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Classical and Quantum – Correspondence or Duality?

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Time in quantum theory, the Wheeler-DeWitt equation and the Born-Oppenheimer approximation,

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Introduction

- The origin of our Universe is quantum.
- The universe in which we live is classical.
- How it is possible?
- The correspondence principle tells us that at some conditions the quantum system behaves as classical.
- How universal is this principle?
- Is the problem of time typical only for quantum cosmology?

Introduction

- I shall try to show that the problem of time in quantum theory is more general than that arising during the reparametrisation invariance of the General Relativity or its modifications or generalisations.
- Moreover, the correspondence principle can be substitute by a more general duality principle.

Wheeler-DeWitt equation, the problem of time in quantum cosmology and reparametrisation invariance

- The Hilbert-Einstein Lagrangian of General Relativity is reparametrisation invariant.
- It contains the Lagrange multipliers N and N^i, lapse and shift functions.
- The dynamical degrees of freedom are connected with the spatial components of the metric g_{ij} and with the non-gravitational fields present in the universe.
- One introduces the conjugate momenta and makes a Legendre transformation in order to use the canonical formalism.
- Then one discovers that the Hamiltonian is proportional to the linear combination of the constraints, multiplied by the Lagrange multipliers.
- Thus, the Hamiltonian vanishes if the constraints are satisfied.

- This can be interpreted as the impossibility of writing down a time-dependent Schrödinger equation.
- One can see this problem from a somewhat different point of view.
- If one applies the Dirac quantisation procedure, then the constraints, wherein the classical phase variables are substituted by the quantum operators, should annihilate the quantum state of the system.

$$\mathcal{H}_i|\Psi\rangle = 0.$$

- Gravitational constraints contain momenta, which classically are time derivatives of fields, but their origin connected with the classical notion of time vanishes in the quantum theory, where momenta are simply operators satisfying some commutation relations.

- The main constraint arising in General Relativity is quadratic in momenta and gives rise to the so called Wheeler-DeWitt equation.
- It looks like that the problem of time in quantum cosmology arises due to a particular combination of the reparametrisation invariance and “quantumness”.

Gianni has given a great contribution to the study of the Wheeler-DeWitt equation, specially in the Born-Oppenheimer approach.

The problem of time in non-relativistic quantum mechanics

Let us imagine an isolated quantum system, which finds itself in an energy eigenstate. Its wave function is

$$\Psi(x_A, t) = e^{-iEt}\psi(x_A),$$

where the time parameter appears only in the phase factor, which does not depend on the variables x_A and is not essential for the definition of the quantum state. Quantum states are determined up to a constant complex phase. All the probability distributions are independent of time.

This situation just coincides with that of the Wheeler-DeWitt equation with the peculiarity that in the case of the Wheeler-DeWitt equation the value of E is always equal to zero.

The problem of time in quantum mechanics and its analogy with the absence of time in the Wheeler-DeWitt equation was analysed in some detail in paper
F. Englert, Quantum physics without time, Physics Letters B228, 111 (1989).

If the set of variables includes more than one element, we can introduce an effective time parameter, identifying it with a certain function of the variables x_A (a quantum clock).

The topic incites an essential interest. We would like to mention the book

E. Anderson, The Problem of Time. Quantum Mechanics Versus General Relativity, Fundamental Theories of Physics, Vol. 190, Springer, 2017,

and two-volume collection of papers

Time in Quantum Mechanics, edited by G. Muga, R. Sala Mayato and I. Egusquiza (Springer, 2008: Vol 1 and 2010: Vol 2),

where different conceptual and experimental aspects of the appearance of time in quantum mechanics are presented.

A very clear presentation of the problem is given in paper A. Schild, Time in quantum mechanics: A fresh look at the continuity equation, Phys. Rev. A 98, 052113 (2018).

Let us consider a quantum system consisting of two subsystems, whose wave function satisfies a time-independent Schrödinger equation with a fixed value of energy. One can always represent the wave function as a product of two functions:

$$\psi(R, r) = \chi(R)\phi(r|R).$$

The function $\chi(R)$ describes a subsystem, which plays the role of quantum clock, while $\phi(r|R)$ describes the subsystem, whose evolution is traced by the quantum clock.

The expression $|\chi(R)|^2$ gives the marginal probability density for the quantum clock and $|\phi(r|R)|^2$ gives the conditional probability for the system under consideration.

The clock-dependent Schrödinger equation for the subsystem under consideration, has the form

$$A\frac{d\ln\chi}{dR}\frac{\partial\phi}{\partial R} = H_{\text{eff}}\phi.$$

We have chosen a convenient gauge fixing of the phase in the decomposition, A is some coefficient and H_{eff} is an effective Hamiltonian for the subsystem.

The left-hand side of this equation does not represent a partial derivative with respect to a time parameter.

if the clock has some particular semiclassical properties and if the wave function χ has a semiclassical form $\chi \sim \exp(iS)$, then the left-hand side of the above equation behaves as a partial derivative with respect to the classical time.

One can underline two important features:

- The exact factorisation of the wave function is always possible and it is always possible to obtain the clock-dependent Schrödinger equation from the time-independent Schrödinger equation.
- A quantum clock does not always give rise to (semi)-classical time.

In some situations it is necessary to use a coarse-graining procedure to obtain a (semi)-classical time from a quantum clock.

