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On unitarity of the scattering operator in non-Hermitian quantum mechanics

by R.G. Novikov and I.A. Taimanov

Abstract. We consider the Schrödinger operator with regular short range complexvalued potential in dimension $d \ge 1$. We show that, for $d \ge 2$, the unitarity of scattering operator for this Hamiltonian at high energies implies the reality of potential (that is Hermiticity of Hamiltonian). In contrast, for d = 1, we present complex-valued exponentially localized soliton potentials with unitary scattering operator for all positive energies and with unbroken PT symmetry. We also present examples of complex-valued regular short range potentials with real spectrum for d = 3. Some directions for further research are formulated.

Keywords: Schrödinger operators, complex potentials, PT symmetry, unitarity of scattering, real spectrum, solitons

AMS subject classification: 81Q05, 81Q12, 81U20, 81U40

1. Introduction

In the present work we consider Schrödinger operators

$$H = -\Delta + v(x), \quad x \in \mathbb{R}^d, \tag{1.1}$$

with complex-valued v.

In particular, in recent years theory of so-called PT potentials attracted a lot of attention in physics, partly because of its importance for developing non–Hermitian quantum mechanics (see, for example, [Ben], [EG], [WB]). We recall that a potential v of the one-dimensional Schrödinger operator H is called a PT potential if it satisfies the condition

$$v(x) = \overline{v(-x)}, \quad x \in \mathbb{R}.$$
 (1.2)

It means that H commutes with the composition of the parity operator $(P\psi)(x) = \psi(\mathcal{P}x)$ and the time-reversal operator T which results in the complex conjugation of wave functions $T\psi(x) = \overline{\psi(x)}$. In higher dimensions by the parity operator \mathcal{P} we mean a linear operator on the configuration space \mathbb{R}^d which is idempotent, i.e., $\mathcal{P}^2 = I$, and inverses the orientation. For instance, in two-dimensions \mathcal{P} is the reflection with respect to some axis. In addition, it is said that H has an unbroken PT symmetry if every eigenfunction of H is also an eigenfunction of the PT operator. This condition guarantees that the eigenvalues of H are real.

Theory of PT potentials was far developed mostly for one-dimensional potentials with the discrete spectrum. The spectacular example of such a potential which attracted a lot of attention is

$$v(x) = ix^3. (1.3)$$

In particular, the work [DDT] proves the conjecture by Bessis and Zinn-Justin that the discrete spectrum for H given by (1.1), (1.3) for d = 1 is real. Recently it was stressed that "very little is known about the nature of PT-symmetric quantum field theory with spacetime dimension D > 1" [ABS]. Also we have to say that mainly there were studied PT potentials without continuous spectra as, for example, the potential in (1.3). However, the study of the scattering operator corresponding to the continuous spectra of one-dimensional potentials was done in [CDV], where it was shown that at positive energies E the scattering matrix S in general is not unitary and satisfies the condition $\bar{S} = S^{-1}$ instead of $S^* = S^{-1}$ for unitary matrices. Recently the problem of studing PT potentials with continuous spectra was stressed in [WB], where it was investigated for one-dimensional potentials.

In the present work we continue studies of the scattering operator for regular short range complex-valued potentials v. These assumptions on v can be specified as (2.2) or, for example, as (3.3).

For the related Schrödinger operator H we consider the wave operators W^{\pm} and the scattering operator S defined by the formulas:

$$W^{\pm} = \lim_{t \to \pm \infty} e^{iHt} e^{-iH_0 t}, \quad H_0 = -\Delta, \tag{1.4}$$

$$S = (W^{-})^* W^+. (1.5)$$

For the case of regular short range real-valued v, i.e. for the Hermitian case, it is well known that: the limits in (1.4) exist in the operator norm sense in $L^2(\mathbb{R}^d)$; S is unitary, that is

$$S^*S = I, \quad SS^* = I;$$
 (1.6)

in impulse representation S can be considered as an integral operator with a kernel of the form

$$S(k,l) = \delta(k-l) - 2\pi i \delta(k^2 - l^2) f(l,k), \quad k,l \in \mathbb{R}^d,$$
(1.7)

where δ is the Dirac function; see, for example, [FM], [N2] and references therein.

