isolated body has an approximate character \[^1\]. It can be used to calculate the statistical characteristics of small subsystems of a macroscopic body, but when calculating such quantities as the total energy and its fluctuations, it leads to obviously incorrect results. Although the calculation errors in this case are not large compared to the quantities themselves and may not be taken into account in the macroscopic approximation, the search for an adequate replacement of distribution Eq. (1) for an adiabatically isolated body is of fundamental importance.

In this search, we use the formulation of the laws of statistics in quantum mechanics \[^2\],\[^3\] and the transparent analogy with quantum dynamics itself available here. It lies in the analogy between the parabolic equation for the density matrix,

\[ \frac{\partial \hat{\rho}}{\partial \beta} = -\hat{H} \hat{\rho}, \]  

where \( \beta = 1/k_B T \), and the Schrödinger equation for the evolution operator,

\[ i\hbar \frac{\partial \hat{U}}{\partial t} = \hat{H} \hat{U}. \]  

It can be seen that the evolution operator

\[ \hat{U} = \exp \left( \frac{1}{i\hbar} \hat{H} t \right) \]  

turns into a density operator (matrix) by a simple replacement

\[ t \rightarrow i\hbar \beta, \]  

i.e., as a result of the transition to imaginary time. In turn, the classical Boltzmann distribution Eq. (1) can be obtained from the mixed coordinate-momentum representation of the logarithm of the density operator due to the relation

\[ \beta H(q, p) = \beta \langle p | \hat{H} | q \rangle = -\langle p | \ln \hat{\rho} | q \rangle, \]  

which is valid if we agree to place the momentum operators in \( \hat{H} \) to the right of the coordinates. In \[^4\], the definition of the partition function of an adiabatically isolated body in the form of a trace of the density operator in the modified quantum theory was proposed. The modification consists in applying the rules of covariant quantization \[^5\] to a dynamical system with reparametrization time invariance. In such a system, proper time is naturally introduced as an additional dynamic variable. Its equation of motion is the law of conservation of energy of the system. In the transition to statistical mechanics, as a result of replacement Eq. (5), we obtain a modified partition function as a function of the energy of an isolated system. In this paper, we will go further in the modification of statistical mechanics, and using relation Eq. (6), we will determine the analogue of distribution Eq. (1) for an isolated body.

The first section formulates the dynamics of an isolated mechanical system in terms of proper time. The second section proposes a quantum version of the modified dynamics and a modified statistical distribution.

II. MECHANICS OF AN ISOLATED BODY

Mechanical laws can be formulated from the outset in a form that explicitly takes into account the complete isolation of the system under consideration from its environment. First of all, it concerns time. Instead of the...
absolute Newton time $t$, we introduce an arbitrary parameter $\tau \in [0, 1]$ and a new dynamic variable $s(\tau)$:

$$s(\tau) = \frac{dt}{d\tau}. \quad (7)$$

Accordingly, we write the action integral in the form

$$I \left[ q, \dot{q}, s \right] = \int_0^1 d\tau sL \left( q, \frac{\dot{q}}{s} \right). \quad (8)$$

Obviously, action Eq. (8) is invariant under an arbitrary change of the parameter $\tau$. The new dynamic variable $s(\tau)$ will play the role of the proper time of the system, if we take into account its equation of motion,

$$\frac{\delta I}{\delta s} = \frac{dW}{d\tau} = 0, \quad (9)$$

where

$$W \equiv \frac{\partial L (q, q')}{\partial q'} \dot{q}_k - L, \quad (10)$$

is the energy, $k = 1, 2, \ldots, K$, $K$ - number of degrees of freedom of the system. Here the prime denotes the derivative with respect to proper time. Indeed, as we know, the first integral of motion

$$W = E \quad (11)$$

allows you to determine your own time by the movement of dynamic variables $q_k(s)$. It remains only to fix the surface of constant energy Eq. (11) as an additional condition in the action integral:

$$\bar{L} (q, q') = L (q, q') + \lambda' W. \quad (12)$$

We have discarded the total derivative $\lambda' E$ in Eq. (12). Note that the arbitrariness in the choice of the parameter $\tau$ is now expressed in the arbitrariness of the interval of motion in proper time $s \in [0, C]$, which is removed only by the additional condition Eq. (11).

