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PARTIAL DIFFERENTIAL EQUATIONS

Dynamics of a Set of Quantum States Generated by a Nonlinear Liouville–von Neumann Equation

A. D. Grekhneva[a,*] **and V. Zh. Sakbaev**[b,c,d,e,**]

[a] *Gromov Flight Research Institute, Zhukovskii, Moscow oblast, 140180 Russia*
[b] *Moscow Institute of Physics and Technology (National Research University), Dolgoprudnyi, Moscow oblast, 141701 Russia*
[c] *Steklov Mathematical Institute, Russian Academy of Sciences, Moscow, 119991 Russia*
[d] *Open Education Institute, Lobachevsky State University of Nizhny Novgorod (National Research University), Nizhny Novgorod, 603950 Russia*
[e] *Institute of Mathematics with Computing Center, Ufa Federal Research Center, Russian Academy of Sciences, Ufa, 450008 Bashkortostan, Russia*
**e-mail: alice-prohorses@yandex.ru*
***e-mail: fumi2002@mail.ru*

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Abstract—A model describing the dynamics of a set of quantum states generated by a nonlinear Schrödinger equation is studied. The relationship between the blow-up of a solution with self-focusing and the transition from pure to mixed states of a quantum system was investigated in [1]. In this context, a natural question is concerned with the dynamics generated by the nonlinear Schrödinger equation in the set of mixed quantum states. The dynamics of mixed quantum states is described by the Liouville–von Neumann equation corresponding to the nonlinear Schrödinger equation. For the former equation, conditions for the global existence of a unique solution of the Cauchy problem and blow-up conditions are obtained.

Keywords: nonlinear Schrödinger equation, quantum state, gradient catastrophe, regularization
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1. FORMULATION OF THE PROBLEM

In this work, we study the evolution of a set of quantum states generated by a nonlinear Schrödinger equation with a potential being a power function of the state probability density in coordinate space:

$$i\frac{du}{dt} = \mathbf{\Delta}u(t) + \mathbf{V}(u(t))u(t), \quad t \in (0,T), \quad T \in (0,+\infty], \tag{1.1}$$

$$u(+0) = u_0, \quad u_0 \in H \equiv L_2([-\pi,\pi]). \tag{1.2}$$

Here, $\mathbf{V}(u) \equiv |u|^p$ with $p \geq 0$ and $\mathbf{\Delta}$ is the Laplacian in the space H whose domain is the space H^2 of functions from the Sobolev space $W_2^2(-\pi,\pi)$ satisfying the homogeneous Dirichlet boundary conditions $u(-\pi) = 0$ and $u(\pi) = 0$. It was shown in [1] that, for low nonlinearity exponents $p \in [0,4)$, the Cauchy problem (1.1), (1.2) generates a continuous group $\mathbf{U}(t)$, $t \in \mathbb{R}$, of nonlinear transformations of the initial data space $H^1 = D(\sqrt{-\mathbf{\Delta}})$ that preserve the H-norm of the solution and the value of the energy functional

$$E(u) = \int_{-\pi}^{\pi}\left(-\frac{1}{2}|\nabla u|^2 + \frac{1}{p+2}|u|^{p+2}\right)dx$$

on the vectors $u(t) = \mathbf{U}(t)u_0$, $t \in \mathbb{R}$. For $p \geq 4$, it will be shown that there are initial data (1.2) for which the solution of the Cauchy problem admits finite-time self-focusing, which is followed by gradient blow-up of the solution.

Nonlinear Schrödinger equations were intensively investigated in the context of mathematical justification of wave self-focusing in nonlinear optical media (see [2]). Nonlinear Schrödinger equations were studied in d-dimensional Euclidean space and its subdomains, and various nonlinear dependences of the interaction potential on the unknown wave function were examined (see [3–7]).

It was shown in [3–6] that the Cauchy problem for a nonlinear Schrödinger equation with a nonlinear potential being a power-law dependence on the unknown function either has a unique global solution or a local solution that blows up when the boundary of the solution existence interval is approached. In the former case, the Cauchy problem determines a one-parameter group of transformations of the initial data space, and, in the latter case, the solution existence interval of the Cauchy problem depends on the initial condition; moreover, the length of the existence interval can take any positive value depending on the choice of the initial data (see [1, 4–6]).

In [8, 9], a regularization procedure was proposed that approximates the Cauchy problem with a blowing-up solution by a directed family of Cauchy problems. By a regularization of the Cauchy problem, we mean a topological space of initial-boundary value problems in which the Cauchy problem under study is a limit point (see [9]). For the Cauchy problem with a polynomial nonlinearity, a regularization is specified as a one-parameter family of Cauchy problems for the nonlinear Schrödinger equation in each of which the nonlinear Hamiltonian is a semi-bounded nonlinear operator (which ensures the global solvability of the regularized Cauchy problem in the space corresponding to the energy functional). Moreover, the directed family of graphs of regularized Schrödinger operators converges to the graph of the Hamiltonian of the Cauchy problem under study on the everywhere dense common domain of these nonlinear operators. In [1, 8] the original Schrödinger equation (1.1) was approximated by its energy regularizations specified by a directed set of energy functionals semi-bounded from below:

$$E_\epsilon(u) = \int_{-\pi}^{\pi}\left(\frac{\epsilon}{2}|\Delta u|^2 - \frac{1}{2}|\nabla u|^2 + \frac{1}{p+2}|u|^{p+2}\right)dx, \quad \epsilon \in (0,1), \quad \epsilon \to +0.$$