The function f arising in (1.7) is known as the scattering amplitude for the potential v. At fixed energy E > 0, this function is defined on

$$\mathcal{M}_E = \{k, l \in \mathbb{R}^d : k^2 = l^2 = E\} = \mathbb{S}_{\sqrt{E}}^{d-1} \times \mathbb{S}_{\sqrt{E}}^{d-1}.$$
(1.8)

In terms of f, the unitarity property (1.6) can be written as

$$f(k,l) - \overline{f(l,k)} = -2\pi i \int_{\mathbb{R}^d} f(k,m) \delta(m^2 - k^2) \overline{f(l,m)} dm, \ (k,l) \in \mathcal{M}_E,$$
(1.9)

which is fulfilled for all E > 0.

As about non-Hermitian Hamiltonians H (i.e. complex potentials v) in fundamental quantum mechanics, as it was mentioned, for example, in [Bar]: "A non-Hermitian Hamiltonian is unacceptable partly because it may lead to complex energy eigenvalues, but chiefly because it implies a non-unitary S matrix, which fails to conserve probability and makes a hash of the physical interpretation."

Therefore, of great interest are non-Hermitian Hamiltonians H for which the scattering operator S is unitary.

In the present work we show that, for the case of regular short range complex-valued potential v in dimension $d \ge 2$, the unitarity property (1.9) fulfilled for arbitrary large Eimplies the reality of v; see Theorem 1 in Section 2. Note that, for the case when complexvalued v is of the Schwartz class on \mathbb{R}^d and unitarity (1.9) is fulfilled for all E > 0, the reality of v follows from Theorem 4.2 in [HN].

In contrast, for d = 1, we present complex-valued (non-real) smooth and exponentially localized soliton potentials v for which the unitarity property (1.9) holds for all E > 0; see Proposition 1 in Section 2. We also show that these examples include v satisfying (1.2) with unbroken PT symmetry for H; see Proposition 2 in Section 2.

Using complex regular short range potentials v_j with unitary scattering operators for all positive energies for d = 1 (e.g., as in Proposition 1), we also obtain complex regular potentials v of the form

$$v(x) = v_1(x_1) + \dots + v_d(x_d), \quad x = (x_1, \dots, x_d) \in \mathbb{R}^d,$$
(1.10)

with unitary scattering operators for all positive energies for $d \ge 2$. However, such potentials are not of short range in \mathbb{R}^d , $d \ge 2$.

In connection with unitarity of the time-evolution operator e^{-iHt} for non-Hermitian H, see Remark 7 in Section 2. In the usual scalar product this unitarity is impossible. But for the case of unbroken PT symmetry the scalar product can be appropriately modified, see [BBJ].

Further structure of the present article is as follows. In Section 2 we present the main results and formulate some directions for further research. In Sections 3, 4, and 5 we prove Theorem 1, Proposition 1 and Proposition 2 mentioned above.

2. Main results

Let

$$W_s^{N,1}(\mathbb{R}^d) = \{ u : \ (1+|x|)^s \partial^J u(x) \in L^1(\mathbb{R}^d), \ |J| \le N \},$$
(2.1)

where $N \in \mathbb{N} \cup 0, s \ge 0$.

Theorem 1. Let v be complex-valued and

$$v \in W_s^{N,1}(\mathbb{R}^d)$$
 for some $N > d-2, \ s > 0, \ d \ge 2.$ (2.2)

Let the unitarity property (1.9) hold for arbitrary large E. Then v is real-valued.

Theorem 1 is proved in Section 3, under the somewhat weaker assumption (3.3) in place of (2.2). The proof is based on technique developed in [F1], [F2], [ER1], [ER2], [N3].

The main idea of this proof consists in the observation that at high energies E the scattering amplitude f(k, l) is approximated by the Fourier transform $\hat{v}(k-l)$ of v and that the right hand side of (1.9) is approximated by zero, and, therefore, \hat{v} has the symmetry implying the reality of v; see formulas (3.4), (3.5), (3.9).

The main idea of the proof of Theorem 1 can be also used for other classes of regular short range potentials in place of (2.2) or (3.3).

