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Measures of Distance in Quantum Mechanics

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Abstract: Combining gravity with quantum theory is still a work in progress. On the one hand, classical gravity is the geometry of space-time determined by the energy–momentum tensor of matter and the resulting nonlinear equations; on the other hand, the mathematical description of a quantum system is Hilbert space with linear equations describing evolution. In this paper, various measures in Hilbert space will be presented. In general, distance measures in Hilbert space can be divided into measures determined by energy and measures determined by entropy. Entropy measures determine quasi-distance because they do not satisfy all the axioms defining distance. Finding a general rule to determine such a measure unambiguously seems to be fundamental.

Keywords: relative entropy; space of metric; distances in Hilbert space

1. Introduction

What defines a metric, that is, a way to measure distances on a given manifold? In the case of classical physics, i.e., non-quantum physics, the answer is provided by the general of relativity (GR). Metrics are determined by the distribution of masses and currents of matter. The modern approach to this problem began with Clifford's work [1] in 1876. Thirty-nine years later, Einstein gave the solution in the form of the general theory of relativity.

The concept of a metric is a basic one and it enters almost every equation of physics. For example, in order to define one of the basic physics operators, the Laplace operator, it is necessary to first determine a metric.

In the case of quantum physics whose states are defined in Hilbert space, there is no such single measure of distance. On the contrary, there are many measures of distance between states, some used in quantum information theory (also applied in research related to quantum gravity, see, e.g., [2]) but none of them follow from some fundamental principle. Since Hilbert space is a vector complex space, one can introduce a metric that is induced from C^N and call this metric canonical. This gives, as a result, the Fubini-Study (FS) metric; this can be used as a basis to determine the distance. In the case when Hilbert space is represented by square-integrable functions $L^2(M)$ on some manifold M, then the scalar product on this Hilbert space is given by the volume form $d\mu$ on M. Again, this scalar product leads to the FS metric. For both finite N and for $L^2(M)$, the largest distance between the points of these Hilbert spaces is normalized to π. However, such a canonical metric does not represent the complexity of the quantum system. Nevertheless, as is well known, the probabilistic interpretation of the quantum system is based on this metric.

Another issue is the geometrization of thermodynamics. There are such metrics as the Weinhold metric or Ruppeiner metric, where the relationship between them is found. However, also in this case, none of the metrics are derived from some fundamental equation. Since the thermodynamics of black holes are widely studied and constitue a well-known topic, the combination of the geometrization of thermodynamics and black holes seems promising. Many papers have been written on this topic, e.g., [3–5].

The fundamental classical concept describing a physical system is the action integral. The energy–momentum tensor of a system results as a variation of the action integral

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with respect to a metric. The general relativity links the energy–momentum tensor to the geometric properties of space-time, i.e., the Riemann tensor. In contrast, the quantum concept describing the system is the density matrix. And there is no theory or relationship that links the density matrix to the quantum properties of space-time, because such concepts do not exist. One may ask: are there any hints in existing theories that would provide such ideas?

A first such hint may be the concept of entropy determined by the density matrix. One should look for an extension of the concept of entropy in way analogous to how energy density and momentum density combine in the energy–momentum tensor.

A second such hint is geometrodynamics [6]. One way to find a quantum theory of gravity is to try to quantize the general theory of relativity using canonical quantization. In this approach, the Wheeler–DeWitt (WDW) equation plays a fundamental role. Many interesting results have been obtained following this way of reasoning, e.g., [7–9]. So, the concepts that allow us to describe quantum space-time should be obtained in the framework of geometrodynamics from the WDW equation. Although this is not a work on quantum gravity (QG), and is only an attempt to find an analogy of the equivalence principle in quantum mechanics, we will mention the two most common and fruitful approaches to the issue of QM as a metric theory, the canonical and covariant approaches. In the 1960s, De Witt presented attempts to quantize the gravitational field in canonical and covariant approaches [10–12]. Since then, much has been understood and achieved but many problems remain.The actual question is whether these approaches are equivalent or not, namely whether or not they possibly represent a single formal theory. Otherwise, the issue should be that of finding out which of them, if any—simply on the basis of general physical principles—may appear as the correct one. Regarding the possible alternative routes to QG theory, covariant quantization should provide hints to the considered problem. The literature on the covariant quantization of gravity is vast, so the authors will cite only two: one [13] and another that is a new approach to the Hamiltonian formulation of gravity [14,15].

Moreover, in quantum field theory in curved space-time (the zero approximation of quantum gravity), the problem of determining the vacuum state of the field arises. There are many vacuum states which are not unitary-related. For example, in the Schwarzschild space-time with a free scalar field, there are three well-known vacuum states: Hartle–Hawking, Boulware and Unruh. Each of these gives different expectation values of the field operators [16]. Another example is de Sitter spacetime with families of vacua states of a quantum scalar field [17]. So, the natural question pertains to the relationship between such states. A good measure to determine these relationships is the distance between them.

