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Wave Functional of the Universe and Time

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Abstract: A version of the quantum theory of gravity based on the concept of the wave functional of the universe is proposed. To determine the physical wave functional, the quantum principle of least action is formulated as a secular equation for the corresponding action operator. Its solution, the wave functional, is an invariant of general covariant transformations of spacetime. In the new formulation, the history of the evolution of the universe is described in terms of coordinate time together with arbitrary lapse and shift functions, which makes this description close to the formulation of the principle of general covariance in the classical theory of Einstein's gravity. In the new formulation of quantum theory, an invariant parameter of the evolutionary time of the universe is defined, which is a generalization of the classical geodesic time measured by a standard clock along time-like geodesics.

Keywords: universe; wave functional; time

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Citation: Gorobey, N.; Lukyanenko, A.; Goltsev, A.V. Wave Functional of the Universe and Time. *Universe* **2021**, *7*, 452. https://doi.org/10.3390/universe7110452

Academic Editors: Stefano Bellucci and Sergei D. Odintsov

Received: 27 October 2021
Accepted: 17 November 2021
Published: 19 November 2021

1. Introduction

The idea of universe expansion, originated at the Big Bang, is widely accepted today, being well founded on clear observational evidence. Arising as a result of solving the equations of Einstein's general theory of relativity (GR), it is the highest achievement of classical (i.e., pre-quantum) physics. At the same time, the basic principles of quantum theory were formulated as applied to atoms and molecules, and their spread to the level of the universe as a whole was inevitable. Dirac laid the foundation for the synthesis of relativistic and quantum principles with his exhaustive analysis of the canonical representation of dynamical theories with singular Lagrangian functions and their quantization [1]. When applied to general relativity, this leads to the modern quantum theory of gravity (QTG) with the Wheeler–DeWitt (WDW) system of equations [2,3] for the wave function of the universe. This theory is based on the canonical representation of the action of general relativity, obtained by Arnovitt, Deser and Misner (ADM; see [4]):

$$I_{ADM} = \int dt \int_{\Sigma} d^3x \left(\dot{g}_{ik} \pi^{ik} - N\mathcal{H} - N_i \mathcal{H}^i \right) \tag{1}$$

(for the case of a closed universe), where the three-dimensional integral is taken over the $3D$ spatial section Σ with the metric tensor g_{ik}, π^{ik} is the momentum canonically conjugate to the metric, N, N_i are arbitrary lapse and shift functions that play the role of Lagrange multipliers, and

$$\mathcal{H}\left(\pi^{ik}, g_{ik}\right) = \frac{1}{\sqrt{g}}\left[Tr\pi^2 - (Tr\pi)^2\right] - \sqrt{g}R, \tag{2}$$

$$\mathcal{H}^i = -2\pi^{ik}_{|k} \tag{3}$$

are Hamiltonian and momentum constraints. In this paper, we use the notations from [4]. In this work, we do not take into account the contribution of the matter fields. Taking it into account does not change the main results of the work. The ADM representation is obtained using the $3+1$-splitting of the $4D$ metric as follows:

$$ds^2 = g_{ik}\left(dx^i + N^i dt\right)\left(dx^k + N^k dt\right) - (Ndt)^2. \tag{4}$$

The shift functions are found by dropping the vector index of the components N^k of the metric $N_i = g_{ik}N^k$. Thus, the Hamilton function in the case of a closed universe is reduced to a linear combination of constraints, Equations (2) and (3), which in the classical theory should be equated to zero as a consequence of the extremum of action (Equation (1)) with respect to N and N_i. Dirac's main conclusion is that constraints (their quantum analogs) should also vanish in quantum theory. More precisely, we arrive at the system of WDW wave equations

$$\widehat{\mathcal{H}}\psi = \widehat{\mathcal{H}}^i\psi = 0. \tag{5}$$

for the wave function of the universe ψ, which ensure its independence from arbitrary parameters N and N_i, including any external coordinate parameter of time. The constraint operators are obtained by substituting the canonical momenta in Equations (2) and (3) to the corresponding differentiation operators as follows:

$$\widehat{\pi}^{ik}(x) = \frac{\hbar}{i}\frac{\delta}{\delta g_{ik}(x)}. \tag{6}$$

We do not discuss here the problem of ordering non-commuting factors.