For example, we expect that the result of Theorem 1 remains valid when assumption (2.2) is replaced by the assumption

$$v \in C^{2}(\mathbb{R}^{d}), \quad d \ge 2,$$

$$|\partial^{J}v(x)| = O(|x|^{-1-\epsilon-|J|}) \quad \text{as} \quad |x| \to \infty \quad \text{for} \quad |J| \le 2 \quad \text{and some} \quad \epsilon > 0.$$
 (2.3)

Under assumption (2.3), one can use technique developed in [EW], [W], [N2].

Apparently, one can also extend the result of Theorem 1 to the N-body Schrödinger operators for which uniqueness of inverse scattering at high energies was proved in [EW], [W], [N2].

Let $\sigma(H)$ denote the spectrum of H defined by (1.1).

In addition to the result of Theorem 1, we also have the following remark with somewhat opposite meaning.

Remark 1. For small potentials v satisfying (2.2) or (3.3), for example, for d = 3, we have that

$$\sigma(H) = [0; +\infty[. \tag{2.4})$$

We present this remark in connection with considerable interest to complex potentials with real spectrum; see, for example, [DDT], [Ben], [WB]. The smallness of v in this remark is considered in the sense of the norm $\|\cdot\|_{\alpha,M}$ defined in (3.1). One can prove this remark using the technique going back to [F2]; see also [FM], [ER1]. Remark 1 does not hold for d = 1 and d = 2.

On the other hand, the result of Theorem 1 does not hold for d = 1. Let

$$v(x) = \frac{-2\kappa^2}{ch^2(\kappa x - \zeta)}, \quad x \in \mathbb{R},$$
(2.5)

where $\kappa, \zeta \in \mathbb{C}$. For real κ and ζ , this potential v is the classical reflectionless real-valued soliton; see [NMPZ], [AC], [FZ] for introduction into the soliton theory. The potential v for complex κ and ζ was also considered in the literature; see, for example, [SLYW], [SYZ].

Proposition 1. Let v be defined by (2.5), where $\kappa \in \mathbb{R}$, $\kappa > 0$, and $Im\zeta \neq 0 \mod(\pi/2)$. Then, in particular: v is infinitely smooth on \mathbb{R} with exponential decay as $|x| \to \infty$; $Imv \neq 0$; the unitarity property (1.9) holds for all E > 0.

Proposition 1 is proved in Section 4 using the Darboux transform theory. For introduction to this theory, see, for example, [TT]. One can also prove Proposition 1 using analytic continuation in ζ . Actually, Proposition 1 follows from explicite formulas including formulas for the scattering amplitude f for the considered potential v. The point is that this f is independent of ζ and is the same that for the real case.

Proposition 2. Let *H* be defined by (1.1), where d = 1, and *v* is as in Proposition 1. Then

$$\sigma(H) = -\kappa^2 \cup [0; +\infty[. \tag{2.6})$$

In addition, if $Re\zeta = 0$, then v is PT-symmetric and this symmetry is unbroken for H.

Proof of Proposition 2 is sketched in Section 5.

Finally, we also have the following remarks.

Remark 2. Apparently, the result of Theorem 1 admits an analog at a fixed positive energy E if v is compactly supported or exponentially decays at infinity as, for example, in [N1].

Remark 3. Possibilities of unitarity of the scattering operator for all positive energies E for singular and/or slowly decaying complex potentials v require additional studies for $d \ge 2$. Such possibilities are also of interest for more complicated non-Hermitian Hamiltonians with decaying at infinity coefficients than H in (1.1) (e.g. for non-Hermitian Schrödinger operator in magnetic field) for $d \ge 2$.

Remark 4. The results of Propositions 1 and 2 admit analogs for complex multisoliton potentials.

Remark 5. Apparently, the following result holds for H defined by (1.1), where v is complex regular and rapidly decaying at infinity, d = 1:

If S is the scattering operator for a real-valued v with discrete spectrum $E_1,...,E_n$, then there is a set of complex (non-real) potentials v_c with the same scattering operator S for all positive energies E and with the same discrete spectrum $E_1,...,E_n$ (and the complex dimension of this set is n).