As a next step, we find the Hamilton function of the modified system. First, we define the canonical momenta:

$$\bar{p}_k = m_{kl} \dot{q}_l (1 - \lambda'), \quad (13)$$

$$\bar{p}_k = W = \frac{1}{2} m_{kl} \dot{q}_k \dot{q}_l + V (q), \quad (14)$$

where the stroke denotes the derivative with respect to proper time and we specified the form of the original Lagrange function:

$$L (q, \dot{q}) = \frac{1}{2} m_{kl} \dot{q}_k \dot{q}_l - V (q). \quad (15)$$

With the help of these equations we find speeds. At first,

$$q'_k = \frac{m_{kl} \dot{p}_l}{(1 - \lambda')}, \quad (16)$$

and then,

$$\lambda' = 1 - \frac{\sqrt{m_{kl} \dot{p}_k \dot{p}_l}}{\sqrt{2(E - V)}}, \quad (17)$$

where Eq. (11) is taken into account. After that, we find the modified Hamilton function:

$$\bar{H} = \sqrt{2(E - V)} \sqrt{m_{kl} \dot{p}_k \dot{p}_l} + E - 2V. \quad (18)$$

Thus, in modified mechanics, the proper time of motion of an isolated body is an indeterminate parameter (before solving the classical equations of motion), and the energy has a fixed value. The two-valued root in Eq. (18) corresponds to two half-cycles of the system’s motion between two cusps in the region of allowed classical motion. After quantization, a root from the elliptic operator will arise, which will need to be given meaning.

In the final step, after quantization, we return to absolute time by simply setting $s = t$. This is acceptable, since the dynamics of an isolated body can itself serve to measure the time $t$. There is no obstacle to this in the new dynamics. Indeed, setting $\bar{p}_k = p_k$, from Eq. (13) we obtain $\lambda' = 0$. Then relation Eq. (17) is equivalent to Eq. (11), and $\bar{H} = E$, as expected for an isolated system with energy $E$. In what follows, we will omit the "tilde" in the designation of canonical momenta.

### III. Statistical Distribution for an Isolated Body

For convenience, we set here $h = k_B = 1$. Let us represent the kernel of the evolution operator of the modified quantum theory as a functional integral on the phase space $[6]$:

$$D \equiv \langle q'' | q', 0 \rangle = \int \prod_s d\bar{q} \exp \left\{ i \int_0^C ds \left[ \bar{p}_k \dot{q}_k - \bar{H} (q, p, E) \right] \right\}. \quad (19)$$

The formal nature of the functional integral in Eq. (19) is aggravated by the presence of a root from the quadratic form of the momenta in the Hamiltonian. We make the
kernel more definite by turning the functional integral Eq. (19) into Gaussian over canonical momenta by introducing integrals over additional variables:

\[
D = \int \prod_s \frac{d^K p_d^K q}{(2\pi)^K} \int_{-\infty}^{+\infty} \prod_s \frac{d\chi}{2\chi (E-V)^{K/2}} \int_{-\infty}^{+\infty} \prod_s QdQ \exp \left\{ i \int_0^C ds \right. \\
\left. - Q + \chi \left( 2(E-V) m^{-1}_{kl} \tilde{p}_k \tilde{p}_l - Q^2 \right) \right\}.
\]

(20)

It is easy to see that integration first over the variable \( \chi \) and then over the variable \( Q^2 \) leads to the original integral Eq. (19). However, now integration over canonical momenta can be done in the first place, and this will be the definition of the square root of the kinetic energy in the modified quantum theory. In order to avoid cumbersome expressions, we agree in what follows to omit numerical factors of type \( 2^\pi \). As a result, we get

\[
D \approx \int \prod_s \frac{d^K q}{\sqrt{E-V}} \Delta [W-E] \exp \left[ i \int_0^C ds (E-2V) \right].
\]