It was shown in [1, 8] that the directed set of solutions to Cauchy problems for regularized Schrödinger equations converges to the solution of Cauchy problem (1.1), (1.2) on the entire solution existence interval of the last. On intervals containing the boundary points of the solution existence interval for problem (1.1), (1.2), the sequence of regularized solutions was established to diverge. Outside the solution existence interval of Cauchy problem (1.1), (1.2), the directed set of solutions to Cauchy problems for the Schrödinger equation with a regularized operator has a limit set in the space $(B(H))^*$ of quantum states equipped with the $*$-weak topology. Equipping the set of regularized problems with the structure of a measurable space with a measure makes it possible to define a one-parameter family of measures on the set of vector quantum states, i.e., a one-parameter family of mixed quantum states.

In this context, we consider the Cauchy problem for the Liouville–von Neumann equation

$$i\frac{d}{dt}\rho(t) = [\mathbf{\Delta} + \mathbf{V}(\rho(t)), \rho(t)], \quad t > 0, \tag{1.3}$$

$$\rho(+0) = \rho_0, \quad \rho_0 \in \Sigma(H), \tag{1.4}$$

where $\Sigma(H)$ is a set of quantum states defined as the intersection of the unit sphere with the cone of positive elements of the space $(B(H))^*$ of linear continuous functionals on the Banach algebra of bounded linear operators $B(H)$. Here, $\mathbf{V}$ is a mapping of some set D from the space of quantum states $(B(H))^*$ to the set of linear operators in H, which to each state $r \in D$ assigns the operator $\mathbf{V}(r)$ of multiplication by a function depending on the state r. If the potential $\mathbf{V}(u)$ in the nonlinear Schrödinger equation (1.1) is the operator of multiplication by the function $(w_u(x))^{p/2}$, where $w_u(x) = |u(x)|^2$ for $x \in (-\pi, \pi)$, then the potential $\mathbf{V}(\rho)$ in the nonlinear Liouville–von Neumann equation (1.3) is the operator of multiplication by the function $(w_\rho(x))^{p/2}$, where

$$w_\rho(x) = \sum_{k=1}^{\infty} p_k |u_k(x)|^2, \quad x \in (-\pi, \pi),$$

provided that the quantum state is specified by the density operator $\rho = \sum_{j=1}^{\infty} p_k \mathbf{P}_{u_k}$ with a set of eigenvalues p_k, $k \in \mathbb{N}$, and an orthonormal basis of eigenvectors $\{u_k\}$. Here and below, $\mathbf{P}_u$ denotes the one-dimensional orthogonal projector onto the linear span of the vector $u \in H$.

Thus, given the Cauchy problem for a nonlinear Schrödinger equation, we can specify a one-parameter family of transformations of the set of quantum states $\Sigma(H)$ into itself that is an extension of the transformation taking each initial value of Cauchy problem (1.1), (1.2) to its solution. Under this extension, a pure state is transformed into a mixed one in the transition through the moment of the gradient blow-up. The task is to extend the family of dynamic transformations from the set of vector states to the set of mixed states and to determine the conditions under which this extended family of transformations is a semigroup. Additionally, we determine the relationship between the extended transformation and the solution of the Cauchy problem for the Liouville–von Neumann equation (1.3), (1.4).

Note that the study of dynamical systems generated by Hamiltonians on an infinite-dimensional phase space, including the Schrödinger equation (see [10]), leads to the study of not only vector states, but also of general ones (i.e., nonnegative linear normed functionals) on the algebra of bounded linear operators and its various subalgebras (see [11, 12]).

In this paper, the Sobolev normal quantum state is defined as a mixture of vector quantum states determined by vectors from a Sobolev space. The Sobolev solution of the Cauchy problem for the Liouville–von Neumann equation (1.3), (1.4) is defined. For the nonlinear Liouville–von Neumann equation, we propose a method of study based on its reduction to a nonlinear Schrödinger equation in an extended Hilbert space. Conditions under which the Cauchy problem (1.3), (1.4) specifies a continuous group of transformations of a set of Sobolev quantum states are obtained, and conditions for finite time blow-up of Sobolev states are derived.

2. LIOUVILLE–VON NEUMANN EQUATION AND THE SCHRÖDINGER EQUATION IN EXTENDED SPACE

Let $H = L_2(\mathbb{R})$ be the Hilbert space of a quantum system and $B(H)$ be the Banach space of bounded linear operators in H. The space of quantum states is defined as the space $B^*(H)$ of linear continuous functionals on the Banach space $B(H)$. The set of quantum states $\Sigma(H)$ is the intersection of the unit sphere with the positive cone in the space $(B(H))^*$ (see [13, 14]).

The space of normal quantum states is defined as the space of trace class operators $T_1(H)$ equipped with the trace norm $\|\cdot\|_1$. The set $S(H)$ of normal quantum states is the intersection of the unit sphere with the positive cone in the space $T_1(H)$ (see [13, 15, 16]).

Definition 1. The *space of Sobolev states* is a subspace $T_1^1(H)$ of the space $T_1(H)$ of normal states such that, for any $\mathbf{A} \in T_1^1(H)$, it is true that $\mathbf{DAD} \in T_1(H)$, where $\mathbf{D} = \sqrt{-\mathbf{\Delta}}$ is a self-adjoint operator in H with the domain

$$H^1 = \{u \in W_2^1([-\pi,\pi]):\ u(-\pi) = u(\pi) = 0\}.$$

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

Note that the operator $-\mathbf{\Delta}$ has a discrete spectrum located on the positive half-line $(0,+\infty)$. Therefore, the spectrum of the self-adjoint operator $\mathbf{D}$ is also discrete and lies on the positive half-line.