In this paper, we propose a metric in a general case of a Hilbert space of a quantum mechanical system. This metric is an infinitely dimensional version of the Fisher–Rao metric on an infinitely dimensional sphere S^∞. We apply such a metric for the simplest quantum systems: a free particle and harmonic oscillator. The "distance" given by the relative entropy is derived and calculated for different quantum systems.

This study is organized as follows. In Section 2, we recall how the distance is determined in classical physics. In Section 3, the metrics in the space of probability distributions are presented and the Fisher–Rao (FR) metric is derived as a condition for the stationarity of the "action integral". In Section 4, we give the metric in the Hilbert space of a quantum mechanical system. In Section 5, we find the FR metrics in the case of a free particle and harmonic oscillator. In Section 6, we present and calculate the "distance" given by the relative entropy. Section 7 is devoted to the conclusions.

2. Measure of the Distance in Space-Time

To determine the distance in space-time M with fixed symmetry and the matter with a given energy–momentum tensor $T_{\mu\nu}$, it is necessary to solve Einstein's equations:

$$G_{\mu\nu}(g) = 16\pi T_{\mu\nu}(g) \tag{1}$$

that is, to determine the metric field g where $G_{\mu\nu}$ is the Einstein tensor. This is a nontrivial task and there are few exact solutions. From the metric "g" obtained in this way, it is necessary to find the line (one-dimensional submanifold) γ along which the distance will be measured. The line γ is parameterized by the affine parameter "s":

$$\gamma = \{x \in M : \; x = x(s)\} \tag{2}$$

and "x"s are coordinates on M. The equation of such a line is found from the stationarity of the functional:

$$\delta L = 0,$$

where

$$L[\gamma] = \frac{1}{2}\int_{s_1}^{s_2} g_{\mu\nu}(x)\frac{dx^\nu}{ds}\frac{dx^\nu}{ds}ds \tag{3}$$

with the fixed boundary points: $x_1 = x(s_1)$ and $x_2 = x(s_2)$. This leads to the geodesic equation:

$$\frac{d^2x^\mu}{ds^2} + \Gamma^\mu_{\nu\rho}\frac{dx^\nu}{ds}\frac{dx^\rho}{ds} = 0, \tag{4}$$

with the *boundary* conditions $x_1 = x(s_1)$ and $x_2 = x(s_2)$. In order to solve this equation in an unambiguous way, it is necessary to give *initial* conditions:

$$x(s_1) = x_1 \;\text{ and }\; \left.\frac{dx}{ds}\right|_{s=s_1} = \dot{x}_1. \tag{5}$$

Thus, one has to express these initial conditions by the boundary conditions. The expression of boundary conditions by initial conditions is unambiguous when the points x_1 and x_2 are "close". The expression "close" means that x_1 and x_2 are not conjugate. Finally, the distance d between points x_1 and x_2 is given by the integral:

$$0 < d(x_1, x_2) = \int_{s_1}^{s_2} \sqrt{\left|g_{\mu\nu}\frac{dx^\nu}{ds}\frac{dx^\nu}{ds}\right|}ds. \tag{6}$$

Since the metric g at each point has a signature $(-,+,+,+)$, there are spatial-like $d^2(x_1, x_2) > 0$, time-like $d^2(x_1, x_2) < 0$ and light-like $d^2(x_1, x_2) = 0$ distances. So, the geodesic is a line of maximum length. A line with a minimum length of zero between two points (causally related) always exists, and it is the sum of zero geodesics.

3. Metrics for Space of Probability Distributions

A random variable $X \in \Omega$ (where the set Ω can be continuous or discrete) is given a probability distribution p:

$$p = p(X; \theta_1, \ldots, \theta_N), \tag{7}$$

where the numbers $(\theta_1, \ldots, \theta_N) \equiv \Theta$ are the parameters of the distribution p belonging to the general case of some manifold M. So, p is the function defined on the Cartesian product $\Omega \times M$ with values between 0 and 1 for each Θ:

$$p : \Omega \times M \to [0, 1]. \tag{8}$$

Moreover, there is the normalization condition:

$$\int_\Omega p(X; \Theta)d\mu = 1, \tag{9}$$

where $d\mu$ is a measure on Ω. This condition defines the manifold M. So, the given probability distribution p determines M; on the other hand, this distribution itself depends on the points of M. Thus, the space of probability distributions is obtained:

$$\mathcal{P} = \{p(X;\Theta)\} \tag{10}$$

as the space of functions over M. Questions arise: how can the distance between two distributions on $\mathcal{P}$ be determined? Is there any distinguished set of metrics on M?