Remark 6. A complete characterization of the scattering operator (and discrete spectrum with their characteristics) for regular short range complex potentials satisfying (1.2) is a natural open problem for d = 1 (where the particular cases when the scattering operator is unitary and when the *PT* symmetry is unbroken are of particular interest). For regular short range real potentials such a characterization was obtained by L.D. Faddeev (modulo a small gap); see [F3], [M], [DT].

Remark 7. Unitarity of the operator e^{-iHt} is impossible for non-Hermitian H in the usual scalar product. Indeed,

$$\begin{aligned} \frac{d}{dt} \langle e^{-iHt} \psi | e^{-iHt} \psi \rangle &= \langle -iHe^{-iHt} \psi | e^{-iHt} \psi \rangle + \langle e^{-iHt} \psi | -iHe^{-iHt} \psi \rangle \\ &= \langle i(H^* - H)e^{-iHt} \psi | e^{-iHt} \psi \rangle \end{aligned}$$

and

$$\frac{d}{dt}\langle e^{-iHt}\psi|e^{-iHt}\psi\rangle=0$$

for all t and ψ if and only if $H = H^*$.

However, for H in (1.1) with unbroken PT symmetry, it is constructed another scalar product with respect to which H is Hermitian and e^{-iHt} is unitary; see [BBJ]. The idea can be illustrated by the following very simple example of an operator in \mathbb{C}^2 . Let

$$H = \begin{pmatrix} 1 & i\varepsilon \\ 0 & -1 \end{pmatrix}$$

where ε is a constant real-valued parameter. It has real-valued eigenvalues $\lambda = 1$ and -1 with the corresponding eigenvectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} -i\varepsilon/2 \\ 1 \end{pmatrix}$ which, for $\varepsilon \neq 0$, are not pairwise orthogonal with respect to the standard Hermitian product on \mathbb{C}^2 . However we can construct another Hermitian product distinguished by the condition that both these vectors have unit norm and are orthogonal to each other. This product is given by the following matrix

$$G = \begin{pmatrix} 1 & -i\varepsilon/2\\ i\varepsilon/2 & 1+\varepsilon^2/4 \end{pmatrix}$$

and it is easy to check that, since $H^{\top}G = G\overline{H}$, the operator H is selfadjoint with respect to this Hermitian product. Therefore, the corresponding evolution operator e^{-iHt} is unitary as it is required by physics.

3. Proof of Theorem 1

Let

$$\mathcal{H}_{\alpha,M} \text{ be the closure of } C_0^{\infty}(\mathbb{R}^d) \text{ in the norm } \|\cdot\|_{\alpha,M}, \\ \|u\|_{\alpha,M} = \|\Lambda^M u\|_{\alpha}, \\ \|w\|_{\alpha} = \sup_{p,\xi \in \mathbb{R}^d, 0 < |\xi| \le 1} (|w(p)| + |\xi|^{-\alpha} |w(p+\xi) - w(p)|), \\ \Lambda^M u(p) = (1 + |p|^2)^{M/2} u(p), \quad p \in \mathbb{R}^d,$$

$$(3.1)$$

where $0 < \alpha \leq 1, M \in \mathbb{R}, \ C_0^{\infty}$ denotes infinitely smooth compactly supported functions. Let

$$\hat{v}(p) = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{ipx} v(x) dx, \quad p \in \mathbb{R}^d.$$
(3.2)

If v satisfies (2.2), then $\hat{v} \in \mathcal{H}_{\alpha,M}$, $\alpha = min(1,s)$, M = N; see [N3]. Therefore, in place of (2.2), we will assume that

$$\hat{v} \in \mathcal{H}_{\alpha,M}$$
 for some $\alpha \in]0,1[, \mathbb{R} \ni M > d-2, d \ge 2.$ (3.3)

The scattering theory, under assumption (3.3), was developed, in particular, in [F2], [ER1], [ER2], [N3].

Under assumption (3.3), the following formulas hold:

$$f(k,l) = \hat{v}(k-l) + O(E^{-\sigma/2}), \quad E \to +\infty,$$
 (3.4)

$$\int_{\mathbb{R}^d} f(k,m)\delta(m^2 - k^2)\overline{f(l,m)}dm = O(E^{-\sigma/2}), \quad E \to +\infty,$$
(3.5)

where $(k, l) \in \mathcal{M}_E$, $0 < \sigma < min(1, M - d + 2)$.