A normal state $\rho \in S(H)$ is called a Sobolev state if $\mathbf{D}\rho\mathbf{D} \in T_1(H)$. Each normal state $r \in T(H)$ can be represented in the form of a nonnegative trace class operator $\mathbf{r}$ with a unit trace having the form

$$\mathbf{r} = \sum_{j=1}^{\infty} p_j \mathbf{P}_{v_j}, \tag{2.1}$$

where $p_j \geq 0$, $\sum_{j=1}^{\infty} p_j = 1$, $\mathbf{P}_v$ is the orthoprojector onto the one-dimensional linear space $\mathrm{span}(v)$, and $\{v_j\}$ is an orthonormal basis in H. Moreover, if $r \in T_1^1(H)$, then the vectors v_j in (2.1) satisfy the condition $v_j \in H^1$ $\forall j \in \mathbb{N}$ and

$$\sum_{j=1}^{\infty} p_j \|\mathbf{D}u_j\|_H^2 < +\infty. \tag{2.2}$$

A pure state of the quantum system with a wave function $u \in L_2(-\pi,\pi)$ specifies a probability distribution on the coordinate space $[-\pi,\pi]$ with an absolutely integrable density $w_u(x) = |u(x)|^2$, $x \in [-\pi,\pi]$. A mixed state with a density operator $\rho = \sum_{k=1}^{\infty} p_k \mathbf{P}_{v_k}$ specifies a probability distribution with an absolutely integrable density

$$w_\rho(x) = \sum_{k=1}^{\infty} p_k |v_k(x)|^2, \quad x \in [-\pi, \pi].$$

If ρ is a Sobolev state, then condition (2.2) implies that $w_\rho \in W_1^1(-\pi,\pi)$. Since each function from the space $W_1^1(-\pi,\pi)$ can be treated (after changing it on a set of measure zero) as a continuous function on the interval $[-\pi,\pi]$, on the set $\Sigma_1(H)$ of Sobolev states, a mapping $\mathbf{V}(\cdot)$ can be defined that takes each state $r \in T_1^1(H)$ to the linear operator $\mathbf{V}(r) \in B(H)$ of multiplication by the continuous function

$$f(w_r(x)) = (w_r(x))^{p/2} = \left(\sum_{k=1}^{\infty} p_k |v_k(x)|^2 \right)^{p/2}, \quad x \in (-\pi, \pi).$$

Here, $p \geq 0$ is a parameter of the nonlinear dependence of the potential on the density (see (1.1), (1.3)).

Lemma 1. *If* ρ *is a Sobolev state, then the operator* $\mathbf{V}(\rho)$ *of multiplication by the function* $f(w_\rho(x)) = (w_\rho(x))^{p/2}$ *is a bounded linear operator in the space* H.

Proof. Since $\rho \in T_1^1(H)$, we have $\rho = \sum_{k=1}^{\infty} p_k \mathbf{P}_{u_k}$, where $p_k \geq 0$ $\forall k \in \mathbb{N}$, $\sum_{k=1}^{\infty} p_k = 1$, and $u_k \in H^1 \, \|u_k\|_H = 1 \, \forall k \in \mathbb{N}$. Therefore, for any $k \in \mathbb{N}$, the function $u_k \in C([-\pi,\pi])$ can be regarded as continuous (after changing it on a set of measure zero); moreover, there exists a constant $B_0 > 0$ such that $\|u_k\|_{C([-\pi,\pi])} \leq B_0 \|u_k\|_{H_1}$ for any $k \in \mathbb{N}$. Therefore, for any $x \in [-\pi,\pi]$,

$$(w_\rho(x))^{p/2} = \left[\left(\sum_{k=1}^{\infty} p_k |u_k(x)|^2 \right)^{1/2} \right]^p \leq \left(\sum_{k=1}^{\infty} p_k |u_k(x)|^2 \right)^p \leq \left(B_0^2 \sum_{k=1}^{\infty} p_k \|u_k\|_{H^1}^2 \right)^p.$$

Thus, if $\rho \in T_1^1(H)$, then the function $\mathbf{V}(\rho)$ is continuous and there exists a constant $c_1 > 0$ such that $\|\mathbf{V}(\rho)\|_{B(H)} \leq c_1 \|\rho\|_{T_1^1(H)}^{2p}$.

Definition 2. A continuous mapping of the interval $[0,T]$, $T > 0$, to the space $T_1^1(H)$ is called a *Sobolev solution of the Cauchy problem* (1.1), (1.2) if

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

To study the Liouville–von Neumann equation, we introduce the extended Hilbert space $\mathcal{H} = \oplus_{k=1}^{\infty} H_k$, where the space H_k is isomorphic to H for each $k \in \mathbb{N}$. As a result, the nonlinear Liouville–von Neumann equation (1.3) for the unknown function with values in the space of quantum states $T_1(H)$ can be considered a nonlinear Schrödinger equation of form (1.1) for the unknown function with values in the space $\mathcal{H}$.