In the geometric approach, the metric is given by the relation (e.g., [18]):

$$g_{ab}(\Theta;F) = \int_\Omega p \frac{\partial F}{\partial \theta^a}\frac{\partial F}{\partial \theta^b} d\mu = \int_\Omega p\left[F'(p)\right]^2 \frac{\partial p}{\partial \theta^a}\frac{\partial p}{\partial \theta^b} d\mu, \tag{11}$$

where F is a function of p and prime means differentiation with respect to p. From this equation, one can obtain an "action integral" S for the function F depending on the one degree of freedom p:

$$S[F] = \int L[F;p]dp,$$

where the Lagrangian $L[F;p]$ for this action is equal to

$$L[F;p] = p\left[F'(p)\right]^2. \tag{12}$$

Hence, the stationarity condition for this "action integral" leads to the Euler–Lagrange equation:

$$\frac{d}{dp}\left(pF'\right) = 0, \tag{13}$$

with the solution:

$$F(p) = k \ln p + F_0, \tag{14}$$

where k and F_0 are integration constants. In this way, the metric for this solution is of the following form:

$$g_{ab}(\Theta) = k^2 \int_\Omega p(X;\Theta)\frac{\partial \ln p}{\partial \theta^a}\frac{\partial \ln p}{\partial \theta^b} d\mu = k^2 \int_\Omega \frac{\partial_a p \partial_b p}{p} d\mu. \tag{15}$$

This is the Fisher–Rao (FS) metric. The other form of this metric is as follows:

$$g_{ab}(\Theta) = -k^2 \int_\Omega p \partial^2_{ab} \ln p d\mu. \tag{16}$$

Hence, the infinitesimal square of length on M has the following form:

$$dl^2 = g_{ab} d\theta^a d\theta^b \tag{17}$$

As an example, we will consider the Gauss distribution:

$$p\left(X;\theta^1,\theta^2\right) = \frac{1}{\sqrt{2\pi}\theta^1} \exp\left[-\frac{\left(X-\theta^2\right)^2}{2\left(\theta^1\right)^2}\right]. \tag{18}$$

Thus, the FR metric is well-known and equal to (for $k = 1$):

$$dl^2 = \frac{1}{\left(\theta^1\right)^2}\left(d\left(\theta^2\right)^2 + 2d\left(\theta^1\right)^2\right). \tag{19}$$

This is the metric on the Poincare upper-half plane **H** defined by the condition $\theta^1 > 0$. Thus, the geodesic distance between two Gauss distributions:

$$p_1 = p(X;\Theta_1) \text{ and } p_2 = p(X;\Theta_2) \tag{20}$$

in this metric is equal to:

$$d(p_1,p_2) = 2\sinh^{-1}\left[\frac{|\Theta_2-\Theta_1|}{2\sqrt{\theta_2^1\theta_1^1}}\right], \tag{21}$$

where $\Theta_a = \left(\theta_a^1, \theta_a^2\right)$, $a = 1,2$, $|\Theta| = \sqrt{(\theta^1)^2 + (\theta^2)^2}$ and $\sinh^{-1} X = \ln\left(X + \sqrt{1+X^2}\right)$. If we omit the stationarity condition, the metric for the Gauss distribution takes the following form:

$$g_{11} = \frac{\sqrt{2}}{\theta^1}\int_{\mathbf{R}^1} p^3(z)\left[F'(p)\right]^2\left[1-4z^2+4z^4\right]dz, \tag{22}$$

$$g_{22} = \frac{1}{\sqrt{2}\theta^1}\int_{\mathbf{R}^1} p^3(z)\left[F'(p)\right]^2 z^2 dz, \tag{23}$$

$$g_{12} = 0, \tag{24}$$

where

$$p(z) = \frac{1}{\sqrt{2\pi}\theta^1}\exp\left(-z^2\right). \tag{25}$$

If we require that the following condition is satisfied:

$$p^3\left[F'(p)\right]^2 = p, \tag{26}$$

then $F(p) = \ln p$ and, again, the FR metric is obtained. So, one can say that, for the Gaussian distribution, the stationarity condition and above condition (which can be referred to as a simplicity condition) give the same result, namely the FR metric.

4. FR Metric in Quantum Mechanics

Quantum mechanics provides probability distributions P expressed by wave functions ψ. In general, the wave function Ψ depends on time t, the parameters of the system ω and the initial state ψ,

$$\Psi = \Psi(x,t,\omega,\psi) \tag{27}$$

where x denotes the spatial coordinates. If $\widehat{H}$ is the time-independent Hamiltonian of the system, then, in the eigenbasis ψ_n of $\widehat{H}$ with eigenvalues E_n, the initial state $\psi = \sum_{n=0} c_n\psi_n(x;\omega)$ evolves as follows:

$$\Psi(x,t,\omega,c) = \exp\left(-it\widehat{H}\right)\psi = \sum_n c_n \exp(-itE_n(\omega))\psi_n(x;\omega). \tag{28}$$

The complex coefficients $c = (c_n)$ are normalized: $\sum_{n=0}|c_n|^2 = 1$. The wave function Ψ can also be expressed via the following:

$$\Psi(x;t,\omega) = \int_{\mathbf{R}^N} d^N y K(x,t;y,0)\psi(y;\omega), \tag{29}$$

propagator $K(y,0;x,t)$ with the initial condition:

$$K(x,0;y,0) = \delta^{(N)}(x-y) \tag{30}$$

and N is the number degrees of freedom. In basis ψ_n, the propagator takes the following form:

$$K(x,t;y,0) = \sum_n \exp(-itE_n(\omega))\psi_n^*(x;\omega)\psi_n(y;\omega) \tag{31}$$

