Dynamics of quantum states generated by Schrödinger equation admitting blow up phenomenon

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Plan

1. The notion of blow up for the solutions of PDE. Classification of blow up phenomena.

2. Cauchy problem for Linear SE with singularities: blow up in Sobolev spaces and in the space L_2.

3. Cauchy problem for NSE: global existense or gradient blow up.

4. Gradient blow up, self-focucing and destruction of the quantum state.

5. Continuation of the dynamics with transition into the space of mixed quantum states.

6. Nonlinear Liuoville – von Neuman equation.

1. The definition of blow up phenomenon in differential equation

The Cauchy problem for some differential equation

$$\mathbf{A}u = f, \tag{1.1}$$

$$f \in Y, \quad u \in X, \quad \mathbf{A} \in \mathcal{M}(X, Y)$$

where X, Y are Banach spaces.

Let $\mathcal{M}(X, Y)$ be some topological space of operators mapping some domain $D \subset X$ to the space Y.

The definition of blow up phenomenon in differential equation

We should define the set-valued map (resolution map)

$$G: \; Z \to 2^X,$$

where 2^X is the set of all subsets of the space X and $Z \equiv Y \times \mathcal{M}(X, Y)$ is topological space endowing with the topology of direct product of topological spaces.

The set-valued map G is defined by the formula

$$G(f, \mathbf{A}) = \mathbf{A}^{-1}(f).$$

The definition of blow up phenomenon in differential equation

$(2^X, \tau)$ is the topological space with the topology generated by the Hausdorff pseudometric

$$r_H(A,B) = max\{\sup_{x\in A} \rho_X(x,B), \sup_{x\in B} \rho_X(x,A)\}, \text{if } A,B \neq \oslash$$

$$r_H(A,\oslash) = r_H(\oslash, A) = +\infty \text{ if } A \neq \oslash;\ \ r_H(\oslash,\oslash) = 0.$$

Let us consider the map G as the map of the topological space $Y \times \mathcal{M}(X,Y)$ into the topological space $(2^X, \tau)$.

Definition 1.1. (Efremova, Sakbaev)
The problem (1.1) possesses the blow up property if $(f, \mathbf{A})$ *is the discontinuity point of the map* G*.*

Classification of the blow up points

The point $(f_0, \mathbf{A}_0)$ is the **removable blow up point** in the space of Cauchy problems $Y \times \mathcal{M}(X, Y)$ if there is the limit $\lim\limits_{(f,\mathbf{A})\to(f_0,\mathbf{A}_0)} G(f, \mathbf{A}) = M$; in this case we define $G(f_0, \mathbf{A}_0) = M$.

The point $(f_0, \mathbf{A}_0)$ is the **unremovable blow up point** in the space of Cauchy problems $Y \times \mathcal{M}(X, Y)$ if $\nexists \lim\limits_{(f,\mathbf{A})\to(f_0,\mathbf{A}_0)} G(f, \mathbf{A})$:

a) the **polar type point** if $\lim\limits_{(f,\mathbf{A})\to(f_0,\mathbf{A}_0)} (\inf\limits_{u\in G(f,\mathbf{A})} \|u\|_X) = +\infty$;

b) the **essential singular point** in other cases.

2. The singular Cauchy problem for the linear Schrodinger equation

The Cauchy problem for Schrodinger equation

$$i\frac{d}{dt}u(t) - \mathbf{L}u(t) = 0,\ t > 0, \tag{2.1}$$

$$u(+0) = u_0,\ u_0 \in H, \tag{2.2}$$

$\mathbf{L}$ is symmetric operator in Hilbert space $H = L_2(\Omega),\ \Omega$ is domain in $R^d,\ d \in \mathbb{N}$.

Let $\Omega = R_+$, let $\mathbf{L}$ be a 2-nd order linear differential operator with nonnegative characteristic form.

$$u \in C(\mathbb{R}_+, H):\ (u(t) - u_0, \psi) = \int\limits_0^t (u(s), i\mathbf{L}^*\psi),\ t \geqslant 0,\ \forall\, \psi \in D(\mathbf{L}^*).$$

The model problem (2.1), (2.2)

$$\mathbf{L}u(x) = i\alpha\frac{\partial}{\partial x}u(x),\ \ x > 0;$$

$$D(\mathbf{L}) = \{u \in W_2^1(R_+):\ \ u(0) = 0\} = \dot{W}_2^1(R_+)$$

$$\mathbf{L}^*u(x) = i\alpha\frac{\partial}{\partial x}u(x),\ \ x > 0;$$

$$D(\mathbf{L}^*) = W_2^1(R_+).$$

Here $\alpha \in R$ be a parameter.
$\mathbf{L}$ is densely defined closed symmetric operator with deficience indexes (n_-, n_+) $(n_\pm = dim(Ker(\mathbf{L}^* \pm i\mathbf{I})))$

$(n_-, n_+) =$
(1,0) if $\alpha < 0$; (0,0) if $\alpha = 0$; (0,1) if $\alpha > 0$.

The correctness of Cauchy problem

Theorem 2.1.