Formula (3.4) is well known (see formula (1.29a) in [N3]) and goes back to [F1]. Formula (3.5) follows from the known formulas:

$$\int_{\mathbb{R}^d} \delta(m^2 - r^2) u(m) dm = \frac{r^{d-2}}{2} \int_{\mathbb{S}^{d-1}} u(r\omega) d\omega, \qquad (3.6)$$

where u is a test function;

$$|f(k,l)| \le 2\|\hat{v}\|_{\alpha,M} (1+|k-l|^2)^{-M/2}, \tag{3.7}$$

where $(k,l) \in \mathcal{M}_E$, $E \ge E_1 = E_1(\alpha, M, \sigma, d, \|\hat{v}\|_{\alpha, M})$, see formula (1.30a) in [N3];

$$(\sqrt{E})^{d-2} \int_{\mathbb{S}^{d-1}} \frac{(1+|k-l|^2)^{M/2}}{(1+|k-\sqrt{E}\omega|^2)^{M/2}(1+|l-\sqrt{E}\omega|^2)^{M/2}} d\omega \le C(d,M,\sigma)E^{-\sigma/2}, \quad (3.8)$$

where $(k, l) \in \mathcal{M}_E$, E > 0; see Lemma 2.2 in [ER1] and Lemma 1.2 in [ER2].

Consider formulas (1.9), (3.4), (3.5) for arbitrary large E, where k-l = p for arbitrary fixed $p \in \mathbb{R}^d$. It is well known that such a choice of k, l is possible for $d \ge 2$.

As a result we obtain that

$$\hat{v}(p) = \overline{\hat{v}(-p)}, \quad p \in \mathbb{R}^d.$$
 (3.9)

Symmetry (3.9) implies that v is real-valued. This completes the proof.

4. Proof of Proposition 1

Recall that, for $z \in \mathbb{C}$,

$$chz = (e^{z} + e^{-z})/2 = (e^{Rez}e^{iImz} + e^{-Rez}e^{-iImz})/2,$$
 (4.1)

$$chz = 0 \Leftrightarrow Rez = 0, \quad Imz = \pi/2 \quad mod(\pi).$$
 (4.2)

Using (2.5) and (4.2), $z = \kappa x - \zeta$, one can see that v is smooth (analytic in $x \in \mathbb{R}$) since $Im\zeta \neq 0 \mod(\pi/2)$.

Using (2.5) and (4.1), $z = \kappa x - \zeta$, one can also see that

$$v(x) = e^{2Re\zeta} e^{2iIm\zeta} e^{-2\kappa x} (1 + O(e^{-2\kappa x})), \quad x \to +\infty,$$

$$v(x) = e^{-2Re\zeta} e^{-2iIm\zeta} e^{2\kappa x} (1 + O(e^{2\kappa x})), \quad x \to -\infty.$$
(4.3)

Therefore, v decays exponentially as $|x| \to \infty$, and $Imv \neq 0$ since $Im\zeta \neq 0 \mod(\pi/2)$.

In a standard way, for the operator H at positive energies E we consider its scattering eigenfunctions $\psi_1(x,k)$, $\psi_2(x,k)$, where $x \in \mathbb{R}$, $k^2 = E$, k > 0, such that

$$\psi_1(x,k) = e^{-ikx} + s_{12}(k)e^{ikx} + o(1), \quad x \to +\infty,$$

$$\psi_1(x,k) = e^{-ikx} + e^{(1)}, \quad x \to +\infty,$$
(4.4)

$$\psi_1(x,k) = s_{11}(k)e^{-i\kappa x} + o(1), \quad x \to -\infty,$$

$$\psi_2(x,k) = e^{ikx} + s_{21}(k)e^{-ikx} + o(1), \quad x \to -\infty,$$

$$\psi_2(x,k) = s_{22}(k)e^{ikx} + o(1), \quad x \to +\infty.$$
(4.5)

Recall that, for d = 1, the scattering operator S can be written as the matrix

$$S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}.$$
 (4.6)

In terms of this matrix the unitarity property (1.9) at fixed E > 0 takes the form

$$S^* = S^{-1}. (4.7)$$

To study spectral properties of the operator H with v given by (2.5), we use, in particular, the Darboux transforms T and \tilde{T} relating the equations

$$-\phi_{xx} = E\phi,\tag{4.8}$$

$$H\psi = -\psi_{xx} + v(x)\psi = E\psi.$$
(4.9)

We consider

$$\omega = e^{-\zeta} e^{\kappa x} + e^{\zeta} e^{-\kappa x}, \qquad (4.10)$$

$$\tau = -\omega_x \omega^{-1}, \tag{4.11}$$

where ω solves (4.8) for $E = (i\kappa)^2$.

