Self-Adjoint Approximations of the Degenerate Schrödinger Operator*

V. Zh. Sakbaev** and I. V. Volovich***

Steklov Mathematical Institute, RAS, Moscow, Russia

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Abstract—The problem of construction a quantum mechanical evolution for the Schrödinger equation with a degenerate Hamiltonian which is a symmetric operator that does not have self-adjoint extensions is considered. Self-adjoint regularization of the Hamiltonian does not lead to a preserving probability limiting evolution for vectors from the Hilbert space but it is used to construct a limiting evolution of states on a $C^*$-algebra of compact operators and on an abelian subalgebra of operators in the Hilbert space. The limiting evolution of the states on the abelian algebra can be presented by the Kraus decomposition with two terms. Both of these terms are corresponded to the unitary and shift components of Wold's decomposition of isometric semigroup generated by the degenerate Hamiltonian. Properties of the limiting evolution of the states on the $C^*$-algebras are investigated and it is shown that pure states could evolve into mixed states.

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1. INTRODUCTION

Degenerate elliptic and parabolic equations are widely studied, see for example [1–3]. Universal boundary conditions for various types of PDE were considered in [4].

It was shown [2, 3] that the solvability of the Cauchy problem for the degenerate differential equation with smooth coefficients in the whole space holds but the degenerate differential equation without smoothness of coefficients can have no solution. We will study an example of the simplest first order differential operator on the semi-line. Note that the boundedness of the domain in Euclidian coordinate space can arise as the result of singularity of coefficients in the complement of this domain (see [5]).

In this paper we concern with the degenerate Schrödinger equation, see [6–8] of the form

$$i\frac{\partial u}{\partial t} = Hu, \tag{1.1}$$

where $-H$ is a second order differential operator with nonnegative characteristic form in a region $G \subset \mathbb{R}^n$. It is assumed that under some boundary conditions $H$ defines a symmetric operator in the Hilbert space $H = L^2(G)$. We are interested in the case when $H$ does not have self-adjoint extensions.

The initial-boundary value problem for the Schrödinger equation (1.1) does not necessary have a solution. In such a case we will use an elliptic regularization and proceed as follows. Consider a family of operators $H_\epsilon$ depending on the parameter $\epsilon > 0$,

$$H_\epsilon = -\epsilon \Delta + H, \tag{1.2}$$

*The text was submitted by the authors in English.
**E-mail: fumi2003@mail.ru
***E-mail: volovich@mi.ras.ru
where $\Delta$ is the Laplace operator. Suppose that $H_\epsilon$ admits a self-adjoint extension (we denote it by the same letter). Let $u_\epsilon(t) = U_\epsilon(t)\varphi$ be a solution of the Cauchy problem

$$i\frac{\partial u_\epsilon}{\partial t} = H_\epsilon u_\epsilon,$$

$$u_\epsilon(0) = \varphi, \quad \varphi \in L^2(G).$$

(1.3)

Here $U_\epsilon(t) = e^{-itH_\epsilon}$ is the unitary evolution operator.

Shrödinger equation with small parameter arises in the study of limit behavior of a class of such quantum systems as electrons and holes in the nonhomogeneous semiconductor materials in the case of large value of effective mass of a particles in one part of materials and small value of effective mass in another (see [8–10]).

The limit of $u_\epsilon(t), \epsilon \to 0$ in the Hilbert space might be not exist, however we will show that in some cases there exists the limit

$$\sigma_t^\varphi(A) = \lim_{\epsilon \to 0} \langle u_\epsilon(t), Au_\epsilon(t) \rangle = \lim_{\epsilon \to 0} \langle \varphi, U_\epsilon^*(t)AU_\epsilon(t)\varphi \rangle$$

(1.5)

for any $\varphi \in H, t \geq 0$ where $A$ is an operator from a subalgebra of the algebra $B(H)$ of bounded operators in $H$.

We will show that $\sigma_t^\varphi$ defines a state (a linear positive functional of norm 1) on a $C^*$-algebra and therefore it can be interpreted as quantum mechanical evolution generated by the Schrödinger operator $H$.

Degenerate Hamiltonians arise in different problems.

1. The theory of semi-classical limit is the theory of the passage to the limit in the family of second order differential operators with the small parameter at the second derivatives. The vanishing of the coefficients with second derivative in the case is the degeneration of Hamiltonians; the limit operator is the first order differential operator which can be symmetric but not self-adjoint operator.

2. Similar effects has the family of Hamiltonians with large mass parameter. In the semiconductors theory (see [9, 10]) the mass of a system is the nonnegative function on the coordinate space which value is the constant in some domain of coordinate space and is the large parameter in the complement of this domain. Then the limit Hamiltonian is the degenerated symmetric but not self-adjoint differential operator of second order in the domain and of first order in its complement (see [5, 7, 8]).

3. Symmetric differential operators arise in the theory of conductance in the geometrical graphs in nano-semiconductors theory (see [5, 11]). The degeneration of the second order coefficients of differential operator on a graph can be the reason of the absence of self-adjoint extensions of this operators.

4. The both of degeneration and nonsmoothness of coefficients of a first order transport equation on a line is the reason of nonexistence or nonuniqueness of its solutions. Hence it is the reason of luck of self-adjointness of the first order operator (see [3, 12]).

5. Positive-operator valued measures (POVM) are used in the quantum measurement theory. Neurmak’s dilation theorem states that a POVM can be lifted to a projection-valued measure. It is used in theory of open quantum systems (see [13–17]).

In the next section we study a simple model of quantum dynamics on the half-line with the symmetric Hamiltonian which does not admit a self-adjoint extension.

2. SCHRÖDINGER EQUATION ON THE HALF-LINE

In quantum mechanics, according to von Neumann’s axioms, observables correspond to self-adjoint operators. However, Hermitian (symmetric) operators which do not admit self-adjoint extensions are also discussed as possible observables (see for example [13]).

It is well known that the momentum operator on a half-line is not self-adjoint. Here we consider the momentum operator on the half-line $\mathbb{R}_+ = \{x \in \mathbb{R} : x > 0\}$ as an example of a degenerate Hamiltonian.