Since the wave function of the universe does not depend on any external time parameter, the problem arises of its dynamic interpretation in terms of the fundamental dynamic variables g_{ik} (and matter fields). This problem was solved by Hartle and Hawking, using the representation of the wave function in the form of a Euclidean functional integral [5] (no-boundary wave function). This integral includes integration over the lapse function N, and in fact, over the parameter of the proper time of the universe, defined as the following integral:

$$c = \int Ndt. \tag{7}$$

Thus, the wave function is also independent of the proper time Equation (7). Hartle, Hawking, and Hertog [6,7] obtained a classical picture of an expanding universe with a scalar field within the framework of the semiclassical approximation for a functional integral, in which the proper time (Equation (7)) takes on the meaning of an evolution parameter. In subsequent works [8], the authors abandon the representation of the wave function by a functional integral, formulating the semiclassical approximation directly for the WDW equation. In [9], a modification of the quantization procedure and functional integral is proposed, in which the (multi-arrow) proper time, without any approximations, acquires the meaning of an evolution parameter. Together with its proper time, a set of additional parameters is introduced into the theory, which forms the distribution of the own mass of the universe. However, these constructions cannot get around the source of the time problem in modern QTG: in correspondence with the physical state of the universe, its Hamiltonian is zero. Thus, the implementation of the principle of general covariance in QTG, proposed by Dirac, leads to the emergence of the problem of time.

In this paper, a version of QTG is proposed, in which the action functional Equation (1) becomes an operator in the space of wave functionals defined on the $4D$ spacetime geometries $g_{\mu\nu}$ (and matter fields). Thus, arbitrary lapse and shift functions N and N_i are also included in this dependence, which ensures the general covariance of the theory—the wave functional corresponding to the physical histories of the evolution of the universe should be an invariant of arbitrary transformations of spacetime coordinates. The quantum principle of least action (QPLA) is formulated, according to which the quantum state of the evolution of the universe is determined by the eigenwave functionals of the action operator, which also depend on the boundary data on the initial and final $3D$ spatial sections Σ. The eigenwave functional has the meaning of the probability density for different trajectories of the evolution of the universe in terms of the internal (coordinate time) between fixed boundary spatial sections. Comparing the new formulation with the standard QTG based on WDW, we note that in the classical general relativity, constraints are integrals of motion. In the same way, we regard canonical quantum gravity based on the WDW equations as a kind of integral form of quantum theory based on the quantum principle of least action.

In Section 2, QPLA is obtained in nonrelativistic quantum mechanics as a formulation of quantum dynamics, equivalent to the Schrõdinger equation. A formulation of the QPLA in the theory of gravity is proposed. In Section 3, an invariant measure on the space of $4D$ geometries is introduced, and the probabilistic interpretation of the wave functional is proposed. In Section 4, based on the probabilistic interpretation of the wave functional, the mean proper time of evolution of the universe between fixed boundary spatial sections is determined. By definition, this time is an invariant of general covariant transformations.

2. Quantum Principle of Least Action in Nonrelativistic Mechanics

To formulate new rules for quantizing the theory of gravity, let us consider the transition to QPLA in ordinary quantum mechanics, where there is no problem of time. It suffices to consider the simplest system with one degree of freedom (particle) described by the Hamiltonian (we assume $m = 1$) as follows:

$$H = \frac{p^2}{2} + U(q,t) \tag{8}$$

In ordinary quantization, canonical variables are replaced by operators (in coordinate representation) as follows:

$$\widehat{q} \equiv q, \quad \widehat{p} \equiv \frac{\hbar}{i}\frac{\partial}{\partial q}, \tag{9}$$

which act in the space of wave functions $\psi(q,t)$. The wave function completely defines the state of the particle at time t. The evolution of a state in time is described by the Schrödinger equation as follows:

$$i\hbar\frac{\partial\psi}{\partial t} = \widehat{H}\psi. \tag{10}$$

where

$$\widehat{H} = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2} + U(q,t) \tag{11}$$

is the Hamilton operator.