Thus, the probability distribution P is equal to

$$P(x;t,\omega,c) = \sum_{m,n} c_m^* c_n I_{mn}(x,t,\omega), \tag{32}$$

where

$$I_{mn}(x,t,\omega) = \int_{\mathbf{R}^{2N}} d^N y d^N z K^*(x,t;y,0)K(x,t;z,0)\psi_m^*(y;\omega)\psi_n(z;\omega) = I_{nm}^*(x,t,\omega) \tag{33}$$

The probability normalization condition is satisfied:

$$\int_{\mathbf{R}^N} d^N x P(x;t,\omega,c) = 1. \tag{34}$$

Thus, for a fixed time t and parameters ω, the FR metric is a function of the complex numbers c_m and the metric has the following components:

$$g_{mn}(c) = -\int_{\mathbf{R}^N} d^N x P \frac{\partial^2 \ln P}{\partial c_m \partial c_n}, \tag{35}$$

$$g_{\overline{m}n}(c) = -\int_{\mathbf{R}^N} d^N x P \frac{\partial^2 \ln P}{\partial c_m^* \partial c_n}, \tag{36}$$

$$g_{\overline{mn}}(c) = -\int_{\mathbf{R}^N} d^N x P \frac{\partial^2 \ln P}{\partial c_m^* \partial c_n^*} = g_{mn}^*(c). \tag{37}$$

Thus, we obtain

$$g_{mn}(c;t,\omega) = \sum_{k,p} c_k^* c_p^* A_{mn}^{kp}(c;t,\omega), \tag{38}$$

$$g_{\overline{m}n}(c;t,\omega) = -\int_{\mathbf{R}^N} d^N x I_{mn}(x,t,\omega) + \sum_{k,p} c_k c_p^* A_{kn}^{mp}(c;t,\omega), \tag{39}$$

where

$$A_{mn}^{kp}(c;t,\omega) = \int_{\mathbf{R}^N} d^N x \frac{I_{km}(x,t,\omega) I_{pn}(x,t,\omega)}{P(x;t,\omega,c)} \tag{40}$$

Since the eigenfunctions ψ_n form a complete and orthogonal system, the first integral on the right-hand side is equal to

$$\int_{\mathbf{R}^N} d^N x I_{mn}(x,t,\omega) = \delta_{mn}. \tag{41}$$

Thus,

$$g_{\overline{m}n}(c;t,\omega) = -\delta_{mn} + \sum_{k,p} c_k c_p^* A_{kn}^{mp}(c;t,\omega). \tag{42}$$

The complex numbers "c" form the infinitely dimensional unit sphere S^∞. Thus, the obtained metric is a metric on S^∞ and has the following form:

$$ds^2 = g_{mn} dc_m dc_n + g_{mn}^* dc_m^* dc_n^* + g_{\overline{m}n} dc_m^* dc_n. \tag{43}$$

This is real since $ds^2 = \left(ds^2\right)^*$. The distance between two states given by two sequences, $c = (c_n)$ and $c' = (c'_n)$, (which are points on S^∞) is given by the length of the geodesic γ originating at c and ending at c'. This geodesic is determined by the above metric. The obtained metric, (38) and (39), is the metric on the infinitely dimensional sphere S^∞.

In the next section, we will use the above formulas for two quantum systems.

5. Metric for Free Particle and Harmonic Oscillator

As the first example, we consider a free quantum particle. The propagator for the free particle (in 1D) of mass m has the following form:

$$K(x,t;y,0) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left[\frac{im(x-y)^2}{2\hbar t}\right] \tag{44}$$

and the wave functions are indexed by the wave vector k:

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} \exp(ikx). \tag{45}$$

The integrals (33) are labeled by the wave vectors k and l. The system has only one parameter m. Thus, inserting above formulas into (33), one obtains

$$I_{kl}(x;t,m) = \frac{m}{(2\pi)^2\hbar t} \int_{\mathbf{R}^2} dydz \exp\left[\frac{-im(x-y)^2}{2\hbar t} + \frac{im(x-z)^2}{2\hbar t}\right] \exp(ikz - ily). \tag{46}$$

This integral is easy to compute and is equal to

$$I_{kl}(x;t,m) = \frac{1}{2\pi} \exp\left[ix(k-l) - \frac{i\hbar t}{2m}\left(k^2 - l^2\right)\right]. \tag{47}$$

In this way, the probability distribution (32) is

$$P(x;t,m,c) = \frac{1}{2\pi} \sum_{k,l} c_k^* c_l \exp\left[ix(k-l) - \frac{i\hbar t}{2m}\left(k^2 - l^2\right)\right], \tag{48}$$

where the parameters space M given by condition (9) is an infinitely dimensional sphere parametrized by the infinite sequence (c_n). Thus, the metric (38) and (39) is determined by the integrals (40). In the considered case, they are given as follows:

$$\begin{aligned} A_{ln}^{kp}(c;t,m) = \frac{1}{2\pi} \exp\left[-\frac{i\hbar t}{2m}\left(k^2 - l^2 + p^2 - n^2\right)\right] \times \\ \times \int_{\mathbf{R}^1} dx \frac{\exp[ix(k-l+p-n)]}{\sum_{r,s} c_r^* c_s \exp\left[ix(r-s) - \frac{i\hbar t}{2m}(r^2 - s^2)\right]}. \end{aligned} \tag{49}$$