Let $\mathbf{L}$ is operator above. Then

1. $\alpha \leqslant 0$ (then $n_+ = 0$) $\Rightarrow$ the operator $-i\mathbf{L}$ is the generator of the isometric semigroup $e^{-it\mathbf{L}}$, $t \geqslant 0$.
The problem (2.1), (2.2) has the unique solution
$u(t) = e^{-it\mathbf{L}}u_0$, $t \geqslant 0$.

2. $\alpha > 0$ (then $n_- = 0$) $\Rightarrow$ the operator $-i\mathbf{L}$ is not the generator of the strong continuous semigroup in the space H.
The problem (2.1), (2.2) has no solution if $u_0 \neq 0$.

The operator $i\mathbf{L}$ is the generator of the isometric semigroup $e^{it\mathbf{L}}$, $t \geqslant 0$; the operator $-i\mathbf{L}^*$ is the generator of the contractive semigroup $e^{-it\mathbf{L}^*}$, $t \geqslant 0$.

Regularization

$$i\frac{d}{dt}u(t) - \mathbf{L}_\epsilon u(t) = \theta_H,\ t > 0,\ \epsilon \in (0,1).$$

$$\mathbf{L}_\epsilon = \mathbf{L} + \epsilon\boldsymbol{\Delta}$$

$$D(\mathbf{L}_\epsilon) = \{u \in W_2^2(R):\ u(0) = 0\} = \dot{W}_2^2(R_+)$$

$$\mathbf{L}_\epsilon = \mathbf{L}_\epsilon^* \ \forall\ \epsilon \in (0,1). \quad \{u_\epsilon(t)\} = \{e^{-i\mathbf{L}_\epsilon t}u_0\}.$$

$$u_\epsilon(t) = e^{-it\mathbf{L}_\epsilon}u_0,\ t \geqslant 0; \quad \epsilon \to 0.$$

Convergence of regularized solution

Theorem 2.2. (Volovich, S., 2017)

1. $\alpha \leqslant 0 \Rightarrow \forall\ T > 0,\ u_0 \in H \lim\limits_{\epsilon \to 0} \sup\limits_{t \in [0,T]} \|u_\epsilon(t) - u(t)\|_H = 0.$

2. $\alpha > 0 \Rightarrow \forall\ T > 0,\ u_0,\ v \in H$

$\lim\limits_{\epsilon \to 0} \sup\limits_{t \in [0,T]} |(v, u_\epsilon(t) - u^*(t))| = 0$, where $u^*(t) = e^{-i\mathbf{L}^* t} u_0$.

$\lim\limits_{t \to +\infty} \|u^*(t)\|_H = 0.$

If $u_0 \in W_2^1(R)$ then

$\|u_\epsilon(t)\|_{W_2^1(R)} \to +\infty$ as $\epsilon \to 0$ for all sufficiently large t.

Blow up for linear Schrodinger equation

Thus the Cauchy problem (2.1), (2.2) can be presented in the form (1.1).
It can admite the blow up phenomenon of polar type.

$$X = C^1(R_+, W_2^2(R_+)); \quad Y = C(R_+, H) \oplus W_2^2(R_+);$$

$$\mathbf{A}u = (i\frac{d}{dt} - \mathbf{L})u \oplus u|_{+0}; \quad \mathbf{f} = 0 \oplus u_0.$$

$$\mathcal{M}(X, Y) = \{\mathbf{A}_\epsilon;\ \epsilon \in (-1, 1)\}.$$

The set of initial-boundary value promlems is the topological space of problems $Z = Y \times \mathcal{M}(X, Y)$ containes the curve

$$\Gamma = \{((0, u_0),\ \mathbf{A}_\epsilon);\ \epsilon \in (-1, 1)\}.$$

$$G((0, u_0), \mathbf{A}_\epsilon) = \{e^{-it\mathbf{L}_\epsilon} u_0,\ \ t \in R_+\}\ \forall\ \epsilon \neq 0.$$

The mapping $G :\ \Gamma \backslash \{(\mathbf{f}, \mathbf{A})\} \to 2^X$ is unbounded and $\lim_{\epsilon \to 0} (\inf_{u \in G((0, u_0), \mathbf{A}_\epsilon)} \|u\|_X) = +\infty.$

The Cauchy problem for degenerated Schrodinger equation

Cauchy problem (2.1), (2.2) has another presentation in the form (1.1).

$$u \in C(\mathbb{R}_+, H): \; u(t) + i \int\limits_0^t \mathbf{L}u(s)ds = u_0, \; t \geqslant 0. \qquad (2.3)$$

$X = C(R_+, H); \quad Y = C(R_+, W_2^{-2}(R_+)); \quad u_0 \in H.$

$\mathbf{A}u \equiv u(t) + i \int\limits_0^t \mathbf{L}u(s)ds; \quad \mathbf{f}_{u_0}(t) = u_0, \; t \geqslant 0.$

Topological space $\mathcal{M}(X, Y)$ is the curve in the set of linear operators $\gamma = \{\mathbf{A}_\epsilon, \; \epsilon \in [0, 1)\} = \mathcal{M}(X, Y)$. Here

$\mathbf{A}_\epsilon u(t) = u(t) + i \int\limits_0^t \mathbf{L}_\epsilon u(s)ds, \; \epsilon \in (-1, 1).$