Consider Hilbert spaces $\mathcal{H} = \oplus_{k=1}^{\infty} H_k$, $\mathcal{H}^1 = \oplus_{k=1}^{\infty} H_k^1$, and $\mathcal{H}^2 = \oplus_{k=1}^{\infty} H_k^2$, where the spaces $H_1, \ldots, H_m, \ldots$ are isomorphic to H, the spaces $H_1^1, \ldots, H_m^1, \ldots$ are isomorphic to H^1, and the spaces $H_1^2, \ldots, H_m^2, \ldots$ are isomorphic to H^2. The operator $\hat{\Delta}$ in the space $\mathcal{H}$ is defined as

$$\hat{\Delta} = \oplus_{j=1}^{\infty} \Delta_j,$$

so that

$$\hat{\Delta}(\oplus_{j=1}^{\infty} u_j) = \oplus_{j=1}^{\infty} \Delta u_j.$$

The nonlinear mapping $\hat{\mathbf{W}}$ of the space $\mathcal{H}^1$ to the space $\mathcal{H}$ is defined as applied to a vector $U = \oplus_{j=1}^{\infty} u_j \in \mathcal{H}^1$ according to the rule

$$\hat{\mathbf{W}}(U)U = \oplus_{j=1}^{\infty} \mathbf{V}\left(\sum_{k=1}^{\infty} p_k(U)\mathbf{P}_{u_k}\right)u_j, \quad U \in \mathcal{H}^1, \tag{2.3}$$

where, for each $\rho = \sum_{j=1}^{\infty} p_j \mathbf{P}_{v_j} \in T_1^1(H)$, the operator $\mathbf{V}(\rho) \in B(H)$ is defined as the operator of multiplication by the function $f(w_\rho(x)) = (w_\rho(x))^{p/2}$.

In equality (2.3), $u_j = \mathbf{P}_{H_j}(U)$, $U \in \mathcal{H}$, and $p_k(U) = \|\mathbf{P}_{H_j}(U)\|_H^2$, where the projector $\mathbf{P}_k: \mathcal{H} \to H_k$ is defined as $\mathbf{P}_k(\oplus_{j=1}^{\infty} u_j) = u_k$.

Along with Cauchy problem (1.3), (1.4), we consider the Cauchy problem for the nonlinear Schrödinger equation (2.4), (2.5)

$$i\frac{d}{dt}U(t) = \hat{\Delta}U(t) + \hat{\mathbf{W}}(U(t))U(t), \quad t > 0, \tag{2.4}$$

$$U(+0) = U_0, \quad U_0 = \oplus_{j=1}^{\infty} u_{0j} \in \mathcal{H}. \tag{2.5}$$

The $\mathcal{H}^1$-solution of the Cauchy problem (2.4), (2.5) on the interval $[0,T]$, $T > 0$, is a mapping $U(\cdot) \in C([0,T], \mathcal{H}^1)$ such that

$$U(t) = \exp(-i\hat{\Delta}t)U_0 - i\int_0^t \exp(-i\hat{\Delta}(t-s))\hat{\mathbf{W}}(U(s))U(s)ds, \quad t \in [0,T]$$

(see [1]).

Theorem 1. *The operator function*

$$\rho(t, \rho_0) = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j(t)}, \quad t \in [0,T],$$

is a Sobolev solution of problem (1.3), (1.4) *with initial data* $\rho_0 = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_{0j}}$ *if and only if the function* $U(t) = \oplus_{j=1}^{m} u_j(t)$*,* $t \in [0,T]$*, is an* $\mathcal{H}^1$*-solution of the Cauchy problem for the nonlinear Schrödinger equation* (2.4), (2.5).

Proof. 1. First, we show that, if $\rho(t)$, $t \in [0,T]$, is a Sobolev solution of the Cauchy problem (1.3), (1.4), then it can be represented in the form

$$\rho(t) = \sum_{k=1}^{\infty} p_k \mathbf{P}_{u_k(t)},$$

where the set of functions $u_k(\cdot)$, $k \in \mathbb{N}$, is such that the function

$$U(t) = \oplus_{k=1}^{\infty} \sqrt{p_k} u_k(t), \quad t \in [0,T],$$

solves the Cauchy problem for the Schrödinger equation (2.4), (2.5) with initial data $U_0 = \oplus_{k=1}^{\infty} \sqrt{p_k} u_k$.

If $\rho(t)$, $t \in [0,T]$, is a Sobolev solution of the Cauchy problem (1.3), (1.4), then the function $f(w_{\rho(t)})$, $t \in [0,T]$ belongs to the space $C([0,T], C[-\pi,\pi])$ and the function $\rho(t)$, $t \in [0,T]$, is a solution of the Cauchy problem for the linear Liouville–von Neumann equation

$$i\frac{d}{dt}\rho(t) = [\mathbf{L}(t), \rho(t)], \quad t \in [0,T], \tag{2.6}$$

with initial condition (1.4) and the time-dependent linear evolution operator $\mathbf{L}(t) = \mathbf{\Delta} + \mathbf{\Lambda}(t)$, where $\mathbf{\Lambda}(t)$ for each $t \in [0,T]$ is a linear bounded operator in $B(H)$ that is the operator of multiplication by the function

$$f(w_{\rho(t)}(x)) = (w_{\rho(t)}(x))^{p/2}, \quad t \in [0,T], \quad x \in [-\pi,\pi].$$

