Some parabolic equations for measures and Gaussian semigroups

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Abstract. This short communication (preprint) is devoted to mathematical study of evolution equations that are important for mathematical physics and quantum theory; we present new explicit formulas for solutions of these equations and discuss their properties. The results are given without proofs but the proofs will appear in the longer text which is now under preparation.

In this paper, infinite-dimensional generalizations of the Euclidean analogue of the Schrödinger equation for anharmonic oscillator are considered in the class of measures. The Cauchy problem for these equations is solved. In particular cases, explicit formulas for fundamental solutions are obtained, which are a generalization of the Mehler formula, and the uniqueness of the solution with certain properties is proved. An analogue of the Ornstein-Uhlenbeck measure is constructed. The definition of Gaussian semigroups is given and their connection with the considered parabolic equations is described.

Keywords: linear evolution equation, Schrödinger equation, parabolic equation, equations for measures, Cauchy problem, exact solution, Gaussian semigroup

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1 Introduction

Quantum mechanics is one of the basic tools of modern science and technology. Quantum computers, small objects in molecular biology, processes involving nano-particles that are important e.g. for constructing new materials with useful properties – all obey the rules of quantum mechanics. Laws of quantum mechanics in its modern understanding are written on the language of functional analysis. In the paper we heavily employ this language and can recommend the following books as a source of terminology and facts that are used without references:

One of the main questions answered by mathematical theories is predicting the future of the system (particle, several particles, airplane, robot, chemical reactor, field, quantum computer etc) based on the information about the laws of evolution (i.e. rules of changing in time) and current state of the system considered. For example, Newton’s laws of classical mechanics help to predict position and velocity of a classical particle based on the knowledge of the acting forces and also initial position and velocity of the particle. In this simple example the second Newton’s law is
the evolution equation (i.e. equation setting the rules of evolution), all possible values of position and velocity is the space of states of the system, and initial position and velocity is the state of the system in the initial moment. The evolution equation together with the initial state are called the initial-value problem, or Cauchy problem, and the solution of this problem is a function that gives the state of the system for all points of non-negative timeline. General theory of evolution equations is closely related with the branch of functional analysis called operator semigroups theory (see for example [5]); in the paper we use notions of this theory without references, but all the facts and terminology we use can be found in standard textbooks [3, 4].

In quantum mechanics the main evolution equation is the Schrödinger equation (see[6, 7]). This is an equation of the form
\[ \psi_t = -iH\psi, \]
where \( \psi \) is the state of a quantum system and \( H \) is the quantum Hamiltonian – linear self-adjoint operator in Hilbert space. The Schrödinger equation is in some sense the quantum analogue the Newton’s equation in classical mechanics, the Hilbert space describes states of the quantum system, and the Hamiltonian describes the process of quantum evolution. The equation \( \psi_t = -H\psi \) is called the Euclidean analogue of the Schrödinger equation; in the case considered in the paper it is a second order parabolic partial differential equation that is connected with both classic and quantum evolution. In the paper the role of \( \psi \) is played by the Borel measure [8, 9, 2], theory of such measures is a part of infinite dimensional analysis [10] [11] [12].