For the next example, we consider a one-dimensional quantum harmonic oscillator with the energy operator:

$$\widehat{H}(m,\omega) = \frac{1}{2m}\widehat{p}^2 + \frac{1}{2}m\omega^2\widehat{x}^2, \tag{50}$$

where m and ω are the mass and frequency, respectively. The eigenstates ψ_n and eigenvalues E_n are equal to

$$\psi_n(x;m,\omega) = \frac{1}{\sqrt{2^n n!}} \left(\frac{\lambda^2}{\pi}\right)^{1/4} \exp\left(-\frac{\lambda^2 x^2}{2}\right) H_n(\lambda x), \tag{51}$$

$$E_n = \hbar\omega(n + 1/2) \tag{52}$$

where $\lambda^2 = m\omega/\hbar$ and H_n are Hermite polynomials with $n = 0, 1, 2, \ldots$ In this case, the wave function $\Psi(x;t,m,\omega)$ is obtained from some initial state $\Psi(x;0,m,\omega) = \psi(x;m,\omega)$:

$$\Psi(x;t,m,\omega) = \int_{\mathbf{R}^1} dy K(y,0;x,t)\psi(y;m,\omega), \tag{53}$$

where the propagator K is equal to

$$K(x,t;y,0) = \frac{\lambda}{\sqrt{2\pi i \sin(\omega t)}} \exp\left[\frac{i\lambda^2}{2}\left(x^2+y^2\right)\cot(\omega t) - \frac{i\lambda^2 xy}{\sin(\omega t)}\right] \tag{54}$$

and

$$K(x,0;y,0) = \delta(x-y).$$

Hence, the probability distribution P takes the following form:

$$P(x;t,m,\omega) = \int_{\mathbf{R}^2} dydz K^*(x,t;y,0)K(x,t;z,0)\psi^*(y;m,\omega)\psi(z;m,\omega). \tag{55}$$

Finally, we obtain

$$P(x;t,m,\omega,c_n) = \frac{\lambda^2}{2\pi\sin(\omega t)} \sum_{n=0} |c_n|^2 |I_n(x;t,m,\omega)|^2, \tag{56}$$

where

$$\begin{aligned} I_n(x;t,m,\omega) = \frac{1}{\sqrt{2^n n!}}\left(\frac{\lambda^2}{\pi}\right)^{1/4} \exp\left[-\frac{i\lambda^2 x^2 e^{-i\omega t}}{2\sin(\omega t)}\right] \times \\ \times \int_{\mathbf{R}^1} dy H_n(\lambda y) \exp\left[\frac{i\lambda^2 e^{i\omega t}}{2\sin(\omega t)}\left(y - xe^{-i\omega t}\right)^2\right]. \end{aligned} \tag{57}$$

So,

$$g_{mn} = -2\delta_{mn}\int_{\mathbf{R}^1} dx |I_n(x;t,m,\omega)|^2 + 4c_m c_n \int_{\mathbf{R}^1} dx \frac{|I_m(x;t,m,\omega)|^2 |I_n(x;t,m,\omega)|^2}{P(x;t,m,\omega,c_n)}. \tag{58}$$

The first integral on the right side is equal to

$$\int_{\mathbf{R}^1} dx |I_n(x;t,m,\omega)|^2 = \frac{2\pi}{\lambda^2}\sin(\omega t). \tag{59}$$

Thus, the metric is

$$g_{mn} = -\delta_{mn}\frac{4\pi}{\lambda^2}\sin(\omega t) + 4c_m c_n \int_{\mathbf{R}^1} dx \frac{|I_m(x;t,m,\omega)|^2 |I_n(x;t,m,\omega)|^2}{P(x;t,m,\omega,c_n)}. \tag{60}$$

As one can see from the above examples, even in the simplest quantum systems, the determination of the Fisher–Rao metric on the infinitely dimensional sphere is a nontrivial task. The coefficients of the metric are given by the integrals (40).

However, if one fixes (c_n) on S^∞, in the case of an oscillator (this procedure can also be applied to the free particle), the parameter space becomes

$$M_{(n)} = \{(m,\omega) : m > 0 \text{ and } \omega > 0\} \subset \mathbf{R}^2. \tag{61}$$