Therefore,

$$\rho(t) = \sum_{k=1}^{\infty} p_k \mathbf{P}_{u_k(t)},$$

where, for each $k \in \mathbb{N}$, the function $u_k\colon [0,T] \to H$ is a solution of the Cauchy problem for the Schrödinger equation

$$i\frac{d}{dt}u_k(t) = (\mathbf{\Delta} + \mathbf{\Lambda}(t))u_k(t), \quad t \in [0,T]; \quad u_k(0) = u_{0k}. \tag{2.7}$$

Therefore, the function

$$U(t) = \oplus_{k=1}^{\infty}\sqrt{p_k}u_k(t), \quad t \in [0,T],$$

solves the Cauchy problem for the Schrödinger equation

$$i\frac{d}{dt}U(t) = (\mathbf{\Delta} + \hat{\mathbf{M}}(t))U(t), \quad t \in [0,T]; \quad U(0) = U_0 = \oplus_{k=1}^{\infty}\sqrt{p_k}u_{0k},$$

where $\hat{\mathbf{M}}(t) \in B(\mathcal{H})$ is a linear operator in $\mathcal{H}$ defined as

$$\hat{\mathbf{M}}(t)(\oplus u_j) = \oplus(\mathbf{\Lambda}(t)u_j).$$

Since

$$\mathbf{\Lambda}(t,x) = \mathbf{V}(\rho(t)) = \left(\sum_{k=1}^{\infty} p_k |u_k(t,x)|^2\right)^{p/2},$$

we have $\hat{\mathbf{M}}(t)U(t) = \hat{\mathbf{W}}(U(t))U(t)$. Therefore, the function $U(t)$, $t \in [0,T]$, solves Cauchy problem (2.4), (2.5) with initial data $U_0 = \oplus_{k=1}^{\infty}\sqrt{p_k}u_{0k}$.

2. Now, let us show that, if the vector function $U(t) = \oplus_{j=1}^{\infty} p_j u_j(t)$, $t \in [0,T]$ is a solution of the Cauchy problem for the nonlinear Schrödinger equation (2.4), (2.5), then the operator function

$$\rho(t,\rho_0) = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j(t)}, \quad t \in [0,T],$$

is a Sobolev solution of problem (1.3), (1.4) with initial data $\rho_0 = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_{0j}}$.

If the vector function $U(t) = \oplus_{j=1}^{\infty}\sqrt{p_j}u_j(t,u_{0j})$, $t \in [0,T]$ is a solution of the Cauchy problem (2.4), (2.5), then this function is a solution of the linear Schrödinger equation with the time-dependent potential

$$\mathbf{M}(t,x) = \hat{\mathbf{W}}(U(t)) = \left(\sum_{j=1}^{\infty} p_j |u_j(t,x)|^2\right)^{p/2}, \quad (t,x) \in [0,T]\times[-\pi,\pi].$$

Therefore, the mapping $[0,T] \to T_1^1(H)$ defined by the equality $\rho(t) = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j(t,u_{0j})}$ is a solution of the Cauchy problem for the linear Liouville–von Neumann equation (2.6) with the time-dependent potential $\mathbf{M}(t,x)$, $(t,x) \in [0,T]\times[-\pi,\pi]$. Therefore, since $\mathbf{M}(t,x) = f(w_{\rho(t)}(x))$, the mapping $[0,T] \to T_1^1(H)$ defined by the equality $\rho(t) = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j(t,u_{0j})}$ is a Sobolev solution of the Cauchy problem for the nonlinear Liouville–von Neumann equation (1.3), (1.4) with initial data $\rho_0 = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_{0j}}$.

Corollary 1. If $\rho(t)$, $t \in [0,T]$, is a Sobolev solution of the Cauchy problem (1.3), (1.4) with initial data $\rho_0 = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j}$, then

$$\rho(t) = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j(t)}, \quad t \in [0,T], \tag{2.8}$$

where, for each $j \in \mathbb{N}$, the function $u_j(t)$, $t \in [0,T]$, is an H^1-solution of the Cauchy problem for Eq. (2.7) with the initial value u_j and the potential $\mathbf{\Lambda}(t) = \mathbf{V}(\rho(t))$, $t \in [0,T]$.

The transformations of the Sobolev space H^1 generated by the nonlinear Schrödinger equation (1.1) have the following properties:

(i) On each H^1-solution of Eq. (1.1), the H-norm of solution values is a constant: $\|u(t,u_0)\|_H = \|u_0\|_H$ $\forall t \in [0,T]$.

(ii) For each H^1-solution of Eq. (1.1), the energy functional preserves a constant value: $E(u(t,u_0)) = E(u_0)$, where

$$E(u) = \int_R \left[-\frac{1}{2}|\mathbf{D}u(x)|^2 + \frac{1}{p+2}|u(x)|^{p+2} \right] dx.$$

Note that a transformation of the Sobolev space may not preserve the inner product of H and the norm of H^1, i.e., the equality $(u(t,u_0),u(t,v_0))_H = (u_0,v_0)_H$, $t \in [0,T]$, and the equality $\|u(t,u_0)\|_{H^1} = \|u_0\|_{H^1}$, $t \in [0,T]$ may not hold. Let us show that a nonlinear transformation of the set of Sobolev states preserves the orthogonality of the vectors in the expansion of the density operator (2.8).

Corollary 2. *Let* $\rho(t)$, $t \in [0,T]$, be a Sobolev solution of the Cauchy problem (1.3), (1.4) with initial data $\rho_0 = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j}$. Then $(u_j(t),u_k(t))_H = (u_j,u_k)_H$ $\forall t \in [0,T]$, where $u_j(t)$, $u_k(t)$, $t \in [0,T]$, are the vectors in the expansion of density operator (2.8).