The curve in the set of initial-boundary value promlems is the topological space of problems

$$Z = \{(\mathbf{f}_{u_0}, \; \mathbf{A}_\epsilon); \; \epsilon \in (-1, 1)\}.$$

Blow up for linear Schrodinger equation

Thus the Cauchy problem (2.3) admites the blow up phenomenon of essential type.

$$X = C(R_+, H); \quad Y = C(R_+, W_2^{-2}(R_+));$$

$$\mathbf{A}u \equiv u(t) + i\int_0^t \mathbf{L}u(s)ds; \quad \mathbf{f} = \mathbf{f}_{u_0}.$$

The curve in the set of Cauchy promlems is the topological space of problems

$$Z = \{(\mathbf{f}_{u_0},\ \mathbf{A}_\epsilon);\ \epsilon \in (-1, 1)\}.$$

$$G(\mathbf{f}_{u_0}, \mathbf{A}_\epsilon) = \{e^{-it\mathbf{L}_\epsilon} u_0,\ t \in R_+\}\ \forall\ (\mathbf{f}_{u_0}, \mathbf{A}_\epsilon) \neq (\mathbf{f}_{u_0}, \mathbf{A}).$$

The mapping $G:\ Z \backslash \{(\mathbf{f}_{u_0}, \mathbf{A})\} \to 2^X$ is bounded but $\nexists \lim\limits_{\epsilon \to 0} G(\mathbf{f}_{u_0}, \mathbf{A}_\epsilon)$.

Cauchy problem for the nonlinear Schrodinger equation on the segment:

$$i\frac{du}{dt} = \mathbf{L}u(t) \equiv -\boldsymbol{\Delta}u(t) - |u(t)|^p u(t),\ \ t \in (0, T); \qquad (3.1)$$

$$u(+0) = u_0; \quad u_0 \in H \equiv L_2(\Omega). \qquad (3.2)$$

where $u_0 \in H = L_2(\Omega),\ T \in (0, +\infty], \qquad p \geqslant 0.$
u is unknown map $[0, T) \to H$ which satisfies (3.1) and (3.2) (see Definition below).

$\boldsymbol{\Delta}$ is Laplace operator on the domain Ω.

$\Omega = \mathbb{R}^d,\ d \in \mathbb{N};$

$\boldsymbol{\Omega} = (-\pi, \pi).$

Solution of nonlinear Cauchy problem

$\Omega = (-\pi, \pi) \subset \mathbb{R}$; $\mathbf{\Delta}$ is Laplace-Dirichlet operator.
$D(\mathbf{\Delta}) = \{u \in W_2^2(-\pi,\pi) : \ u(-\pi) = 0 = u(\pi)\}$.
$H^l = D((-\mathbf{\Delta})^{l/2})$, $l \in 0, 1, \ldots$.

Definition

The function u is called H^l-solution for Cauchy pronlem (3.1), (3.2) with some $l \in \mathbf{N}$ if $u \in C([0,T), H^l)$ and

$$u(t) = e^{-it\mathbf{\Delta}} u_0 - i \int_0^t e^{-i(t-s)\mathbf{\Delta}}[|u(s)|^p u(s)]ds, \ t \in [0, T). \quad (3.3)$$

Let $N(u) = \|u\|_H^2$, $G(u) = \int\limits_\Omega |x|^2 |u|^2 dx$, $\ u \in H$;

$$E(u) = \int\limits_\Omega [\frac{1}{2}|\nabla u\|^2 - \frac{1}{p+2}|u|^{p+2}]dx, \ u \in H^1$$

(energy functional).

The local solvability of nonlinear Cauchy problem

Theorem 3.1. (Zhiber, Zakharov)
Let $\Omega = (-\pi, \pi)$, *and* $p \geqslant 0$. *Then the following statement holds:*
$\forall \quad \rho > 0 \quad \exists \quad T_* = T_*(\rho) > 0$ *such that if* $u_0 \in H^1$ *and* $\|u_0\|_{H^1} \leqslant \rho$ *then the Cauchy problem (1), (2) has the unique* H^1*-solution* $u_{u_0} = \mathcal{R}(u_0) \in C([0, T_*], H^1)$.

Lemma 3.1. If $u_0 \in H^1$ then $N(u_{u_0}(t)) = N(u_0)$, $t \in [0, T_*)$;
$E(u_{u_0}(t)) = E(u_0)$, $t \in [0, T_*)$.

The global existence

$$E(u) = \int\limits_{\Omega} [\frac{1}{2}|\nabla u\|^2 - \frac{1}{p+2}|u|^{p+2}]dx, \ \ u \in H^1$$

Theorem 3.2. (Zhiber, Zakharov)
If $0 \leqslant p < 4$ then for any $u_0 \in H^1$ Cauchy problem (1), (2) has the unique H^1-solution on the semiaxe R_+.

Let $p \in [0, 4)$.
Then one-parametric family $\mathbf{V}_t$, $t \in \mathbb{R}$ of mappings $H^1 \to H^1$ acting by the rule $\mathbf{V}_t u_0 = u_{u_0}(t)$, $t \in \mathbb{R}$ is defined.

