

Complex Scaling and Selfadjoint Dilations.*

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October 12, 2002

1 Introduction.

Singularities of the scattering matrix play an important role during investigation of the large time behaviour of quantum systems. Only singularities, corresponding to bound states, produce eigenfunctions which belong to the same Hilbert space, where the operator is selfadjoint. It follows that positions of eigenvalues can be defined easily. But resonance "eigenfunctions" - solutions of the stationary equation, corresponding to the resonance energies - are not elements of the main Hilbert space. The method of complex scaling for the Schroedinger equation with an analytic potential connects resonances of the initially selfadjoint operator with eigenvalues of some scaled operator [1],[3]. The scaled operator has eigenfunctions corresponding to these complex eigenvalues. The positions of the resonances can be derived numerically. However, it is very hard to introduce any self-consistent scattering theory for nonselfadjoint operators. This fact is connected with nonunitarity of the evolution operator for such Hamiltonians. If the imaginary part of the scaled operator has a definite sign, then it is possible that the scaled operator or its adjoint is a dissipative operator. The evolution semigroup defined by one of these operators is contractive and can be dilated to some unitary group [7]. The generator of this group is a selfadjoint dilation of the dissipative scaled operator ([2]), i.e. operator which restriction on a certain subspace coincide with nonselfadjoint one. Note that this definition of dilation is not related to complex rotation, which is sometimes also called complex dilation. This construction allows us to consider the spectral problem for the scaled operator from the scattering theory point of view because we include the nonselfadjoint problem into the selfadjoint one.

In this paper we shall analyze this idea for the simplest model operator obtained by perturbation of the boundary condition. Such operator defines the scaled operator with a finite rank of nonselfadjointness. First we show that this operator during the complex scaling reproduce the behaviour of an operator with an analytic potential.

*Published in *International Journal of Quantum Chemistry*, **46** (1993), 415-418.

Then we shall construct a functional model of a selfadjoint dilation of the scaled operator with the help of additional incoming and outgoing channels ([5]). It will be shown that the reflection coefficient, obtained for the scaled operator, is a matrix element of the general scattering matrix for selfadjoint dilation. Connections between scattering characteristics of the dilation and spectrum of the scaled operator will be shown.

2 Boundary condition for the operator .

We define a selfadjoint operator in the Hilbert space $H = L_2(0, \infty)$ by the formula

$$L_h = -\frac{d^2}{dx^2} \quad (1)$$

on the functions with square integrable second derivative($W_2^2(\mathbf{R}_+)$), satisfying boundary condition:

$$\frac{du}{dx} \Big|_{x=0} = h u \Big|_{x=0}, h \in \mathbf{R} \quad (2)$$

For an arbitrary real constant h the operator L_h is a selfadjoint operator on it's domain. We have to note that in the case of a complex constant h the operator is no longer a selfadjoint one.

The spectrum of the operator consists of the branch $[0, \infty)$ of the continuous spectrum and may be one eigenvalue on the negative half-axis. Eigenfunctions of continuous spectrum are:

$$\psi(k, x) = e^{-ikx} - S(k)e^{ikx} \quad (3)$$

where scattering matrix $S(k)$ can be calculated from the boundary condition:

$$S(k) = \frac{h + ik}{h - ik} \quad (4)$$

This S-matrix is a meromorphic function on the complex plane k , unitary on the real axis. The singularity of the scattering matrix is situated on the imaginary axis. It defines a bound state or a resonance. If $h < 0$, then the function

$$\psi_0(x) = e^{hx} \quad (5)$$

is an eigenfunction, corresponding to a bound state with the energy $E_0 = -h^2$. When $h > 0$ the singularity corresponds to a resonance. In this case the function $\psi_0(x) = e^{hx}$ increases at infinity exponentially and does not belong to L_2 .

3 Complex Scaling.

Following ref. [1] and [3] we shall consider an unitary transformation in $L_2(0, \infty)$:

$$U(z) : u(x) \Rightarrow \sqrt{z}u(zx), z \in \mathbf{R}_+ \quad (6)$$

This transformation is unitary for positive real values of the parameter z only. Hence the scaled operator

$$\hat{L}_h(z) = U(z)L_hU^{-1}(z) \quad (7)$$

is a self adjoint operator for real positive z . The transformation $U(z)$ can be continued to complex values of the parameter z . Then the operator becomes nonselfadjoint with a complex branch of continuous spectrum $\bar{z}^2 \times [0, \infty)$. In order to use a possibility to compare the scaled operator with the nonperturbed operator on half axis we shall multiply operator $\hat{L}_h(z)$ by a complex constant:

$$L_h(z) = z^2\hat{L}_h(z). \quad (8)$$

The branch of the continuous spectrum becomes real, i.e. it coincides with the essential spectrum of the unperturbed operator. The new operator is a selfadjoint operator for real values of the parameter z again. We shall calculate the operator $L_h(z)$, which is an operator in $L_2(0, \infty)$. First of all, we shall restore the differential expression:

$$(L_h(z)u)(x) = z^2U(z)\left(-\frac{d^2}{dx^2}\right)\frac{1}{\sqrt{z}}u\left(\frac{x}{z}\right) = z^2U(z)\left(-\frac{1}{z^2\sqrt{z}}u''\left(\frac{x}{z}\right)\right) = -\frac{d^2}{dx^2}u(x)$$