We have that:

$$v = 2\tau_x,\tag{4.12}$$

$$\omega^{-1} = e^{\zeta} e^{-\kappa x} (1 + O(e^{-2\kappa x})), \quad x \to +\infty,$$

$$\omega^{-1} = e^{-\zeta} e^{\kappa x} (1 + O(e^{2\kappa x})), \quad x \to -\infty,$$
(4.13)

$$\tau = -\kappa + O(e^{-2\kappa x}), \quad x \to +\infty,$$

$$\tau = \kappa + O(e^{2\kappa x}), \quad x \to -\infty,$$
(4.14)

assuming in (4.13), (4.14) that $Re\kappa > 0$; in addition, under the assumptions of Proposition 1, ω^{-1} and τ are smooth in a similar way with v.

In addition, due to well-known results of the Darboux transform theory, we have that: if ϕ satisfies (4.8) and

$$\psi = T\phi = \phi_x + \tau\phi, \tag{4.15}$$

then ψ satisfies (4.9); the function ω^{-1} satisfies

$$H\omega^{-1} = (i\kappa)^2 \omega^{-1}; (4.16)$$

if ψ satisfies (4.9) and

$$\phi = \tilde{T}\psi = \psi_x - \tau\psi, \qquad (4.17)$$

then ϕ satisfies (4.8); if ϕ satisfies (4.8), then

$$\tilde{T}T\phi = ((i\kappa)^2 - E)\phi.$$
(4.18)

Let

$$\phi_1 = \frac{e^{-ikx}}{-(ik+\kappa)}, \quad \phi_2 = \frac{e^{ikx}}{ik-\kappa}, \quad x \in \mathbb{R}, \quad k^2 = E, \quad k > 0.$$
(4.19)

Under the assumptions of Proposition 1, using (4.14)-(4.18) one can see that: there are unique ψ_1 , ψ_2 , which satisfy (4.9), E > 0, and have asymptotics of the form (4.4), (4.5); in addition,

$$\psi_1 = T\phi_1, \quad \psi_2 = T\phi_2,$$
(4.20)

$$s_{11} = s_{22} = \frac{ik - \kappa}{ik + \kappa}, \quad s_{12} = s_{21} = 0, \quad k > 0.$$
 (4.21)

As a corollary of (4.21), we have, in particular, the unitarity property (4.7). This completes the proof.

5. Proof of Proposition 2

The eigenfunctions ψ_1 , ψ_2 of the continuous spectrum $\sigma_c(H) = [0; +\infty)$ are given by formulas (4.19), (4.20), where $k \ge 0$.

The function ω^{-1} is the bound state with $E = -\kappa^2$; see formulas (4.13), (4.16).

Using formulas (4.14)-(4.18), one can see that there are no other linearly independent solutions of (4.9), $E \in \mathbb{C}$, with appropriate behavior at infinity.

Therefore, formula (2.6) holds. For complete proof of (2.6) one can use the technique of direct scattering presented, for example, in [F3].

Next, let $Re\zeta = 0$.

Property (1.2) follows from (2.5), (4.1).

Using (4.13), one can see that

$$\overline{\omega^{-1}(-x)} = \omega^{-1}(x), \quad x \in \mathbb{R}.$$
(5.1)

Using (4.4), (4.5), (4.20), (4.21), one can see that

$$\overline{\psi_j(-x,k)} = \overline{s_{jj}(k)}\psi_j(x,k), \quad x \in \mathbb{R}, \ k \ge 0, \ j = 1, \ 2.$$
(5.2)

Therefore, all eigenfunctions of H are also eigenfunctions of the PT-operator. This completes the proof.

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