To change the quantization rules, let us look at the classical canonical form of this theory from a different angle: we consider the trajectory of the particle $q(t)$ as a whole, together with the corresponding function $p(t)$, as a complete set of canonical variables, enumerated by a continuous parameter t [10]. Both of these functions are still found for given boundary values from the condition for the extremum of the action in the canonical form as follows:

$$I = \int_0^T dt\Big[\dot{q}p - H(q,p,t)\Big]. \tag{12}$$

Let us formulate new quantization rules directly for action (Equation (12)) as a functional of the mentioned continuous set of canonical variables. Now, one should expect that the state of the system, instead of the wave function $\psi(q,t)$ given at each time instant, is described by the wave functional $\Psi[q(t)]$, which depends on the entire trajectory. Accordingly, we implement the generalized canonical variables by the following operators:

$$\widehat{q}(t) \equiv q(t), \quad \widehat{p}(t) \equiv \frac{\widetilde{\hbar}}{i}\frac{\delta}{\delta q(t)}, \tag{13}$$

acting in the space of wave functionals. Here, $\widetilde{\hbar}$ is the "generalized" Planck constant, which differs from the "usual" dimension: $[\widetilde{\hbar}]$ = J· sec^2 . This follows from the fact that the variational derivative, according to its definition,

$$\delta\Psi = \int_0^T dt \frac{\delta\Psi}{\delta q(t)} \delta q(t), \tag{14}$$

has a dimension that differs from the dimension of the ordinary partial derivative with respect to the coordinate by exactly the factor sec^{-1} [11]. We write the following:

$$\widetilde{\hbar} = \hbar \cdot \varepsilon, \tag{15}$$

where ε is some value of the dimension of time. The new implementation of generalized canonical variables allows, after substituting them in Equation (12), to define the action operator on the space of wave functionals as follows:

$$\widehat{I} = \int_0^T dt \left[\frac{\widetilde{\hbar}}{i} \dot{q}(t) \frac{\delta}{\delta q(t)} + \frac{\widetilde{\hbar}^2}{2} \frac{\delta^2}{\delta q^2(t)} - U(q(t), t) \right]. \tag{16}$$

Using this operator, we formulate the basic law of motion of a particle in quantum mechanics instead of Schrödinger's equation (Equation (10)) as follows. The physical state of motion of a particle is described by an eigenfunctional for the action operator (Equation (16)) as follows:

$$\widehat{I}\Psi = \Lambda\Psi, \tag{17}$$

where Λ is the corresponding eigenvalue. This quantity, by definition, does not depend on the specific trajectory $q(t)$, except for its boundary points $q_0 = q(0)$ and $q_T = q(T)$. This statement is called the quantum principle of least action.

Let us show that a consequence of the QPLA for the simplest theory considered here is the Schrödinger equation (Equation (10)). The correspondence is established for some singular family of wave functionals in the limit $\varepsilon \to 0$. We define this family as follows. Any trajectory $q(t)$ can be approximated by a broken line. For this, we divide the time interval $[0, T]$ into small intervals of length $\varepsilon = T/N$ by points $t_n = n\varepsilon$. Take a broken line with vertices $q_n = q(t_n)$, which is an approximation of the trajectory $q(t)$ and coincides with it in the limit $\varepsilon \to 0$. Let $\psi(q, t)$ be some wave function. Consider the function of the vertices of the polyline as follows:

$$\Psi(q_n) = \prod_{n=0}^{N} \psi(q_n, t_n). \tag{18}$$

In the limit $N \to \infty$, we obtain the trajectory functional $\Psi[q(t)]$. We write the wave function in an exponential form as follows:

$$\psi(q, t) = \exp\left[\frac{i}{\hbar} R(q, t)\right], \tag{19}$$

where $R(q, t)$ is some complex function. Then Equation (18) can be represented as follows:

$$\Psi(q_n) = \exp\left[\frac{i}{\hbar\varepsilon} \sum_{n=0}^{N} \varepsilon R(q_n, t_n)\right]. \tag{20}$$

In the limit $\varepsilon \to 0$, we obtain the wave functional of the exponential form as follows:

$$\Psi[q(t)] = \exp\left[\frac{i}{\widetilde{\hbar}} \int_0^T dt R(q(t), t)\right], \tag{21}$$

in which, however, the infinitely small quantity ε is explicitly present. This is the singularity of the considered class of wave functionals. Nevertheless, the operator of action Equation (16) on this class of functionals is defined insofar as it also contains this infinitesimal quantity and their mutual cancellation will occur.