The new operator is defined on the functions which after the U - transformation satisfy the boundary conditions (2), hence:

$$\frac{d}{dx}u\left(\frac{x}{z}\right)\Big|_{x=0} = hu\left(\frac{x}{z}\right)\Big|_{x=0} \Rightarrow \frac{d}{dx}u(x)\Big|_{x=0} = zh u(x)\Big|_{x=0} \quad (9)$$

Thus we have just proved the equality:

$$L_h(z) = L_{zh}(1) = L_{zh} \quad (10)$$

Corresponding continuous spectrum eigenfunctions have the same form, as for initial operator. So one can again introduce a reflection coefficient $S_z(k)$, which coincides with the scattering matrix in a selfadjoint case:

$$S_z(k) = \frac{zh + ik}{zh - ik} = \frac{h + ikz^{-1}}{h - ikz^{-1}} = S(z^{-1}k) \quad (11)$$

The scaled operator can have only one complex eigenvalue which is a singularity of the reflection coefficient. Let us suppose that $z = e^{i\theta}$ then the reflection coefficient for the scaled operator coincide with the S-matrix of the initial operator rotated on the angle θ on the k -plane and 2θ on the energy plane. This behaviour of the singularities

of the scattering matrix reproduce the usual behaviour for the Schroedinger operator with an analytical potential.

Eigenfunctions and bound state energy (resonance energy) are analytic functions of the parameter z . Hence one can obtain all the characteristics of the scaled operator by analytic continuation of the corresponding characteristics of the initial one. Thus the scattering matrix is an analytic continuation of the initial scattering matrix. The bound state eigenfunction is an analytic continuation of the bound state or a resonance eigenfunction.

4 Selfadjoint Dilation of the Scaled Operator.

The calculated scaled operator has an imaginary part of definite sign. Moreover, it is possible to prove that the operator or it's adjoint is a dissipative operator. In this section we shall construct selfadjoint dilation of the scaled operator i.e. a selfadjoint operator which restriction on a certain subspace coincides with the scaled operator. Such dilation can be obtained for dissipative operators only. In our notations dissipative operator has a spectrum in a closed lower halfplane. Hence the imaginary part of the parameter zh is supposed to be negative: $\Im(zh) < 0$; $2\Im(zh) = -\alpha^2$. This restriction is not essential because operators L_z and $L_{\bar{z}}$ are adjoint one to another. This condition means, that we shall choose scaling parameter z from one of the half planes (depending on the *sign* h). The functional model for this case was constructed by B.S.Pavlov ([2]).

One can define the general operator \mathcal{L} in the Hilbert space

$$\mathcal{H} = L_2(-\infty, 0) \oplus H \oplus L_2(0, \infty) \ni \mathcal{U} = (u_-, u, u_+) \quad (12)$$

by the formula:

$$\mathcal{L}\mathcal{U} = \begin{pmatrix} \frac{1}{i} \frac{d}{ds} u_-(s) \\ -\frac{d^2}{dx^2} u(x) \\ \frac{1}{i} \frac{d}{ds} u_+(s) \end{pmatrix} \quad (13)$$

on the domain of functions, satisfying boundary condition:

$$\begin{aligned} \left(\frac{du}{dx} - zh u \right) |_{x=0} &= \alpha u_-(0) \\ \left(\frac{du}{dx} - \bar{z} \bar{h} u \right) |_{x=0} &= \alpha u_+(0) \end{aligned} \quad (14)$$

One can prove that the operator \mathcal{L} is a selfadjoint dilation of the operator $L_h(z)$. We shall restrict ourselves by calculation of the boundary form of the operator:

$$\begin{aligned} &\langle \mathcal{L}\mathcal{U}, \mathcal{V} \rangle - \langle \mathcal{U}, \mathcal{L}\mathcal{V} \rangle = \\ &= -i (u_-(0)\bar{v}_-(0) - u_+(0)\bar{v}_+(0)) + u'(0)\bar{v}(0) - u(0)\bar{v}'(0) = \end{aligned}$$

$$\begin{aligned}
&= \frac{-i}{\alpha^2} \left((u'(0) - zhu(0))(\bar{v}'(0) - z\bar{h}\bar{v}(0)) - (u'(0) - z\bar{h}u(0))(\bar{v}'(0) - zh\bar{v}(0)) \right) + \\
&\quad + u'(0)\bar{v}(0) - u(0)\bar{v}'(0) = 0.
\end{aligned} \tag{15}$$

To prove that the operator \mathcal{L} is a dilation of the operator $L_h(z)$ one can show for $\Im\lambda > 0$ that:

$$\mathbf{P}_H(\mathcal{L} - \lambda)^{-1} |_{H} = (L_h(z) - \lambda)^{-1} \tag{16}$$