Lemma 3.2. One-parametric family $\mathbf{V}_t$, $t \in \mathbb{R}$ is the one-parametric group of continuous nonlinear mappings $H^1 \to H^1$. In addition, $E(\mathbf{V}_t u_0) = E(u_0)$, $t \in \mathbb{R}$ for all $u_0 \in H^1$.

Gradient blow up phenomenon

Theorem 3.3. (Zhiber, Zakharov)
Let $p \geqslant 4$, *and* $u_0 \in H^3$ *satisfy the condition* $E(u_0) < 0$. *Then there is a number* $T^* \geqslant T_*$ *(see Theorem 1) such that supremum* T_1 *of the* H^1*-solution existence interval of the Cauchy problem (3.1), (3.2) satisfies the inequalities* $T_* \leqslant T_1 \leqslant T^*$.
Moreover, the limit equalities hold:

$$\lim_{t \to T_1 - 0} \|u(t)\|_{H^1} = +\infty;$$

$$\lim_{t \to T_1 - 0} \|u(t)\|_{L_{p+2}} = +\infty.$$

Remark. If $p > 0$ then there is $u_0 \in H^1$ such that $E(u_0) < 0$.

Reglarizatio of NSE

Unboundedness of level surfaces of the energy functional $E(u)$ in the space H^1 is the reason of the gradient catastrophe for large p. The regularization of NSE (3.1) is the one-parameter family of the nonlinear Schrödinger equations such that its energy functional has the bounded level surfaces.
For example,

$$i\frac{d}{dt}u = \mathbf{L}_\epsilon u \equiv \boldsymbol{\Delta} u + V_\epsilon(|u|)u,\ t > 0, \quad \epsilon \in (0,1),\ \epsilon \to 0, \quad (3.4)$$

$$V_\epsilon(|u|) = \frac{1}{1+\epsilon^2|u|^{2p+4}}|u|^{p+2},\ \epsilon \in (0,1).$$

The regularized energy functional for every $\epsilon \in (0,1)$ has the form

$$E_\epsilon(u) = \int_{-\pi}^{\pi}[\frac{1}{2}|\nabla u|^2 - \frac{1}{\epsilon(p+2)}\,\mathrm{arctg}(\epsilon|u|^{p+2})]dx,\ u \in H^1.$$

Solution of regularized problem

Let $\epsilon \in (0,1)$, $T \in (0,+\infty]$, and $l \in \mathbb{N}$. A function $u_\epsilon \in C([0,T), H^l)$ is called the H^l-solution of the Cauchy problem (3.2), (3.4) on the segment $[0,T)$ if it satisfies the equality

$$u_\epsilon(t) = e^{-i\boldsymbol{\Delta} t}u_0 + \int\limits_0^t e^{-i\boldsymbol{\Delta}(t-s)}V_\epsilon(|u_\epsilon(s)|)u_\epsilon(s)ds,\ \ t \in [0,T).$$

Theorem 3.5. (S.) *Let $\epsilon > 0$, $p \geqslant 0$. Then for any $u_0 \in H^1$ the Cauchy problem (3.2), (3.4) on the interval $[0,+\infty)$ has the unique H^1-solution $u_\epsilon(t;u_0)$; moreover, functionals $N(u)$ and $E_\epsilon(u)$ take constant values on the range of a solution $u_\epsilon(t;u_0)$, $t \geqslant 0$.*

$$u_\epsilon(t;u_0) = \mathbf{W}_\epsilon(t)u_0,\ \ t \geqslant 0;\ \ u_0 \in H^1.$$

The continuous semigroup $\mathbf{W}_\epsilon(t)$, $t \geqslant 0$, of nonlinear mappings of the space H^1 has the unique continuous continuation onto the continuous semigroup of nonlinear mappings on the space H.

Convergence of the solutions of regularized problem

Theorem 3.6. (S.)
Let $u_0 \in H^1$. *Let* $T_1 \in (0, +\infty)$ *be supremum of the interval, on which the* H^1*-solution* $u(t; u_0)$, $t \in [0, T_1)$, *of the Cauchy problem (3.1), (3.2) exists. Then for any* $T \in (0, T_1)$ *the directed family* $\{u_\epsilon(t; u_0),\ t > 0,\}$ *of solutions of the problems (3.2), (3.4) converges to the solution* $u(t; u_0)$, $t \in [0, T_1)$ *of the problem (3.1), (3.2) in the sense of the equality*

$$\lim_{\epsilon \to 0} \sup_{t \in [0,T]} \|u_\epsilon(t; u_0) - u(t; u_0)\|_H = 0 \ \forall\ T \in [0, T_1).$$

If $p = 4$ *and* $T \geqslant T_1$ *then there is no infinitesimal sequence* $\{\epsilon_k\}$ *such that the sequence* $\{u_{\epsilon_k}\}$ *converges in the space* $C([0, T], H)$.

Blow up for NSE

If the conditions of theorem 3.3 are satisfied then the Cauchy problem (3.1), (3.2) admites

1) the blow up phenomenon of polar type in the spaces $W_2^1(\Omega)$, $L_{p+2}(\Omega)$, $C_b(\Omega)$.

2) the blow up phenomenon of essential type in the space H.