Consider the expression

$$\Lambda = \frac{\widehat{I}\Psi}{\Psi} \tag{22}$$

on an arbitrary trajectory $q(t)$ with given boundary points and find a condition under which it does not depend on the interior points of this trajectory. The first term in the action operator Equation (16) gives the following contribution to Equation (22):

$$\begin{aligned}\int_0^T dt\dot{q}(t)\frac{\partial R(q(t),t)}{\partial q} &= R(q_T,T) - R(q_0,0) \\ &\quad - \int_0^T dt\frac{\partial R(q(t),t)}{\partial t}.\end{aligned} \tag{23}$$

The second term in Equation (16) requires more attention. Its calculation rests on the following expression:

$$\frac{1}{2}\int_0^T dt\left[-\left(\frac{\partial R(q(t),t)}{\partial q}\right)^2 + i\widetilde{\hbar}\frac{\delta\partial R(q(t),t)}{\delta q(t)\partial q}\right]. \tag{24}$$

Here the second term is determined if we take into account the following:

$$\frac{\delta}{\delta q(t)}q(t) = \frac{\delta}{\delta q(t)}\int_0^T dt'\delta(t-t')q(t') = \delta(0) = \frac{1}{\varepsilon} \tag{25}$$

as $\varepsilon \to 0$ (more precisely, on an interval of length ε of our partition of the time interval $[0, T]$). Then, taking into account Equation (15), the second term is equal to the following:

$$\frac{1}{2}\int_0^T dti\hbar\frac{\partial^2 R(q(t),t)}{\partial q^2} \tag{26}$$

Putting everything together (including the contribution of the third term in Equation (16), we obtain the following:

$$\begin{aligned}\Lambda &= R(q_T,T) - R(q_0,0) \\ &\quad + \int_0^T dt\left[-\frac{\partial R(q(t),t)}{\partial t} - \frac{1}{2}\left(\frac{\partial R(q(t),t)}{\partial q}\right)^2\right. \\ &\quad \left. + \frac{i\hbar}{2}\frac{\partial^2 R(q(t),t)}{\partial q^2} - U(q(t),t)\right]\end{aligned} \tag{27}$$

It is easy to verify that if the wave function (Equation (19)) is a solution to the Schrödinger equation (Equation (10)), the integral in Equation (27) is equal to zero for any trajectory $q(t)$, and Λ depends only on the boundary points of this trajectory. Thus, singular exponential wave functionals in the form of Equation (21) satisfy the QPLA (Equation (17)) if the wave function (Equation (19)) is a solution to the Schrödinger equation (Equation (10)).

The probabilistic interpretation of the wave functional $\Psi[q(t)]$ follows from the probabilistic interpretation of the wave function: it determines the probability of a particle moving along trajectories from a small neighborhood $q(t)$ (more precisely, it represents the probability of locating the particle in a succession of T/ε measurements of the position near the assigned points $q(n\varepsilon)$, with $n = 1, ..., T/\varepsilon$) by the formula

$$dP[q(t)] = |\Psi[q(t)]|^2 \prod_t dq(t) \tag{28}$$

under the following appropriate normalization condition:

$$\int |\Psi[q(t)]|^2 \prod_t dq(t) = 1. \tag{29}$$

3. Quantum Principle of Least Action in the Theory of Gravity

We can transfer all the previous constructions in full to the QTG, taking as the initial the canonical form of the ADM action (Equation (1)). As a complete set of canonical variables, we now consider the trajectories of motion in time of the 3D geometry and the corresponding canonical momentum $\left(g_{ik}(x,t), \pi^{ik}(x,t)\right)$ as a whole. Thus, time, along with the spatial coordinates, now plays the role of a numbering index. The lapse and shift functions N and N_i remain arbitrary functions of spacetime coordinates. Accordingly, we introduce another operator realization of canonical momenta in quantum theory in the form of partial variational derivatives with respect to time

$$\widehat{\pi}^{ik}(x,t) = \frac{\widetilde{\hbar}}{i} \frac{\delta}{\delta_0 g_{ik}(x,t)} \tag{30}$$

in the space of wave functionals $\Psi[g_{ik}(x,t)]$. The partial variational derivative in Equation (30) is defined as follows:

$$\delta\Psi = \int_0^T dt \int_\Sigma d^3x \frac{\delta\Psi}{\delta_0 g_{ik}(x,t)} \delta g_{ik}(x,t). \tag{31}$$