We call a \( n \)-dimensional anharmonic oscillator a system consisting of \( n \) one-dimensional interacting oscillators. The Schrödinger equation for the wave function \( \psi(t; x_1, \ldots, x_n) \) of a quantum \( n \)-dimensional anharmonic oscillator has the form (6):
\[ ih \cdot \psi_t = -\frac{1}{2} \sum_{j=1}^{n} \frac{\psi''_{xx_j}}{m_j} + \frac{1}{2} \sum_{j=1}^{n} k_j x_j^2 \cdot \psi + V \cdot \psi, \]
where \( m_1, \ldots, m_n \) are the masses of one-dimensional oscillators, \( k_1, \ldots, k_n \) are the stiffness of their springs. This equation can be rewritten in a more general way. To do this, we will define two diagonal matrices: the matrix \( B_n \) with diagonal elements \( 1/(hm_j) \), \( j = 1, \ldots, n \), and the matrix \( C_n \) with diagonal elements \( k_j/\hbar \), \( j = 1, \ldots, n \). In addition, we denote by \( \psi''_{xx} \) the Hesse matrix with elements \( \psi''_{xx_j x_k} \), \( j, k = 1, \ldots, n \). Then the equation (1) can be written as:
\[ \psi_t = i \left[ \frac{1}{2} \text{tr}(B_n \psi''_{xx}) - \frac{1}{2} (C_n x, x) \cdot \psi - V \cdot \psi \right]. \]
Removing the imaginary unit on the right side, we get the Euclidean analog of the equations (1) and (2):
\[ \psi_t = \frac{1}{2} \text{tr}(B_n \psi''_{xx}) - \frac{1}{2} (C_n x, x) \cdot \psi - V \cdot \psi. \]
Next, we turn to the infinite-dimensional analog of this equation. In the infinite-dimensional case, there is, in particular, the following fundamental difference from the \( n \)-dimensional case: in an infinite-dimensional Hilbert space, there is no analog of the Lebesgue measure (see [13]). The presence of the Lebesgue measure is important because in quantum mechanics, the square of the modulus of the wave function is equal to the density of the coordinate distribution relative to this measure. The absence of its analog in the infinite-dimensional case leads to the idea of using not only the wave function \( \psi \), but also the “wave” measure \( \mu \) to describe a quantum system. In this case, the probability of the falling of system coordinates into the set \( A \), is equal to the integral \( \int_A \psi d\mu \).
Thus, we come to the following problem: solve the analog of the equation (3) with respect to measures defined on an infinite-dimensional Hilbert space. More precisely, we solve equations of the next form in our work:

$$\mu'_t = \frac{1}{2} \text{tr}(B\mu'') - \left[ (B\mu', \cdot) + \text{tr} D \cdot \mu \right] - \frac{1}{2} (C \cdot \cdot)\mu + V \cdot \mu. \quad (4)$$

To determine the differential operators included in the right-hand side of the equation, as well as to solve the equation itself, we use the Fourier transform method (see [14]). This method seems to us the most convenient. We give more precise definitions in the next section.

2 Preliminaries and problem setting

Let $\mathcal{H}$ be a separable Hilbert space, $B_\mathcal{H}$ is $\sigma$-algebra of its Borel subsets, $\mathcal{M}(\mathcal{H})$ is the set of Borel measures on $B_\mathcal{H}$, $\mathcal{U}_\mathcal{H}$ is the algebra of cylindrical subsets in $\mathcal{H}$, $\mathcal{M}_c(\mathcal{H})$ is the family of cylindrical measures on $\mathcal{U}_\mathcal{H}$. Next let $B$, $C$ and $D$ be bounded linear operators on $\mathcal{H}$, at that $B$, $C$ are symmetric and nonnegative, and $B$ is nuclear.

**Definition 1.** We will call the function $\hat{\mu}(y) = \int_\mathcal{H} e^{i(x,y)} d\mu(x)$, where $y \in \mathcal{H}$, Fourier transform of the measure $\mu \in \mathcal{M}_c(\mathcal{H})$.

**Definition 2.** If $\mu \in \mathcal{M}(\mathcal{H})$, then let us denote through $\text{tr}(B\mu'')$ such a measure $\lambda \in \mathcal{M}_c(\mathcal{H})$, that $\hat{\lambda}(\varphi) = - (B\varphi, \varphi)\hat{\mu}(\varphi)$ (of course, if it exists), and through $[(B\mu', \cdot) + \text{tr} D \cdot \mu]$ — such $\nu \in \mathcal{M}_c(\mathcal{H})$, that $\hat{\nu}(\varphi) = - \hat{\mu}_{D\varphi}(\varphi)$ (here the derivative is understood in the sense of Gato).

**Definition 3.** The family of measures $\{\mu(t)\}_{t \geq 0}$ is called differentiable (weakly differentiable) if for all $A \in \mathcal{U}_\mathcal{H}$ and $t > 0$ there exists $\frac{d}{dt} (\mu(t))(A)$ (respectively, if for all functions $f_c$ lying in the class $C_{bc}(\mathcal{H}, \mathbb{R})$ of continuous bounded cylindrical functions from $\mathcal{H}$ to $\mathbb{R}$, there exists $\frac{d}{dt} \int_\mathcal{H} f_c(x) d(\mu(t))(dx)$).

**Remark 1.** It is known that if the family $\mu(t)$ is differentiable, then the set function $\frac{d}{dt} \mu(t): A \mapsto \frac{d}{dt} (\mu(t))(A)$ is a cylindrical measure (see [15]).