Proof. It suffices to recall that, by Corollary 1, the functions $u_j(t)$, $u_k(t)$, $t \in [0,T]$, are solutions of the Cauchy problem for the linear Schrödinger equation (2.7) with initial data u_j and u_k, respectively, and with the potential $\mathbf{\Lambda}(t) = \mathbf{V}(\rho(t))$, $t \in [0,T]$. Since $\mathbf{V}$ is a common potential for the evolution of the vector functions,

$$\frac{d}{dt}(u_j(t),u_k(t))_H = -i[(\mathbf{\Delta} + \mathbf{V}(\rho(t)))u_j(t),u_k(t))_H - (u_j(t),(\mathbf{\Delta} + \mathbf{V}(\rho(t)))u_k(t))_H] = 0.$$

Remark. Theorem 1 shows that the Cauchy problem for an unknown function with values in the space of density operators of the quantum system is equivalent to the Cauchy problem for an unknown function with values in the extended Hilbert space. Moreover, the extended Hilbert space describes quantum dynamics on a graph (see [17]) formed by a finite or countable set of edges with specially chosen boundary conditions (homogeneous Dirichlet conditions on each edge) and with a special nonlinear interaction potential determined by equality (2.3).

3. LOCAL SOLVABILITY OF THE CAUCHY PROBLEM FOR THE LIOUVILLE–VON NEUMANN EQUATION

Relying on the established equivalence between the Cauchy problems for the Liouville–von Neumann equation (1.3), (1.4) and the nonlinear Schrödinger equation (2.4), (2.5) and using the results of [1, 18], we can prove the following assertion.

Theorem 2. *Suppose that* $p \geq 0$. *Assume that the initial state* (1.4) *is specified by the density operator*

$$\rho_0 = \sum_{j=1}^{\infty} p_j \mathbf{P}_{u_j}, \tag{3.1}$$

where $\{u_j, j = 1,\ldots,m,\ldots\}$ *is an orthonormal system of vectors of the space* H. *Additionally, suppose that* $\rho_0 \in T_1^1(H)$. *Then, for any* $M > 0$, *there exists* $\delta > 0$ *such that, if* $\|\rho_0\|_{T_1^1(H)} < M$, *then the Cauchy problem* (1.3), (1.4) *has a unique Sobolev solution on the interval* $[-\delta,\delta]$.

Proof. The existence, on the interval $[-\delta, \delta]$, of a Sobolev solution to the Cauchy problem (1.3), (1.4) with initial data (3.1) is equivalent to the existence, on the same interval, of a solution to Cauchy problem (2.4), (2.5) with initial data $U_0 = \oplus_{j=1}^{\infty}\sqrt{p_j}u_j$. In [1, 18], a local existence and uniqueness theorem for Cauchy problem (2.4), (2.5) in the case $p \geq 0$ was proved by applying the same methods as in [3, 4, 8]. By Theorem 1, that result implies the assertion of Theorem 2.

4. ENERGY CONSERVATION

On the set $T_1^1(H)$ of Sobolev states, we define a functional E that maps each Sobolev state ρ to the number

$$E(\rho) = -\frac{1}{2}\mathrm{Tr}(\mathbf{D}\rho\mathbf{D}) + \int_{\mathbb{R}} \frac{1}{p+2}(\rho(x,x))^{p/2+1}dx.$$

Theorem 3. *Suppose that* $p \geq 0$. *Assume that the initial state* (1.4) *is specified by density operator* (3.1). *Additionally, suppose that* $u_j \in H^1\ \forall j \in \mathbb{N}$ *and* $\rho_0 \in T_1^1(H)$. *If* $\rho(t)$, $t \in [0,T]$, *is a Sobolev solution of problem* (1.3), (1.4), *then* $E(\rho(t)) = E(\rho_0)$ *for* $t \in [0,T]$.

Proof. Note that $E(\rho(t)) = \mathscr{E}(U(t))$, where

$$\mathscr{E}(U) = -\frac{1}{2}(\nabla U, \nabla U)_{\mathscr{H}} + \int_R F(|U(x)|^2)dx.$$

Here,

$$(\nabla U, \nabla U)_{\mathscr{H}} = \sum_{j=1}^{\infty} p_j(\mathbf{D}u_j, \mathbf{D}u_j)_H, \quad |U(t,x)|^2 = \sum_{j=1}^{\infty} p_j|u_j(t,x)|^2,$$

where the function U is given by $U = \oplus_{j=1}^{\infty}\sqrt{p_j}u_j$ and $F(s) = \dfrac{1}{p+2}s^{\frac{p+2}{2}}$.

The conservation of the energy $\mathscr{E}$ for vector functions $U(t)$, $t \in [0,T]$, solving the Cauchy problem (2.4), (2.5) was established in [1, 18]. Therefore, the assertion of Theorem 3 follows from Theorem 1.

5. GLOBAL SOLUTION

Theorem 4. *Suppose that* $p \in [0,4)$ *and* $\rho_0 \in T_1^1(H)$. *Then the Cauchy problem* (1.3), (1.4) *has a unique Sobolev solution on the entire real line* $\mathbb{R}$.