Spatial coordinates in this definition play the role of numbering indices. Operators of momenta of matter fields are realized in a similar way. For comparison, we recall that in the generally accepted implementation of QTG, the wave function of the universe ψ is actually the functional of the $3D$ metric $g_{ik}(x)$ (and matter fields) on the spatial section Σ, and the variational derivative is determined by the following relation:

$$\delta\psi = \int_\Sigma d^3x \frac{\delta\psi}{\delta_0 g_{ik}(x)} \delta g_{ik}(x). \tag{32}$$

In such an implementation, modification (Equation (15)) of the Planck constant is not required. Substituting the operators of momenta (Equation (30)) into action (Equation (1)), we obtain the operator of the action of the ADM in the modified QTG as follows:

$$\widehat{I}_{ADM} = \int dt \int_\Sigma d^3x \left(\dot{g}_{ik}\widehat{\pi}^{ik} - N\widehat{\mathcal{H}} - N_i\widehat{\mathcal{H}}^i\right), \tag{33}$$

where, as we agreed, the momentum operators (Equation (30)) in all expressions are on the right. Now, let us formulate the quantum principle of least action in the theory of gravity as a spectral problem for the action operator:

$$\widehat{I}_{ADM}\Psi = \Lambda_{ADM}\Psi. \tag{34}$$

Here, the eigenvalue Λ_{ADM} is a (complex) function of $3D$ geometries g^0_{ik}, g^T_{ik} on two boundary spatial sections Σ_0, Σ_T of $4D$ Lorentz spacetime. The eigenvector—the wave functional Ψ—depends on all components of the $4D$ spacetime metric between the boundary spatial sections, including arbitrary Lagrange multipliers N and N_i. The desired wave functional $\Psi\left[g_{\mu\nu}(x,t)\right]$, which describes the physical history of the evolution of the universe, must be an invariant of general covariant transformations, and this is ensured by its dependence on N and N_i.

4. Interpretation of the Wave Functional of the Universe and Time

As it should be in quantum theory, the wave functional describes the evolution of the universe in a probabilistic way. However, this description must be covariant. Since the wave functional itself is an invariant, one should also introduce an invariant measure of integration on the set of $4D$ spacetime geometries between the given boundary spatial sections Σ_0, Σ_T. Such a measure was constructed in the works of Faddeev and Popov [12,13], and here we use the ready result:

$$\begin{aligned} d\mu_{FP}[g_{\mu\nu}] &= \Delta_h[g_{\mu\nu}] \times \\ &\times \prod_x \left(\prod_\beta \delta\left(\partial_\alpha\left(\sqrt{-g} g^{\alpha\beta}\right)\right) \times \right. \\ &\left. \times (-g)^{\frac{5}{2}} \prod_{\mu \leqslant \nu} dg^{\mu\nu} \right), \end{aligned} \tag{35}$$

where additional gauge harmonicity conditions are used, and $\Delta_h[g_{\mu\nu}]$ is the corresponding Faddeev–Popov determinant. Thus, the probability that the universe evolved in a small neighborhood of a given $4D$ spacetime geometry $g_{\mu\nu}(x,t)$ is given by the following expression:

$$dP[g_{\mu\nu}(x,t)] = \left|\Psi[g_{\mu\nu}(x,t)]\right|^2 d\mu_{FP}[g_{\mu\nu}(x,t)] \tag{36}$$

with the following additional normalization condition:

$$\int \left|\Psi[g_{\mu\nu}(x,t)]\right|^2 d\mu_{FP}[g_{\mu\nu}(x,t)] = 1. \tag{37}$$

Now we can answer the question: what physical (invariant) time separates the boundary spatial sections Σ_0, Σ_T? Here the parameter T is an arbitrary coordinate time, which is fixed by us for convenience. As a physical measure of time between two spatial sections, it is natural to take geodesic time, measured by a clock moving along a time-like geodesic. More precisely, in a given $4D$ spacetime geometry $g_{\mu\nu}(x,t)$, we take a family of geodesics orthogonal to the initial spatial section Σ_0 and calculate the average over this family (integral over Σ_0) of the geodesic distance between the boundary spatial sections Σ_0, Σ_T as follows:

$$\left\langle \int_{\Sigma_0}^{\Sigma_T} \sqrt{-g_{\mu\nu} dx^\mu dx^\nu} \right\rangle_{\Sigma_0}. \tag{38}$$

Now this value should be averaged over all possible $4D$ spacetime geometries between the given boundary spatial sections Σ_0, Σ_T as follows:

$$S = \int \left\langle \int_{\Sigma_0}^{\Sigma_T} \sqrt{-g_{\mu\nu} dx^\mu dx^\nu} \right\rangle_{\Sigma_0} d\mu_{FP}[g_{\mu\nu}]. \tag{39}$$

Integral Equation (39) gives the mathematical expectation for the proper time between two boundary states of the universe on the spatial sections Σ_0, Σ_T.