**Definition 4.** Let $\mathcal{L} : \mathcal{M}(\mathcal{H}) \to \mathcal{M}_c(\mathcal{H})$ be some linear operator with the domain $D_{\mathcal{L}}$. The family of measures $\{\mu(t)\}_{t \geq 0}$, lying in $D_{\mathcal{L}}$, is called weak solution of the equation $\mu'_t = \mathcal{L} \mu$ with initial conditions $\mu_0 \in \mathcal{M}(\mathcal{H})$, if the next two conditions are met:

1) $\frac{d}{dt} \int_\mathcal{H} f_c(x) d(\mu(t))(x) = \int_\mathcal{H} f_c(x) d[\mathcal{L}(\mu(t))](x)$ for any continuous cylindrical bounded function $f_c$ on $\mathcal{H}$;

2) $\lim_{t \to +0} \int_\mathcal{H} f(x) d(\mu(t))(x) = \int_\mathcal{H} f d\mu_0$ for any continuous bounded function $f$ on $\mathcal{H}$.

**Definition 5.** We call the fundamental solution of such an equation, the family of its solutions is $G_x(t)$, $t \geq 0$, depending on the parameter $x \in \mathcal{H}$, with initial conditions $G_x(0) = \delta_x$.

First let consider the following evolution equation:

$$\mu'_t = \frac{1}{2} \text{tr}(B\mu'') - \left[ (B\mu', \cdot) + \text{tr} D \cdot \mu \right] - \frac{1}{2} (C \cdot \cdot)\mu + \alpha \mu. \quad (5)$$

We will look for its fundamental solution in the form of

$$G_x(t) = s(t) \exp \left\{ - \frac{1}{2} (P(t)x, x) \right\} \Gamma(Q(t), R(t)x), \quad (6)$$
where

1) function \( s : \mathbb{R}_+ \to \mathbb{C} \) is continuous; \( P, Q \) and \( R \) are continuous mappings from \( \mathbb{R}_+ \) to \( L(\mathcal{H}, \mathcal{H}) \), with \( P \geq 0 \), and \( P, Q \) are symmetric;
2) \( \Gamma(Q(t), R(t)x) \) is Gaussian measure with the correlation operator \( Q(t) \) and the mean \( R(t)x \).
3) \( s(0) = 1, P(0) = 0, Q(0) = 0, R(0) = I \) (here \( I \) is a unit operator).

**Definition 6.** Family of measures \( G_x(t), t \geq 0 \), of the form (2) we call a Gaussian semigroup, if it satisfies the above conditions 1) – 3), and also has the semigroup property:
\[
\int_{\mathcal{H}} G(t)(y)G(s)(x)(dy) = G(t + s)(x), \text{ for any } t, s \geq 0.
\]

### 3 Results

#### 3.1 Explicit formulas for solutions of evolution equation

**Theorem 1.** If the weak fundamental solution of (5) has the form (6) and has properties 1), 2) and 3), then the functions \( P, Q, R \) and \( s \) satisfy a system of equations and initial conditions
\[
s'(t) = -\frac{1}{2} s \cdot \text{tr}(CQ) + \alpha s \quad \text{with} \quad s(0) = 1 \quad P(0) = 0 \quad Q(0) = 0 \quad R(0) = I.
\]

**Theorem 2.** If \( P, Q, R \) and \( s \) are the solution of (3), then the family of measures of the form (6) is the (strong) fundamental solution of the equation (5) and is a Gaussian semigroup. Also, if \( \mu_0 \in \mathcal{M}(H) \) and \( \int_{\mathcal{H}} |x|^2 d\mu < \infty \), then the family \( \mu(t) = \int_{\mathcal{H}} G_x(t) \mu_0(dx) \), \( t > 0 \), is the solution of (5) with the initial condition \( \mu_0 \).