We obtain that the values of solution of regularizing problem has no limit in the space H as $t \to T_1$, $\epsilon \to 0$ both for LSE and NSE admiting blow up phenomenon.

Then we should construct the evolution equation for dynamics of mixed quatnum states – Liouville - von Neuman equation, GKSL-equation for quantum state and Schrodinger equation in extended space.

4. Blow up phenomenon for solution and the destruction of quantum state

Let
$B(H)$ be the Banach algebra of bounded linear operators in the space H.

$\mathcal{A}$ be a C^*-subalgebra of Banach algebra $B(H)$.

$T_1(H)$ be the Banach space of trace class operators.

$B^*(H)$ be the Banach space conjugated to the space $B(H)$.

$\Sigma(H) = S_1(B^*(H)) \bigcap (B^*(H))_+$ be the set of quantum states.

$\Sigma_p(H)$ be the set of pure vector states, i.e. the following states $\rho_\varphi,\ \varphi \in S_1(H):\ \langle \rho_\varphi, \mathbf{A} \rangle = (\mathbf{A}\varphi, \varphi)$.

$\Sigma_n(H) = S_1(\sigma_1(H)) \bigcap (T_1(H))_+$ be the set of normal states.

Criteria of pure and normal state

$\Sigma_p(H)$ – the set of pure states.

$$\rho_u : \ B(H) \to \mathbb{C}, \quad \langle \rho_u, \mathbf{A} \rangle = (u, \mathbf{A}u)_H, \ \mathbf{A} \in B(H).$$

$\Sigma_n(H)$ – the set of normal states.

$\rho = \sum_{k=1}^{\infty} p_k \rho_{u_k}, \ \{u_k\}$ *is ONB*.

Let

$\mathcal{P}(H)$ be the set of finite dimensional orthogonal projectors;

$\mathcal{P}_1(H)$ be the set of 1-dimensional orthogonal projectors;

Lemma 4.1.

The state ρ is pure iff $\sup\limits_{u \in \mathcal{P}_1(H)} \langle \rho, \mathbf{P}_u \rangle = 1$.

The state ρ is normal iff $\sup\limits_{\mathbf{P} \in \mathcal{P}(H)} \langle \rho, \mathbf{P} \rangle = 1$.

Blow up phenomenon, self-focusing and state destruction

Definition

A solution $u(\cdot; u_0)$ of the Cauchy problem for Schrodinger equation admits

1) a gradient blow up phenomenon if there exists a number $T_1 \in (0, +\infty)$ such that $\lim\limits_{t \to T_1 - 0} \|u(t; u_0)\|_{H^1} = +\infty$;

2) a self-focusing phenomenon at the point $x_1 \in \Omega$ if there exists a number $T_1 \in (0, +\infty)$ such that
$\lim\limits_{t \to T_1 - 0} \int\limits_{\Omega} |x_1 - x|^2 |u(t, x; u_0)|^2 dx = 0,$

3) a pure state destruction if there are numbers $T_1 \in (0, +\infty)$ and a sequence $\{t_k\}$ such that $t_k \to T_1 - 0$, and a sequence $\{u(t_k; u_0)\}$ weakly converges to $u_* \in H$ such that $\|u_*\| < \|u_0\|$.

4) a normal state destruction if there are numbers $T_1 \in (0, +\infty)$ and a sequence $\{t_k\}$ such that $t_k \to T_1 - 0$ and the ineqaulity $\sup\limits_{\mathbf{P} \in \mathcal{P}(H)} [\lim\limits_{k \to \infty} \langle \rho_{u(t_k, u_0)}, \mathbf{P} \rangle] < 1$ holds.

Blow up phenomenon, self-focusing and state destruction

Point out the correlations between phenomena of the gradient blow up, the destruction of a pure state and the solution self-focusing.

Theorem 4.1. *Let* $T_1 \in (0, +\infty)$ *and* $u(t; u_0)$, $t \in [0, T_1)$ *be an* H^1*-solution of the Cauchy problem for Schrodinger equation in the space* $H = L_2(\Omega)$, Ω *is a domain in* R^d, $d = 1, 2$.
Then the following implications are valid $d) \Rightarrow c) \Rightarrow b) \Rightarrow a)$.
Here conditions $a)$, $b)$ *and* $c)$ *mean the following:*
a) a solution admits the gradient blow up for $t \to T_1 - 0$;
b) a solution admits the destruction of pure state for $t \to T_1 - 0$;
c) a solution admits the destruction of normal state for $t \to T_1 - 0$;
d) a solution admits the self-focusing phenomenon for $t \to T_1 - 0$.
Moreover, $a) \Rightarrow b)$ *for Cauchy problem (3.1), (3.2) for NSE with* $p = 4$.

Remark. Let Ω be a domain in the space R^d. Then the blow up in the Sobolev space $W_2^l(R^d)$ is the consequence of the destruction of pure state for $l \geqslant \frac{d}{2}$.