Proof. By Theorem 1 on the equivalence of Cauchy problems (1.3), (1.4) and (2.4), (2.5), it suffices to show that the solution of Cauchy problem (2.4), (2.5) is globally extendable. Let $\|\rho_0\|_{T_1^1(H)} = M$. If $U_0 = \oplus_{j=1}^{y}\sqrt{p_j}u_{0,j}$, then $U_0 \in \mathscr{H}_1$ and $\|U_0\|_{\mathscr{H}^1}^2 = \|\rho_0\|_{T_1^1(H)}$. According to Theorem 2 (see [18]), there exists $\delta = \delta(M)$ such that the Cauchy problem (2.4), (2.5) has a unique $\mathscr{H}^1$-solution $U(t, U_0)$, $t \in [0,\delta]$, on the interval $[0,\delta]$.

Let T^* be the supremum of the set of lengths of intervals on which the Cauchy problem (1.3), (1.4) has a Sobolev solution and, hence, the Cauchy problem (2.4), (2.5) has an $\mathscr{H}^1$-solution. It was established in [1, 18] that either $T^* \in (0,+\infty)$ and $\lim_{t\to T^*-0}\|U(t)\|_{\mathscr{H}^1} = +\infty$ or $T^* = +\infty$ and $\overline{\lim}_{t\to+\infty}\|U(t)\|_{\mathscr{H}^1} < +\infty$.

In [1] it was shown that, for the H^1-solution u of the Cauchy problem (1.1), (1.2) with $p \in [0,4)$, the condition $F(s) \leq Cs^{p/2+1}$ implies that $\sup_{t\in[0,T^*)}(\nabla U(t), \nabla U(t))_{H^1}$ is bounded. Let us prove that a similar assertion holds for the $\mathscr{H}^1$-solution of Cauchy problem (2.4), (2.5) and, hence, for the Sobolev solution of Cauchy problem (1.3), (1.4).

By Theorem 3, for any $t \in [0,T^*)$, it is true that

$$\frac{1}{2}\|\nabla U(t)\|_{\mathscr{H}}^2 = -E(\rho_0) + \int_{-\pi}^{\pi} F\left(\sum_{k=1}^{\infty} p_k(U)|u_k(t,x)|^2\right)dx, \tag{5.1}$$

where $F(s) = \dfrac{1}{p+2}s^{1+p/2}$.

The potential energy

$$\int_{-\pi}^{\pi} F\left(\sum_{k=1}^{\infty} p_k(U)|u_k(t,x)|^2\right)dx = \frac{1}{p+2}\|f(t,\cdot)\|_{p+2}^{p+2},$$

where

$$f(t,x) = \left(\sum_{k=1}^{\infty} p_k|u_k(t,x)|^2\right)^{1/2}, \quad x \in (-\pi,\pi), \quad t \in [0,T^*),$$

is estimated from above in terms of the kinetic energy $\frac{1}{2}\|\nabla U(t)\|_{\mathcal{H}}^2$.

Following the approach used in [5, 18], if $f \in C([0,T^*), H^1)$, then, in view of the Gagliardo–Nirenberg–Brezis inequality (see [1, 19]), for each $p \in [0,4)$, there exists a constant $c_2 > 0$ such that

$$\|f(t)\|_{p+2} \le c_2 \|f(t)\|_H^{1-\theta} \|f(t)\|_{H^1}^{\theta} \quad \forall t \in [0,T^*), \tag{5.2}$$

where $\theta = \frac{p}{2p+4} \in (0,1)$.

Note that $\|f(t)\|_2 = 1 \; \forall t \in [0,T_1)$. Additionally,

$$\nabla f(t,x) = \frac{1}{2}\left(\sum_{k=1}^{\infty} p_k|u_k(t,x)|^2\right)^{-1/2}\left[\sum_{k=1}^{\infty} p_k(\nabla\bar{u}_k(t,x)u_k(t,x) + \bar{u}_k(t,x)\nabla u_k(t,x))\right].$$

It follows that

$$|\nabla f(t,x)| \le \left(\sum_{k=1}^{\infty} p_k|u_k(t,x)|^2\right)^{-1/2} \sum_{k=1}^{\infty} p_k\,|u_k(t,x)|\,|\nabla u_k(t,x)|,$$

so, according to the Cauchy–Schwarz inequality,

$$|\nabla f(t,x)| \le \left(\sum_{k=1}^{\infty} p_k|\nabla u_k(t,x)|^2\right)^{1/2}.$$

Therefore,

$$\|\nabla f(t)\|_H^2 \le \|\nabla U(t)\|_{\mathcal{H}}^2 \quad \forall t \in (0,T^*).$$

Since $U(t) \in \mathcal{H}^1 \; \forall t \in [0,T^*)$, we have $f(t,\cdot) \in H^1 \; \forall t \in [0,T^*)$ and the estimate

$$\|f(t)\|_{H^1} \le c_1 \|U(t)\|_H + \|U(t)\|_{\mathcal{H}^1}$$

holds for any $t \in (0,T^*)$.

Therefore, according to inequality (5.2),

$$\int_{-\pi}^{\pi} F\left(\sum_{k=1}^{\infty} p_k(U)|u_k(t,x)|^2\right)dx \le C_1 + C_2\left(\frac{1}{2}\|\nabla U(t)\|_{\mathcal{H}}^2\right)^{\beta} \quad \forall t \in [0,T^*),$$

where $\beta = (p+2)\theta = \frac{p}{2} \in (0,2)$; hence, by virtue of (5.1),

$$\frac{1}{2}\|\nabla U(t)\|_{\mathcal{H}}^2 \le C_3 + C_2(\|\nabla U\|_{\mathcal{H}}^2)^{\beta} \quad \forall t \in [0,T_*).$$

Therefore, $T_* = +\infty$ (see [3, 18]).