The validity of the following two theorems can be easily verified by direct substitution:

**Theorem 3.** If \( C = 0 \), then
\[
\begin{align*}
\frac{d}{dt} s(t) &= e^{\alpha t}, \\
\frac{d}{dt} P(t) &= 0, \\
\frac{d}{dt} Q(t) &= \int_0^t \exp\{D^*s\}B \exp\{Ds\} ds, \\
\frac{d}{dt} R(t) &= \exp\{D^*t\}.
\end{align*}
\]

**Theorem 4.** If \( D = 0 \), then
\[
\begin{align*}
\frac{d}{dt} s(t) &= e^{\alpha t} \cdot \det^{-1/2}(\cosh(t\sqrt{CB})), \\
\frac{d}{dt} P(t) &= C(\tanh(t\sqrt{CB}))/\sqrt{CB}, \\
\frac{d}{dt} Q(t) &= (\tanh(t\sqrt{CB})/\sqrt{CB})B \text{ and} \\
\frac{d}{dt} R(t) &= \cosh^{-1}(t\sqrt{CB})
\end{align*}
\]

**Remark 2.** Even functions of \( \sqrt{CB} \) are defined using Maclaurin series, which, due to parity, will contain only integer powers of the operator \( CB \).

**Theorem 5.** Let \( G_x(t) \) be a Gaussian semigroup. Then there are operators \( B, C, \) and \( D \) belonging to \( L(\mathcal{H}, \mathcal{H}) \), with \( B = B^* \), \( C = C^* \), and nuclear \( B \geq 0 \), and a number \( \alpha \) such that for the equation they define of the form (2), \( G_x(t) \) will be the fundamental solution.
3.2 One statement about uniqueness

Using some ideas from [16], we prove that the solution of (1) is unique. The result is stated in the following theorem.

**Theorem 6.** Let $C = 0$, $\eta \in \mathcal{M}(H)$. Then, if $\int_{\mathcal{H}} |x|^2 \, d\eta < \infty$, then there is at most one solution $\{\mu(t)\}_{t > 0}$ of the equation (5) with the initial condition $\eta$ satisfying the condition $\sup_{0 < t \leq T} \int_{\mathcal{H}} |y|^2 \|\mu(t)\| \, (dy) < \infty$ for any $T > 0$ (here $\|\mu(t)\|$ is variation of measure $\mu(t)$). In addition, a solution satisfying this condition exists.

3.3 Construction of conditional generalized Ornstein-Uhlenbeck measure

Let’s denote by $G_x(t)$ the fundamental solution of the equation

$$
\mu'_t = \frac{1}{2} \text{tr}(B \mu''_t) - \left[ (D \mu'_t, \cdot) + \text{tr} D \cdot \mu \right] - \frac{1}{2} (C, \cdot)_\mu.
$$

Let the symbol $C_{x,A}^T$ means, for fixed $T > 0$, $x \in \mathcal{H}$ and $A \in B_\mathcal{H}$, the space of all continuous functions $f$ on the segment $[0, T]$, taking values in $\mathcal{H}$, such that $f(0) = x$ and $f(T) \in A$. For any set of points $0 < t_1 < \ldots < t_n < T$ and sets $A_1, \ldots, A_n \in B_\mathcal{H}$, the subsets $I_{A_1, \ldots, A_n} = \{ f \mid f(t_i) \in A_i, i = 1, \ldots, n \}$ form a semiring $K$ in $C_{x,A}^T$. Let’s set the measure $U_{x,A}^T$ on it by the equality

$$
U_{x,A}^T(I_{A_1, \ldots, A_n}) = \int_{A_1} [G_x(t_1)](dy_1) \int_{A_2} [G_x(t_2 - t_1)](dy_2) \cdot \ldots \cdot 
\int_{A_n} [G_x(t_n - t_{n-1})](dy_n)[G_x(T - t_n)](A).
$$

**Theorem 7.** The measure $U_{x,A}^T$ on $K \subset C_{x,A}^T$ has unique countably-additive continuation to Borel measure on $C_{x,A}^T$. Moreover, its continuation $U_{x,H}^T$ is a gaussian measure.

**Definition 7.** We will call a conditional generalized Ornstein-Uhlenbeck measure the measure $U_{x,A}^T$, described in theorem 7 (see also [17]).

3.4 Existence of a solution of the equation with potential

Here we use just constructed measure $U_{x,A}^T$ on the set of functions $C_{x,A}^T$ (such functions can be called trajectories in the Hilbert space $\mathcal{H}$) to represent solutions of the evolutionary equation of type (1) as an integral (see for example [18]).