The manifold $M_{(n)}$ is two-dimensional with coordinates given by two positive numbers, m and ω. This space corresponds to a set of harmonic oscillators with different masses

m and frequencies ω being in the same state given by the sequence (c_n). Hence, the probability distribution related to the eigenstate ψ_n is

$$p_n(x; m, \omega) = \frac{1}{2^n n!} \frac{\lambda}{\sqrt{\pi}} \exp\left(-\frac{\lambda^2 x^2}{2}\right) H_n^2(\lambda x) \tag{62}$$

and the Fisher–Rao metric $g^{(n)}$ on $M_{(n)}$ obtained from (16) has the following components (with $k = 1$):

$$g_{mm}^{(n)} = \frac{1}{2m^2}\left(1 - n^2 - n\right), \tag{63}$$

$$g_{\omega\omega}^{(n)} = \frac{1}{2\omega^2}\left(1 - n^2 - n\right), \tag{64}$$

$$g_{m\omega}^{(n)} = \frac{1}{4m\omega}\left(1 - n^2 + 3n\right). \tag{65}$$

The line element $dl_{(n)}^2$ is equal to

$$dl_{(n)}^2 = a\frac{dm^2}{m^2} + a\frac{d\omega^2}{\omega^2} + b\frac{dmd\omega}{m\omega}, \tag{66}$$

where $a = \left(1 - n^2 - n\right)/2$, $b = \left(1 - n^2 + 3n\right)/2$. The coordinates U and V are defined as follows:

$$U = \ln\left[\frac{\omega}{\omega_0}\left(\frac{m}{m_0}\right)^{b/(2a)}\right], \tag{67}$$

$$V = \ln\frac{m}{m_0}, \tag{68}$$

The metric (66) takes a diagonal form:

$$dl_{(n)}^2 = a dU^2 + \eta(n) dV^2 \tag{69}$$

with

$$\eta(n) = \frac{1}{8}\frac{\left(1 - n^2 - 5n\right)\left(3 - 3n^2 + n\right)}{1 - n^2 - n}. \tag{70}$$

The constants m_0 and ω_0 have the mass and s^{-1} dimensions, respectively, and have to be determined. Since $m_0\omega_0/\hbar$ has a dimension of $(length)^{-2}$, we make following ansatz:

$$\lambda_0^2 = \frac{m_0\omega_0}{\hbar} = l_{Pl}^{-2} = \frac{c^3}{\hbar G},$$

where l_{Pl} is the Planck length. So,

$$\omega_0 m_0 = \frac{c^3}{G}.$$

For the successive n, the metric takes the following form:

$$dl_{(0)}^2 = \frac{1}{2}dU^2 + \frac{3}{8}dV^2,$$

$$dl_{(1)}^2 = -\frac{1}{2}dU^2 + \frac{5}{8}dV^2,$$

$$dl_{(2)}^2 = -\frac{5}{2}dU^2 - \frac{13}{8}dV^2.$$

It can be seen from this that, for $n \geq 2$, the distance becomes purely imaginary.

6. Entropy as a Measure of Distance in Hilbert Space

The measure of a "distance" between states, $\widehat{\rho}$ and $\widehat{\sigma}$, is the relative entropy S_{rel}:

$$S_{rel}(\widehat{\rho}||\widehat{\sigma}) = Tr[\widehat{\rho}\log\widehat{\rho} - \widehat{\rho}\log\widehat{\sigma}]. \tag{71}$$

It can be rewritten as follows:

$$S_{rel}(\widehat{\rho}||\widehat{\sigma}) = S[\widehat{\sigma}] - S[\widehat{\rho}] + Tr[(\widehat{\sigma} - \widehat{\rho})\log\widehat{\sigma}], \tag{72}$$

where

$$S[\widehat{\sigma}] = -Tr(\widehat{\sigma}\log\widehat{\sigma})$$

is the von Neumana entropy. The entropy S_{rel} is positive : $S_{rel}(\widehat{\rho}||\widehat{\sigma}) \geq 0$ and is equal to zero if $\widehat{\rho} = \widehat{\sigma}$. Thus, one can consider this entropy as the square of the "distance" between states ([18], p. 44). We compute this distance for pure states. Let the pure states have the form: $\widehat{\sigma} = diag(0,\ldots,1,0,\ldots,0)$ (1 is in a-th place) and $\widehat{\rho} = diag(0,\ldots,1,0,\ldots,0)$ (1 is in b-th place). Since $(I-\widehat{\sigma})^n = I - \widehat{\sigma}$ and

$$\ln(\widehat{\sigma}) = \ln[I - (I-\widehat{\sigma})] = -\sum_{n=1}\frac{(I-\widehat{\sigma})^n}{n}$$

one obtains that $S_{rel}(\widehat{\rho}||\widehat{\sigma})$ is equal to

$$S_{rel}(\widehat{\rho}||\widehat{\sigma}) = -Tr[(\widehat{\sigma} - \widehat{\rho})(I-\widehat{\sigma})]\sum_{n=1}\frac{1}{n}. \tag{73}$$

Using relations $\widehat{\sigma} = \widehat{\sigma}^2$ and $Tr(\widehat{\sigma}\widehat{\rho}) = 0$, we finally obtain

$$S_{rel}(\widehat{\rho}||\widehat{\sigma}) = Tr[\widehat{\rho}]\sum_{n=1}\frac{1}{n} = +\infty. \tag{74}$$

Hence, the square of the "distance" between two pure states is infinite. In the case when $\widehat{\sigma}$ is a pure state and $\widehat{\rho}$ is a mixed state, then

$$\begin{aligned} S_{rel}(\widehat{\rho}||\widehat{\sigma}) = -S[\widehat{\rho}] - Tr[\widehat{\rho}\log\widehat{\sigma}] = \\ (1 - Tr\widehat{\rho}\widehat{\sigma})\sum_{n=1}\frac{1}{n} - S[\widehat{\rho}]. \end{aligned} \tag{75}$$

However, in this case, this square of the "distance" can be finite, because the difference of the infinity sum of the harmonic series and entropy of the mixed state (which can also be infinity) could give finite results.