5. Regularized dynamics in the set of states for NSE

Let $p \geqslant 0$, $\epsilon > 0$. The group $\mathbf{T}_\epsilon$ acts on an element $\rho_{u_0} \in \Sigma_p(H)$ by the rule

$$\mathbf{T}_\epsilon(t)\rho_{u_0} = \rho_{\mathbf{W}_\epsilon(t)u_0}, \ t \in \mathbb{R}, \ \rho_{u_0} \in \Sigma_p(H).$$

Regularized nonlinear Liouville-von Neumann equation

$$i\frac{d}{dt}\rho(t) = [\mathbf{\Delta} + \mathbf{f}_\epsilon(\rho(t)), \rho(t)], \ t > 0. \tag{5.1}$$

Here $\mathbf{f}_\epsilon(\rho(t))\varphi = V_\epsilon((w_{\rho(t)})^{\frac{1}{2}})\varphi, \ \varphi \in H$;

$$\int_\Omega w_{\rho(t)}(x)|\varphi(x)|^2 dx = (\rho(t)\varphi, \varphi)_H, \ \forall \ \varphi \in H.$$

We study the limit points of the directed family in weak-* topology of the space $(B(H))^*$

$$\mathbf{T}_\epsilon \rho_{u_0} = \rho_\epsilon(t, \rho_{u_0}), \ \epsilon \to 0.$$

Random dynamics in the set of quantum states

Let $\mathcal{A}^*$ be the σ-algebra of subsets generated by the family of functionals $\{\Phi_{\mathbf{A}}: \ \rho \to \rho(\mathbf{A}), \ \mathbf{A} \in B(H)\}$ on the set $\Sigma(H)$.

Let $W_0(0,1)$ be the set of nonnegative finite additive measures on the measurable space $((0,1), 2^{(0,1)})$ concentrated in an arbitrary punctured right half-neighborhood of the point 0 and normalized by the equality $\nu((0,1)) = 1$. Here $2^{(0,1)}$ is the σ-algebra of all subsets of the interval (0, 1).

The solutions of regularized Cauchy problems (3.2), (3.4) and the measure ν on the measurable space $((0,1), 2^{(0,1)})$ define the random process with values in the set $\Sigma_p(H)$.

$$((0,1), 2^{(0,1)}, \nu) \times \mathbb{R} \quad \to \quad (\Sigma_p(H), \mathcal{A}^*)$$

$$(0,1) \times \mathbb{R} \to \Sigma_p(H); \qquad (\epsilon, t) \to \rho_{\mathbf{W}_\epsilon(t)u_0}$$

Quantum states and the measures on the unite sphere $S_1(H)$

Proposition 5.1. *For any* $\rho \in \Sigma(H)$ *there is the measure* $\nu : \ 2^{S_1(H)} \to [0,1]$ *such that*

$$\langle \rho, \mathbf{A} \rangle = \int\limits_{S_1(H)} (u, \mathbf{A}u) d\nu(u) \quad \forall \quad \mathbf{A} \in B(H) \tag{5.2}$$

If the measure ν *in (5.2) is countable additive then the state* ρ *is normal.*

We can identify

1) the quantum state,

2) the mean value of the random variable with values in the measurable space of pure quantum states $(\Sigma_p(H), \mathcal{A}^*)$.

The continuation of solution by the random process

Let $(E, \mathcal{A}, \nu)$ be a measurable space with the measure where $E = (0,1),\ \mathcal{A} = 2^{(0,1)},\ \nu \in W_0(0,1)$.

$$(E, \mathcal{A}, \nu) \to (\Sigma(H), \mathcal{A}^*)$$

Then for any $u_0 \in H$ the directed family of problems (3.2), (3.4) defines the random process $\rho_{u_\epsilon(t,u_0)}$ with the values in $\Sigma_p(H)$.

$$\mathcal{T} :\ E \times \mathbb{R} \times \Sigma_p(H) \to \Sigma_p(H); \qquad \mathcal{T}_\epsilon(t)\rho_{u_0} = \rho_{\mathbf{W}_\epsilon(t)u_0}$$

The mean values of the random processes are

$$\mathrm{M}\mathcal{T} = \mathcal{T}^\nu : \quad \mathcal{T}^\nu(t)\rho_{u_0} = \int\limits_E \rho_{u_\epsilon(t,u_0)} d\nu(\epsilon);$$

$$\langle \mathcal{T}^\nu(t)\rho_{u_0}, \mathbf{A}\rangle = \int\limits_E \langle \rho_{u_\epsilon(t,u_0)}, \mathbf{A}\rangle d\nu(\epsilon)\ \forall\ \mathbf{A} \in B(H).$$

Limit points of regularized solutions

Theorem 5.1. *For any $t \geqslant 0$ and $u_0 \in H^1$ the equality holds:*

$$\mathrm{Ls}_{\epsilon\to 0}\mathbf{T}_\epsilon(t)\rho_{u_0} = \bigcup_{\nu\in W_0(0,1)} \mathcal{T}^\nu(t)\rho_{u_0},$$

where $\mathrm{Ls}_{\epsilon\to 0}\mathbf{T}_\epsilon(t)\rho_{u_0}$ is the set of all limit points of the directed set $\mathbf{T}_\epsilon(t)\rho_{u_0}$, $\epsilon \in (0,1)$, $\epsilon \to 0$, in the $*$-weak topology of the space $B^*(H)$.