**Theorem 8.** Let $V : \mathbb{R}_+ \times \mathcal{H} \to \mathbb{C}$ be a function, continuous by the totality of variables, and there are functions $C_1, C_2 \in L_{1, loc}(\mathbb{R}_+)$ and number $0 \leq r \leq 2$, such that for any $t \in \mathbb{R}$, $x \in \mathcal{H}$, the next inequalities are satisfied:

$$
|V(t, x)| \leq C_1(t) \exp\{\sigma\|x\|^r\} \quad \text{and} \quad \text{Re} V(t, x) \leq C_2(t)\sigma\|x\|^r.
$$

Then the equation $\nu'_t = \frac{1}{2} \text{tr}(B \nu'') - [(D \nu', \cdot) + \text{tr} D \nu] + V \nu$ has a weak fundamental solution $G^V_x(t)$ of the form

$$
[G^V_x(t)](A) = \int_{C_{x,A}^T} \exp\{\int_0^t V(s, q(s)) \, ds\} U_{x,A}^T(dq),
$$

where $A \in B_\mathcal{H}$. Also, if $\nu_0 \in \mathcal{M}(\mathcal{H})$ and $\int_{\mathcal{H}} \exp\{\|x\|^r\} \nu_0(dx) < \infty$, then the formula $[\nu(t)](A) = \int_{\mathcal{H}} G^V_x(t)(A) \nu_0(dx)$, $A \in B_\mathcal{H}$, sets the weak solution of this equation with the initial condition $\nu_0$. 
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References

[1] Moretti V. Spectral Theory and Quantum Mechanics. Springer. 2017. 950 p.
[2] Bogachev V.I., Smolyanov O.G. Real and Functional Analysis. Springer. 2020. 586 p.
[3] Hille E., and Phillips R.S. Functional Analysis and Semi-groups. American Mathematical Society. 1996. 819 p.
[4] Engel K.-J., Nagel R. One-Parameter Semigroups for Linear Evolution Equations. Springer-Verlag. New York. 2000. 609 p.
[5] Remizov I.D. Explicit formula for evolution semigroup for diffusion in Hilbert space.// Infinite Dimensional Analysis, Quantum Probability and Related Topics. 2018. V. 21, no. 4. 1850025, 35 p. DOI: 10.1142/S021902571850025X.
[6] Landau L.D., Lifshitz E.M. Quantum Mechanics: Non-Relativistic Theory. V. 3. Butterworth-Heinemann. 2010. 694 p.
[7] Glimm J., Jaffe A. Quantum Physics : A Functional Integral Point of View. Springer-Verlag. New York. 1987. 535 p.
[8] Kuo H.-H. Gaussian Measures in Banach Spaces. Springer-Verlag. Berlin, Heidelberg. 1975. 228 p.
[9] Bogachev V.I. Gaussian measures. // Mathematical Surveys and Monographs. American mathematical society. 1998. V. 62. 449 p. DOI: 10.1090/surv/062
[10] Aliprantis C.D., Border K.C. Infinite Dimensional Analysis: A Hitchhiker’s Guide. Springer, 2006. 716 p.
[11] Da Prato G. An Introduction to Infinite-Dimensional Analysis. Springer Science and Business Media. 2006. 215 p.
[12] Bogachev V.I., Smolyanov O.G. Topological Vector Spaces and Their Applications. Springer. 2017. 466 p.
[13] Weil A. l’Integration dans les group topologiques et ses application. Hermann. 1951. 162 p.
[14] Averbukh V.I., Smolyanov O.G., Fomin S.V. Generalized functions and differential equations in linear spaces. II. Differential operators and their Fourier transforms. // Tr. Mosk. Mat. Obs. M., MSU. 1972. V. 27, pp. 249–262.
[15] Dunford N.J., Schwartz J.T. *Linear Operators. Part I: General Theory*. Wiley-Interscience. 1988. 872 p.

[16] Smolyanov O.G. *A method of proof of the uniqueness theorem for evolutionary differential equations*. // Mathematical Notes of the Academy of Sciences of the USSR. 1979. V. 25, pp. 135–140. DOI: 10.1007/BF01142724

[17] Gaveau B. *Noyau des probabilites de transition de certains operateurs d’Ornstein-Uhlenbeck dans l’espace de Hilbert*. // C. R. Acad. Sci. Paris, Serie I. 1981. V. 293, pp. 469–472. DOI: 10.3792/pjaa.59.8

[18] Mazzucchi S. *Mathematical Feynman Path Integrals And Their Applications*. World Scientific. 2009. 225 p. DOI: 10.1142/7104.