The construction proposed here also allows one to determine an analog of the no-boundary of the Hartle and Hawking wave function. To do this, one should go to the Euclidean form of the action of ADM, Equation (1), and QPLA, Equation (34). The transition to the Euclidean $4D$ metric in the representation of Equation (4) is achieved by a simple replacement:

$$N \longrightarrow iN. \tag{40}$$

The canonical momentum of the $3D$ ADM metric, according to its definition (see [4]), changes as follows: $\pi \to -i\pi$. As a result, the canonical action of ADM is transformed into the Euclidean form: $I_{ADM} \longrightarrow -iI^{E}_{ADM}$. In the Euclidean form of QPLA, one can search for a solution in the form of a real wave functional defined on $4D$ Euclidean geometries with one boundary spatial section or no boundaries at all. The return to the Lorentzian signature of the $4D$ metric is carried out in the found solution by rotating in the N complex plane (where possible), inverse to Equation (40).

In conclusion, we note that the singular character of the QPLA in this formulation, which assumes the passage to the limit $\varepsilon \to 0$ in Equation (15), admits regularization by adding to the Hilbert–Einstein action with the Lagrange function $-1/\varkappa^2\sqrt{-g}R$ the square of scalar curvature (the theory with the Lagrangian function $-1/\varkappa^2 R + \sigma^2 R^2$). In this theory, the Lagrange function contains second-order derivatives of the metric. Its canonical analysis and standard quantization are carried out in [14] based on the approach developed by Ostrogradsky for theories with higher derivatives [15]. The modified Lagrange function contains an additional dimensional parameter $\varkappa\sigma$, which serves as a measure of the theory's nonlocality. Within the framework of the approach proposed in this paper to the formulation of the QPLA, the nonlocality of the dynamics does not prevent the possibility of determining the set of generalized canonical variables formed by their values at all times. In this case, the canonical momenta conjugate to the metric $g_{ik}(x,t)$ should be defined as the variational derivatives of the action with respect to the velocities $\dot{g}_{ik}(x,t)$. The resulting canonical action are nonlocal, and in the QPLA formulation, the modified Planck constant should be set equal to the following:

$$\widetilde{\hbar} = \hbar \cdot \varkappa\sigma. \tag{41}$$

In the limit $\sigma \to 0$, we return to the original singular form of the QPLA.

5. Conclusions

The wave function in the generally accepted QTG, if we follow the canonical structure of the ADM action (Equation (1)), describes the state of the universe at a particular moment of coordinate time. However, the formulation of the principle of general covariance in quantum theory, according to Dirac, requires the removal of this time parameter from consideration as being non-physical. This is achieved by the conditions for the vanishing of quantum constraints. In this case, the wave function contains information about the history of the evolution of the universe only in integral form in its phase. Recovery of this information is possible in the semiclassical approximation, and this procedure is called the holographic principle in [7,8]. The introduction of the wave functional, which is an atlas of the history of the universe in coordinate time, allows us to speak about this history explicitly. QPLA allows one to define a solution that is invariant with respect to general covariant transformations. Thus, an alternative embodiment of the principle of general covariance in the quantum theory of gravity is proposed, which includes coordinate time together with arbitrary lapse and shift functions. This implementation is close to its formulation in the classical GR theory of Einstein. This makes it possible to determine in the quantum theory the invariant parameter of the evolutionary time of the universe, which generalizes the concept of proper time measured along time-like geodesics.

In this paper, we do not discuss the nonlocal version of the theory of gravity associated with the addition of terms that are quadratic in curvature. The probabilistic interpretation of the wave functional in the nonlocal theory requires more attention. In the case of the nonlocal modification of the theory of gravity, a connection between the time of nonlocality and the scale of energies in the universe takes place. However, this is the subject of a separate study.

Author Contributions: Investigation, N.G. and A.L.; Draft review and editing, N.G., A.L. and A.V.G. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data sharing not applicable.

Acknowledgments: We would like to thank V.A. Franke for the useful discussions.

Conflicts of Interest: The authors declare no conflict of interest.

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