The multy-valued dynamical mappings

$$\mathbf{T}(t)\rho_{u_0} = \bigcup_{\nu\in W_0(0,1)} \mathcal{T}^\nu(t)\rho_{u_0}$$

should be endowed with the structure of random process. For this aim the measure on the set $\bigcup_{\nu\in W_0(0,1)} \mathcal{T}^\nu(t)\rho_{u_0}$ should be introduced for any $t \geqslant 0$.

The continuation of solution by the random process

Theorem 5.2. *Let $\nu \in W_0(0,1)$, $u_0 \in H^1$, and $[0, T_1)$ be the existence interval of the H^1-solution for Cauchy problem (3.1), (3.2).*
Then the mean value of random process $\rho_{u_\epsilon(t;u_0)}$, $t \in \mathbb{R}_+$, defines the one-parameter family of quantum states

$$\mathcal{T}^\nu(t)\rho_{u_0} = \rho^\nu(t, \rho_{u_0}); \quad \rho^\nu(t, \rho_{u_0}) = \int\limits_{(0,1)} \rho_{u_\epsilon(t,u_0)} d\nu(\epsilon),\ t \in \mathbb{R}_+$$

which has the following properties

i) $\rho^\nu(t, \rho_{u_0}) = \rho_{u(t;u_0)}\ \forall\ t \in [0, T_1)$;

ii) $\rho^\nu(t, \rho_{u_0}) \in \Sigma(H)\ \forall\ t \geqslant 0$;

iii) $\rho^\nu(T_1, \rho_{u_0}) \notin \Sigma_n(H)$ *if* $p = 4,\ T_1 < +\infty$.

The continuation of solution by the random process

The one-parametric family of dynamical mappings $\mathcal{T}^{\nu}(t)$, $t \geqslant 0$, can be presented as the partial trace of one-parametric semigroup of nonlinear mappings of pure states set in the extended Hilbert space.

$$\mathcal{H} = L_2((0,1), 2^{(0,1)}, \nu, H).$$

$$U_0(\epsilon) = u_0,\ \epsilon \in (0,1).$$

$$\mathcal{U}(t)U_0(\epsilon) = u_\epsilon(t, u_0),\ \ t \geqslant 0,\ \ \epsilon \in (0,1).$$

$\mathcal{U}(t) :\ \mathcal{H} \to \mathcal{H}$ is the one-parametric group of nonlinear mappings.

Theorem 5.3. *Let* $\nu \in W_0(0,1)$, $u_0 \in H$. *Then* $\mathcal{T}^{\nu}(t)\rho_{u_0}$ *is the partial trace of pure vector state* $\rho_{\mathcal{U}(t)U_0} \in \Sigma_p(\mathcal{H})$ *which is defined as the restriction of the state* $\rho_{\mathcal{U}(t)U_0}$ *onto* C^* *subalgebra* $\mathcal{A}_H = B(H) \otimes \mathbf{I}_E :\ \ \mathbf{A} \otimes \mathbf{I}_E U(\epsilon) = \mathbf{A}U(\epsilon),\ \epsilon \in (0,1),\ \ \mathbf{A} \in B(H)$.

$$\langle \mathcal{T}^{\nu}(t)\rho_{u_0}, \mathbf{A}\rangle = (\mathcal{U}(t)U_0, (\mathbf{A} \otimes \mathbf{I}_E)\mathcal{U}(t)U_0),\ \ \mathbf{A} \in B(H).$$

The continuation of solution by the random process

The solution of Cauchy problem (3.1), (3.2) is continued on the semiaxe $[0, +\infty)$
by the random process $\mathcal{T}\rho_{u_0}: \ E \times \mathbb{R}_+ \to \Sigma_p(H)$
$\Leftrightarrow$
by the one-parametric family of quantum states $\mathcal{T}^{\nu}(t)\rho_{u_0}, \ t \geqslant 0$.

One-parametric family $\mathcal{T}^{\nu}(t), \ t \geqslant 0$, is not a semigroup.

The sequence of iterations $\{\mathcal{S}_n(t) = (\mathcal{T}^{\nu}(\frac{t}{n}))^n, \ t \geqslant 0\}$ can be approximation of some averaged semigroup (Volovich, Sakbaev 2018).

6. Liouville von Neuman equation for the dynamics of mixed Sobolev states

The space of normal states is the space of trace-class operators $T_1(H)$ endowed with the trace norm $\|\cdot\|_1$.
The set $\sigma_1(H)$ of normal states is the intersection of the unite sphere with the positive cone on the space $T_1(H)$.

Definition

The space of Sobolev states is the subspace $T_1^1(H)$ of the normal state space $T_1(H)$ such that for any $\mathbf{A} \in T_1^1(H)$ the condition $\mathbf{DAD} \in T_1(H)$ holds where $\mathbf{D} = \sqrt{-\boldsymbol{\Delta}}$.

The space $T_1^1(H)$ endowed with the norm $\|\mathbf{A}\|_{1,1} = \|\mathbf{A}\|_1 + \|\mathbf{DAD}\|_1$.

Dynamics in the space of quantum states

Sobolev states set $\Sigma_p^k(H) = \{\rho_u,\ u \in H^k \bigcap S_1(H)\},\ k \in \mathbb{N}$.
The family of dynamical mappings of the set $\Sigma_p^k(H)$ is investigated.