Thermal States and Relative Entropy

The thermal state is defined by the maximum entropy S and fixed energy E. Thus, for an energy operator $\widehat{H}$, a density matrix $\widehat{\sigma}$ is equal to

$$\widehat{\sigma}_t(\beta) = \frac{1}{Z}\exp\left(-\beta\widehat{H}\right), \tag{76}$$

where $Z = Tr\left[\exp\left(-\beta\widehat{H}\right)\right]$ and $\beta = 1/(k_B T)$ is the Lagrange multiplier, which has interpretations of the inverse of temperature T. The relative entropy S_{rel} between the states $\widehat{\sigma}_t$ and $\widehat{\rho}$ takes the following form:

$$S_{rel}(\widehat{\rho}||\widehat{\sigma}_t) = \beta Tr\left(\widehat{\rho}\widehat{H}\right) - \beta Tr\left(\widehat{\sigma}_t\widehat{H}\right) - (S[\widehat{\rho}] - S[\widehat{\sigma}_t;\beta]), \tag{77}$$

where $S[\widehat{\sigma}_t;\beta]$ is the maximum entropy S and the term $Tr\left(\widehat{\sigma}_t\widehat{H}\right)$ is fixed energy E:

$$Tr\left(\widehat{\sigma}_t\widehat{H}\right) = E(\beta). \quad (78)$$

Hence,

$$S_{rel}(\widehat{\rho}||\widehat{\sigma}_t) = \beta Tr\left(\widehat{\rho}\widehat{H}\right) - S[\widehat{\rho}] + S[\widehat{\sigma}_t;\beta] - \beta E(\beta). \quad (79)$$

The last two terms are related to free energy: $F(\beta) = E - S/\beta$. Finally, the relative entropy is equal to

$$S_{rel}(\widehat{\rho}||\widehat{\sigma}_t) = \beta Tr\left(\widehat{\rho}\widehat{H}\right) - S[\widehat{\rho}] - \beta F(\beta). \quad (80)$$

If $\widehat{\rho}$ is also a thermal state with an energy operator $\widehat{h}$

$$\widehat{\rho}_t(b) = \frac{1}{U}\exp\left(-b\widehat{h}\right), \quad (81)$$

where $U = Tr\exp\left(-b\widehat{h}\right)$, then their relative entropy is

$$S_{rel}(\widehat{\rho}_t||\widehat{\sigma}) = -S[\widehat{\rho}_t;b] - \frac{1}{U}Tr\left[\exp\left(-b\widehat{h}\right)\log\widehat{\sigma}\right]. \quad (82)$$

The other form of the last equation is

$$S_{rel}(\widehat{\rho}_t||\widehat{\sigma}_t) = S[\widehat{\sigma}_t;\beta] - S[\widehat{\rho}_t;b] - \beta Tr\left(\widehat{\sigma}\widehat{H}\right) + \frac{\beta}{U}Tr\left[\exp\left(-b\widehat{h}\right)\widehat{H}\right]. \quad (83)$$

In this way, the relative entropy for two thermal states with the fixed energy operators $\widehat{H}$ and $\widehat{h}$ is parametrized by the two positive numbers β and b, with an interpretation of the inverse temperatures (modulo Boltzman constant).

When $\widehat{H} = \widehat{h}$, the last relation becomes

$$S_{rel}(\widehat{\rho}_t||\widehat{\sigma}_t) = S[\widehat{\sigma}_t;\beta] - S[\widehat{\rho}_t;b] + \beta E(b) - \beta E(\beta). \quad (84)$$

As an example, we will find the relative entropy for a free scalar field in thermodynamic equilibrium. Such a field is equivalent to an infinite set of non-interacting harmonic oscillators with a maximum entropy S and fixed energy E. The entropy is equal to

$$S[\widehat{\sigma}_t;\beta] = 2^4\frac{\pi^5 k_B}{45}\frac{1}{(\hbar c)^3}\frac{V}{\beta^3}, \quad (85)$$

and the energy $E(\beta)$ is equal to

$$E(\beta) = \frac{4\pi\cdot 3!}{(\hbar c)^3\beta^4}V\frac{\pi^4}{90} + E_0 \quad (86)$$

where E_0 is the infinite ground-state energy and V is the volume of space. Hence, the relative entropy takes the following form:

$$S_{rel}(\widehat{\rho}_t||\widehat{\sigma}_t) = \frac{4\pi^5 V k_B}{45(\hbar c)^3\beta^3}\left[1 - 4\left(\frac{\beta}{b}\right)^3 + 3\left(\frac{\beta}{b}\right)^4\right]. \quad (87)$$