(22)

Here

\[
\Delta [W-E] \equiv \text{Re} \int_0^\infty \prod_s (i\eta)^{(K-1)/2} d\eta \times \exp \left[ i \int_0^C ds \frac{\eta}{4} \left( \frac{1}{2} m^2_{kl} q_k' q_l' + V - E \right) \right].
\]

(23)

where \( \eta = 1/\chi (E-V) \) is the new integration variable. As expected, functional Eq. (23) limits integral Eq. (22) to trajectories that lie entirely on the surface of constant energy \( E \). For such trajectories, the exponent under the integral sign in Eq. (22) exactly coincides with the initial action of the system.

Thus, the presence of the square root of the quadratic pulse shape in the modified Hamilton function Eq. (18) is the source of the generalized \( \delta \)-function Eq. (23) in the modified propagator Eq. (22). This is just what is needed to solve another problem of covariant quantum theory, the problem of time \( C \). A similar problem of determining the propagator of a relativistic particle within the framework of the rules of covariant quantum theory \( 8 \) is completed by additional integration over proper time within \( 0 \leq C < \infty \) with the trivial measure \( \mu = 1 \).

In our problem, the proper time on an arbitrary trajectory \( q(s) \) is determined two-valued by two directions of motion, so we should integrate along the full axis \(-\infty < C < \infty \). It should be borne in mind that the time of movement on the trajectory \( q(s) \) is a functional of the trajectory: \( C = C[q(s)] \). Therefore, an additional integral over proper time in the propagator should be placed before the final summation over all admissible trajectories.

Now the purpose of the proposed modification of mechanics is clear: the generalized \( \delta \)-function Eq. (23) will allow removing additional integration over proper time in covariant quantum theory and giving the propagator a dynamic meaning, and after the transition to imaginary proper time, a statistical meaning to the density matrix. The resulting proper time, and in statistical mechanics, the reciprocal temperature of an adiabatically isolated body is random variable in this theory. Thus, we obtain the following representation of the density matrix of an adiabatically isolated body:

\[
\tilde{\rho}(q'', q') = \int \prod_s \frac{d^K q}{\sqrt{V-E}} \times \int_{-\infty}^{+\infty} dC \Delta \left[ V - \frac{1}{2} m^2_{kl} q_k' q_l' - E \right] \\
\times \exp \left[ - \int_0^C ds (E-2V) \right].
\]

(24)

From the quantum mechanical density matrix Eq. (24), we proceed to the modification of the classical Boltzmann distribution Eq. (1) for an adiabatically isolated body using relation Eq. (6):

\[
\tilde{f}(q, p, E) = A \exp \left[ B(q, p, E) \right],
\]

(25)

where

\[
B(q, p, E) = \langle q | \ln \tilde{\rho} | p \rangle.
\]

(26)

IV. CONCLUSIONS

Thus, the statistical distribution for an adiabatically isolated body is defined within the framework of the formalism of reparameterization invariant mechanics and the corresponding covariant quantization procedure. The indeterminate proper time parameter arising in this formalism also plays the role of an indefinite body temperature in modified statistical mechanics. This is how it should be in a system that is devoid of contact with the
environment and whose energy is fixed. It must also be assumed that the nominal distribution Eq. (25) in accordance with the ergodic hypothesis [9] describes the relative time that the system spends in the vicinity of the point \((q_k, p_k)\) of the phase space when moving on the surface of constant energy \(E\).

Distribution Eq. (25) can only be used for a macroscopic body with a large amount of mechanical energy. In this case, the continuous law of conservation of mechanical energy Eq. (9) is obviously substantiated in quantum theory in the semiclassical approximation. At the same time, the modification of the classical statistical distribution proposed here is justified.

The next step for studying the statistics of an isolated system is the calculation of the distribution density Eq. (25) for the simplest system - an ensemble of harmonic oscillators. This will be the subject of subsequent works.

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