For $p \in [0,4)$ the group $\mathbf{T}$ (see Theorem 3.2) acts on an element $\rho_{u_0} \in \Sigma_p(H)$ by the rule

$$\mathbf{T}(t)\rho_{u_0} = \rho_{\mathbf{V}(t)u_0} \equiv \rho(t, \rho_{u_0}),\ t \geqslant 0,\ \rho_{u_0} \in \Sigma_p^1(H).$$

Then the function $\mathbf{T}(t)\rho_{u_0}$ satisfies the following nonlinear Liouville-von Neumann equation with the initial condition

$$i\frac{d}{dt}\rho(t) = [\mathbf{\Delta} + \mathbf{f}(\rho(t)), \rho(t)],\ t > 0; \qquad (6.1)$$

$$\rho(+0) = \rho_0,\ \rho_0 \in \Sigma(H), \qquad (6.2)$$

$$\mathbf{f}(\rho(t))\varphi(x) = (w_{\rho(t)}(x))^{\frac{p}{2}}\varphi(x),\ \varphi \in H,$$

where $\int\limits_\Omega w_{\rho(t)}(x)|v(x)|^2 dx = (v, \rho(t)v)\ \forall\ v \in H$.

$w_{\rho(t)}(x) = \sum\limits_{k=1}^{\infty} p_k(t)|u_k(t,x)|^2$ for $\rho(t) = \sum\limits_{k=1}^{\infty} p_k(t)\rho_{u_k(t)}$.

Sobolev solution of Liouville von Neuman equation

Definition

A continuous mapping $\rho: \ [0, T] \to T_1^1(H), \ T > 0$, is called Sobolev solution of Cauchy problem (6.1), (6.2), if

$$\rho(t) = e^{-i\mathbf{\Delta} t}\rho(0)e^{i\mathbf{\Delta} t} +$$

$$+\int_0^t e^{-i\mathbf{\Delta}(t-s)}[\mathbf{f}(\rho(s))\rho(s) - \rho(s)\mathbf{f}(\rho(s))]e^{i\mathbf{\Delta}(t-s)}ds, \ t \in [0, T].$$

The energy functional of LvN equation is $E: \ T_1^1(H) \to \mathbb{R}$

$$E(\rho) = \frac{1}{2}\mathrm{Tr}(\mathbf{D}\rho\mathbf{D}) - \int_{\mathbb{R}} F(w_{\rho(t)}(x))dx,$$

where $F(w_{\rho(t)}(x)) = \frac{1}{p+2}(w_{\rho(t)}(x))^{\frac{p}{2}+1}$.
The main idea is to consider the Liouville von Neuman equation as the Schrodinger equation in the extended space.

Local Sobolev solution of LvN equation

Theorem 6.1. *Let* $p \geqslant 0$. *Let the initial data (6.2) is given by the density operator*

$$\rho_0 = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j}, \tag{6.3}$$

where $\{u_j, j = 1, ..., m, ...\}$ *is orhthonormal basis of vectors in the space* H. *Let* $\rho_0 \in T_1^1(H)$. *For any* $M > 0$ *there is the number* $\delta > 0$ *such that if* $\|\rho_0\|_{T_1^1(H)} < M$, *then the Cauchy problem (6.1), (6.2) has the unique Sobolev solution on the segment* $[-\delta, \delta]$.

Theorem 6.2. *Let* $p \geqslant 0$. *Let the initial data (6.2) is given by the density operator (6.3) and* $\rho_0 \in T_1^1(H)$. *If* $\rho(t)$, $t \in [0, T]$ *is the Sobolev solution of Cauchy problem (6.1), (6.2) then* $E(\rho(t)) = E(\rho_0)$, $t \in [0, T]$.

Global existense and blow up of Sobolev solutions

Theorem 6.3. *Let* $p \in [0, 4)$ *and* $\rho_0 \in T_1^1(H)$. *Then Sobolev solution of Cauchy problem (6.1), (6.2) exists and unique on the whole axe* $\mathbb{R}$.

Theorem 6.4. *Let* $p \in [4, +\infty)$ *and* $\rho_0 \in T_1^3(H)$. *If* $E(\rho) > 0$ *then there is a real* $T_1 \in (0, +\infty)$ *such that a Sobolev solution of Cauchy problem (6.1), (6.2) exists on the segment* $[0, T_1)$ *only. Moreover this solution* $\rho(t, \rho_0)$, $t \in [0, T_1)$ *in unigue on the segment* $[0, T_1)$ *and*

$$\lim_{t \to T_1 - 0} \|\rho(t, \rho_0)\|_{T_1^1} = +\infty.$$

Conclusions

The following questions are studied:

Regularization of Cauchy problem as the topological space of initial-boundary value problems.

The set of limit points of directed set of regularizing problems.

The relationship between the phenomena of gradient blow up, self-focusing and destruction of quantum state.

Blow up and destruction of the state for nonlirear Schrodinger and nonlinear Liouville - von Neuman equations.

The extension of one-parametric family of dynamical mappings on the quantum state set through the moment of blow up.

Thank you for attention