Consequently, the Sobolev solution of Cauchy problem (1.3), (1.4) is extendable to the half-line R_+ and the set of its values in the space $T_1^1(H)$ is bounded.

6. BLOW-UP OF THE SOLUTION

Theorem 5. *Suppose that* $p \in [4, +\infty)$ *and* $\rho_0 \in T_1^3(H)$. *If* $E(\rho) > 0$, *then there exists a number* $T_1 \in (0, +\infty)$ *such that the Cauchy problem* (1.3), (1.4) *has a Sobolev solution only on the interval* $[0, T_1)$. *Moreover, the Sobolev solution* $\rho(t, \rho_0)$, $t \in [0, T_1)$, *is unique on the interval* $[0, T_1)$ *and*

$$\lim_{t \to T_1 - 0} \|\rho(t, \rho_0)\|_{T_1^1} = +\infty. \tag{6.1}$$

Proof. To prove Theorem 5, it suffices to show that there is $T_1 \in (0, +\infty)$ such that the Cauchy problem (2.4), (2.5) with initial data $U_0 = \oplus_{j=1}^{\infty} \sqrt{p_j} u_{0,j}$ has an $\mathcal{H}^1$-solution only on the interval $[0, T_1)$. Moreover, the $\mathcal{H}^1$-solution $U(t, U_0)$, $t \in [0, T_1)$, is unique on the interval $[0, T_1)$ and

$$\lim_{t \to T_1 - 0} \|U(t, U_0)\|_{\mathcal{H}^1} = +\infty.$$

First, we note that, if $\rho_0 \in T_1^3(H)$, then $U_0 \in \mathcal{H}^3$. Therefore, if $U(\cdot, U_0) \in C([0, T_1), \mathcal{H}^1)$ is an $\mathcal{H}^1$-solution of the Cauchy problem (2.4), (2.5) with initial data $U_0 = \oplus_{j=1}^{\infty} \sqrt{p_j} u_{0,j}$, then $U(\cdot, U_0) \in C([0, T_1), \mathcal{H}^3)$. Hence, if

$$G(t) = \int_{-\pi}^{\pi} x^2 |U(t,x)|^2 dx = \sum_{k=1}^{\infty} p_k \int_{-\pi}^{\pi} x^2 |u_k(t,x)|^2 dx, \quad t \in [0, T_1),$$

then an analysis of the dynamics of $G(t)$, $t \in [0, T_1)$, suggests that the solution of the Cauchy problem exhibits a gradient blow-up and self-focusing at the point $x_0 = 0$ (see [1]).

Following [3, 18], we show that

$$\frac{d^2}{dt^2} G(t) \le 8 \|\nabla U(t)\|_{\mathcal{H}}^2 - 4 \int_{-\pi}^{\pi} \left[|U(t,x)|^2 f(|U(t,x)|^2) - F(|U(t,x)|^2) \right] dx, \quad t \in (0, T_1),$$

where $f(s) = (s)^{p/2}$ and $F(s) = \int_0^s f(t) dt = \frac{1}{p+2} (s)^{p/2+1}$.

Then, for $p \ge 4$, on the solution existence interval $(0, T_1)$, it holds that

$$\frac{d^2}{dt^2} G(t) \le 8 \|\nabla U(t)\|_{\mathcal{H}}^2 - 2p \int_{-\pi}^{\pi} F(|U(t,x)|^2) dx = -2pE(U(t)) + (8 - 2p) \|\nabla U(t)\|_{\mathcal{H}}^2 \le -2pE(U_0).$$

This inequality implies that the solution existence interval is bounded from above. Following the approach used in [3], we obtain (6.1).

Remark. The fact that the norm of the $\mathcal{H}^1$-solution to the Cauchy problem (2.4), (2.5) (or, equivalently, the $T_1^1(H)$-norm of the Sobolev solution to problem (1.3), (1.4)) grows unboundedly as $t \to T_1 - 0$ does not necessarily mean the existence of a mixed-state component $u_k(t, \cdot)$, $t \in [0, T_1)$ whose H^1-norm grows unboundedly as $t \to T_1 - 0$.

7. CONCLUSIONS

Conditions on the parameters of the nonlinear operator of the nonlinear Liouville–von Neumann equation were obtained under which the Cauchy problem (1.3), (1.4) defines a one-parameter group of linear transformations of the space $T_1^1(H)$ of Sobolev quantum states. It was shown that the violation of these conditions leads to the blow-up of the Sobolev solution to Cauchy problem (1.3), (1.4).

In [1] for the Cauchy problem (1.1), (1.2) for the nonlinear Schrödinger equation, a procedure was proposed for extending its H^1-solution beyond the blow-up time T_1 with the help of a mapping of the time half-line $[0, +\infty)$ to a quantum-state space $\Sigma(H)$ determined by regularizing the original problem (1.1), (1.2). Considered in this work, the Liouville–von Neumann equation (1.3) has an advantage over Schrödinger equation (1.1) in that the solution of Eq. (1.3), its regularization, and the limit points of the family of regularized solutions are all mappings of the time half-line $[0, +\infty)$ to the state space $\Sigma(H)$.

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