Really, for every $f \in H$ we have:

$$(\mathcal{L} - \lambda)^{-1} \begin{pmatrix} 0 \\ f \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ (L_h(z) - \lambda)^{-1}f \\ -i\alpha((L_h(z) - \lambda)^{-1}f)(0)e^{i\lambda s} \end{pmatrix}$$

Then from the translational invariance of the subspace H we have:

$$\mathbf{P}_H(\mathcal{L} - \lambda)^{-1}\mathbf{P}_H = \mathbf{P}_H i \int_{-\infty}^0 e^{i(\mathcal{L}-\lambda)t} dt \mathbf{P}_H$$

which follows that \mathcal{L} is a dilation of $L_h(z)$.

Constructed selfadjoint operator has a purely continuous spectrum. Corresponding eigenfunctions can be divided onto two sets. The first set is connected with incoming waves in the space $L_2(-\infty, +\infty)$, so-called incoming solutions in Lax-Phillips scattering theory:

$$\Psi^i(\lambda) = \begin{pmatrix} \frac{1}{\sqrt{2\pi}}e^{i\lambda s} \\ -S_{21}\frac{1}{2\sqrt{\pi k}}e^{ikx} \\ S_{11}\frac{1}{\sqrt{2\pi}}e^{i\lambda s} \end{pmatrix}, \lambda \in (-\infty, +\infty), k = \sqrt{\lambda} \tag{17}$$

$$S_{11} = \frac{z\bar{h} - ik}{zh - ik}, S_{21} = \frac{\alpha\sqrt{2k}}{zh - ik}.$$

The second set is produced by incoming solutions in space H , so-called radiating eigenfunctions in Lax-Phillips theory:

$$\Psi^r(\lambda) = \begin{pmatrix} 0 \\ \frac{1}{2\sqrt{\pi k}}e^{-ikx} - S_{22}\frac{1}{2\sqrt{\pi k}}e^{ikx} \\ S_{12}\frac{1}{\sqrt{2\pi}}e^{i\lambda s} \end{pmatrix}, \lambda \in [0, +\infty), k = \sqrt{\lambda} \tag{18}$$

$$S_{22} = \frac{zh + ik}{zh - ik}, S_{12} = -\frac{\alpha\sqrt{2k}}{zh - ik}.$$

The introduced matrix of transition coefficients:

$$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \tag{19}$$

is the scattering matrix in the outgoing spectral representation for the pair of operators \mathcal{L} and $\mathcal{L}_0 \oplus L_\infty$, where operator \mathcal{L}_0 is operator of the first derivative on the real axis: $\mathcal{L}_0 = \frac{1}{i} \frac{d}{dx}$. One can see that the reflection coefficient $S_z(k)$ for the nonselfadjoint operator is a matrix element of the unitary scattering matrix for a selfadjoint dilation of this operator. In the limit $z \rightarrow 1$, the scattering matrix \mathbf{S} transforms into a diagonal matrix:

$$\mathbf{S} \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & S(k) \end{pmatrix},$$

which corresponds to the case of nonconnected channels.

5 Resume.

It was shown in a model situation that the complex scaled problem can be included into a selfadjoint one. Thus we received a possibility to consider all the objects of the selfadjoint theory. Among other things, it is possible to introduce an unitary scattering matrix. It seems that these ideas can be generalized for a problem with an analytic potential with an imaginary part with a definite sign. The connections with Lax-Phillips scattering theory can be very useful for the further investigation of complex scaled operators.

We are indebted to prof. B.S.Pavlov for a continuous interest for this work.

References.

1. J.Aguilar, J.M.Combes "A Class of Analytic Perturbations for One-Body Schroedinger Hamiltonians", Commun. Math.Phys. 22, 269-279(1971).
2. B.S.Pavlov "Dilation Theory and Spectral Analysis of Nonselfadjoint Differential Operators", Proc. 7-th Winter School, Drogobych, 1974, ed. B.S.Mitjagin, Moscow,1976; English translation: Amer. Math. Soc. Transl. (2) Vol. 115, 1980.
3. E.Balslev, J.M.Combes "Spectral Properties of Many-Body Schroedinger Operators with Dilation-analytic Interactions", Commun.Math.Phys. 22, 280-294(1971).
4. B.Simon "Methods of Modern Mathematical Physics" vol. IV, Academic Press, 1978, pp. 183-191.
5. P.D.Lax, R.S.Phillips "Scattering Theory", Academic Press, NY, 1989 (IIInd edition).
6. V.M.Adamjan, D.Z.Arov "On unitary couplings of semiunitary operators", Mat. Issled. 1 (1966), no. 2, 3-64; English translation: Amer. Math. Soc. Transl. (2) Vol. 95, 1970, 75-129.
7. B.Sz.-Nagy, C.Foias "Harmonic Analysis of Operators on Hilbert Space", Akademiai Kiado, Budapest, 1970.