If the parameter β is in the vicinity of b

$$\beta = b + \delta \quad (88)$$

for $0 < \delta/b << 1$, then their relative entropy is equal to

$$S_{rel}(\widehat{\rho}_t(\delta)||\widehat{\rho}_t(b+\delta)) = \frac{4\pi^5 V k_B}{45(\hbar c)^3} 6\frac{\delta^2}{b^5} + O\left(\delta^3\right). \tag{89}$$

Taking the interpretation of relative entropy as the square of the distance between states, the above relationship can be written as an expression for a one-dimensional (one parameter b) metric:

$$dl^2 = A\frac{db^2}{b^5}, \tag{90}$$

where $A = 8\pi^5 V k_B / \left[15(\hbar c)^3\right]$. In terms of the energy E, the last formula takes the following form:

$$dl^2 = \frac{k_b}{8}\left[\frac{4\pi^5 V}{15(\hbar c)^3}\right]^{1/4} E^{-5/4} dE^2. \tag{91}$$

So, the distance in this metric between two states of a free scalar field with fixed energies $E_2 > E_1$ is equal to

$$d(E_1, E_0) = \frac{1}{3}\sqrt{8k_B}\left[\frac{4\pi^5 V}{15(\hbar c)^3}\right]^{1/8}\left(E_2^{3/8} - E_1^{3/8}\right). \tag{92}$$

7. Conclusions

The method of determining the metric and distance in classical and quantum physics is shown in the diagram below. The left column refers to classical physics and the right column refers to quantum physics:

$$\begin{array}{ccc}
(E, \mathbf{p}) & & (\widehat{\rho}, ?) \\
\downarrow & & \downarrow \\
(T_{\mu\nu}) & & (S, ?) \\
\downarrow & & \downarrow \\
\left((T_{\mu\nu}), \left(R^{\mu}_{\nu\rho\sigma}\right)\right) & & \mathcal{H} \\
\downarrow \text{(EP)} & \Longleftarrow & \downarrow \\
\delta\int(R + \Lambda + L_m) = 0 & ? & \widehat{H}\psi = i\partial_t\psi \\
\downarrow & & \downarrow \\
d = d\left(x, y; (g_{\mu\nu})\right) & & d(\widehat{\rho}, \widehat{\sigma}) = \dots
\end{array},$$

where (EP) means the equivalence principle. As follows, EP is the key idea that is needed to determine the geometry of space-time. Question marks indicate unknown complementary concepts. It can be said that the ambiguity in determining the distance or metric in quantum physics (e.g., [19–21]) is due to the lack of a counterpart for the equivalence principle.

Moreover, there is an intriguing relationship between pure states and the Kasner metric in $n+1$ dimensional space-time. This metric describes vacuum cosmological solutions and has the following form:

$$ds^2 = dt^2 - \sum_{a=1}^{n} t^{2p_a} dx_a^2,$$

where the numbers $p_1, \dots, p_n$ obey two constraints:

$$\sum_{a=1}^{n} p_a = \sum_{a=1}^{n} p_a^2 = 1.$$

Thus, formally, one can consider these numbers $\{p_a\}$ as the eigenvalues of a certain density matrix $\widehat{\rho}$ corresponding to a pure state.

The obtained metric (38) and (39) on an infinitely dimensional sphere S^{∞} is given by the integrals (40) and was obtained as the FR metric for the infinitely dimensional Hilbert space. It is known that, when the Hilbert space is CP^N, then the FR metric becomes the Fubini–Study metric. Thus, the metric (38) and (39) should be reduced to the Fubini–Study in the case of finite dimensions. But this is not obvious. The sphere S^{∞} should be modeled by some kind of limit of N-dimensional spheres S^N:

$$\text{“}\lim_{N\to\infty}\text{”} S^N = S^{\infty}.$$

Moreover, the metrics on S^N have to be invariant under the unitary grup $U(N)$. For finite N, the normalization condition leads to an odd value of $N = 2n + 1$, so the sphere S^{2n+1} is represented as the homogenous manifold:

$$\frac{U(n+1)}{U(n)} \simeq S^{2n+1}.$$

From the other side, CP^n is also represented as the homogenous manifold:

$$\frac{S^{2n+1}}{S^1} \simeq CP^n.$$

One of the $U(n)$ invariant metrics is the Fubini–Study (FS) metric. But there are other metrics which remain hidden. In the FS metric, the volume of CP^N is equal to

$$vol_{FS}\left(CP^N\right) = \frac{\pi^N}{N!}.$$

Hence, for $N \to \infty$, the volume in the FS metric tends to zero. It can be seen from this that the FS metric does not lead to the metric (38) and (39).

In the case of a measure related to relative entropy, completely different distances are obtained (e.g., [22–25]), which should not be surprising. Without some fundamental principle, each measure is equally appropriate. In this article, we have presented only very specific measures. Of course, there are more of them.

One of the unsolved problems in quantum cosmology is finding the “norm” of the universe’s wave function. In this case, the WDW equation is defined on a minisuperspace and the wave function is known for different boundary conditions [26–33]. So, the use of the approach outlined in this work is most reasonable. Finding the “distance” for the wave functions describing the expanding universe and the collapsing universe is a task to be accomplished. A more difficult issue is the “distance” between states associated with black holes. These issues will be addressed in our next paper.

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