In cosmology the corresponding models were studied in the papers:

A. Tronconi, G. P. Vacca and G. Venturi, The Inflaton and time in the matter gravity system, Phys. Rev. D 67, 063517 (2003);

A. Yu. Kamenshchik, A. Tronconi, T. Vardanyan and G. Venturi, Quantum Gravity, Time, Bounces and Matter, Phys. Rev. 97, 123517 (2018).

Difference

In quantum mechanics the wave function $\psi(R, r)$ is normalisable and both the system under consideration and the clock can be treated to some extent on equal footing.

The solutions of the Wheeler-DeWitt equation are non-normalizable, because the configuration space on which they are defined contains some superfluous (gauge or non-physical) degrees of freedom.

The variables r should be chosen to make the wave function $\phi(r|R)$ normalisable and to satisfy the Schrödinger equation with some effective Hamiltonian, while the variable R and the wave function $\chi(R)$ play an auxiliary role and serve for the introduction of the quantum clock and, sometimes, of the classical time.

Classical motion behind a quantum state

Some analogue of the classical time can be introduced even in the system with one degree of freedom:
A. Sommerfeld, Wave Mechanics, London, Methuen, 1930;
E. G. Peter Rowe, The classical limit of quantum mechanical hydrogen radial distributions, European J. Physics 8, 81 (1987);
L. Pauling and E. B. Wilson, Introduction to Quantum Mechanics, Reading, MA: Addison-Wesley, 1935.

- Let us consider a particle with one spatial coordinate and a stable probability distribution for this coordinate.
- One can suppose that behind this probability distribution there is a classical motion which we can observe stroboscopically.
- We can detect its position many times and obtain a probability distribution for this position.

- Classically this measured probability is inversely proportional to the velocity of the particle.
- The higher is the velocity of a particle in some region of the space the less is the time that it spends there.
- In quantum mechanics this probability is given by the squared modulus of its wave function.

$$\psi^*(x)\psi(x) = \frac{1}{|v(x)|T},$$

where T is a normalising time scale.

In paper by Rowe the probability distributions for the energy eigenstates of the hydrogen atom with a large principal quantum number n were studied.
The distributions with the orbital quantum number l having the maximal possible value $l = n - 1$, being interpreted as above, describe the corresponding classical motion of the electron on the circular orbit.

The state with $l = 0$ cannot produce immediately a correct classical limit. One should apply a coarse-graining procedure based on the Riemann - Lebesgue theorem.

nother interesting example: the harmonic oscillator with a large value of the quantum number n. In this case, making a coarse-graining of the probability density one can again reproduce a classical motion of the oscillator (Pauling).

Inverse problem: quantum state and Hamiltonian behind a classical motion

- Usually, when one studies the question of the classical-quantum correspondence, one looks for the situations where this correspondence is realised.
- It is reasonable to suppose that such situations are not always realised.
- Moreover, they can be rather exceptional.
- Here we would like to attract attention to another phenomenon: a particular quantum-classical duality between the systems governed by different Hamiltonians.

Example

Let us suppose that we have a classical motion of the harmonic oscillator, governed by the law

$$x(t) = x_0 \sin \omega t.$$

The velocity is

$$\dot{x}(t) = \omega x_0 \cos \omega t.$$

We can believe that behind this classical motion there is a stationary wave function

$$\psi(x) = \frac{1}{\sqrt{\pi}(x_0^2 - x^2)^{1/4}} e^{if(x)} \theta(x_0^2 - x^2),$$

where θ is the Heaviside theta-function and f is a real function.

Applying the energy conservation law and the stationary Schrödinger equation we can find the corresponding potential for the quantum problem:

$$V(x) = \frac{m\omega^2 x_0^2}{2} + \frac{\hbar^2}{2m}\left(\frac{1}{2(x_0^2 - x^2)} + \frac{5x^2}{4(x_0^2 - x^2)^2} + if'' + if'\frac{x}{x_0^2 - x^2} - f'^2\right), \quad \text{if } x^2 < x_0^2.$$

To guarantee the reality of the potential and, hence, the hermiticity of the Hamiltonian, we must choose the phase function f such that

$$f' = C\sqrt{x_0^2 - x^2},$$

where C is a real constant.

Then the potential is equal to

$$V(x) = \frac{m\omega^2 x_0^2}{2}$$
$$+\frac{\hbar^2}{2m}\left(\frac{1}{2(x_0^2 - x^2)} + \frac{5x^2}{4(x_0^2 - x^2)^2} + C^2(x^2 - x_0^2)\right),$$
$$\text{if } x^2 < x_0^2.$$

Then for $x^2 > x_0^2$ we can treat the potential as an infinite since there the wave function is zero.

Conclusions

- The example constructed above is a rather artificial.
- We have elaborated it to hint at the possibility of encountering similar effects in cosmology .
- One can imagine a situation where behind the visible classical evolution of the universe looms a quantum system, whose Hamiltonian is quite different from the classical Hamiltonian governing this visible classical evolution.
- It was Gianni who has attracted our attention to the paper by Rowe and the books by Sommerfeld and Polling, leading us to a new hypothesis about the possibility of a classical-quantum duality.

- Another research line initiated by Gianni: the Pauli-Zeldovich mechanism for the cancellation of the ultraviolet divergences in vacuum energy.
- This mechanism arises because bosons and fermions give contributions of the opposite signs.