On calculation of the inverse of multidimensional harmonic oscillator on Schwartz space

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Introduction

Classical harmonic oscillator operator $u(t) \rightarrow -u''(t) + t^2u(t)$, $t \in R$, defined on Schwartz nuclear space S(R) of rapidly decreasing functions on one dimensional Euclidean space R is largely used in quantum mechanics for white noise analysis [1]. In this report p -dimensional analogy of harmonic oscillator operator $u(t) \rightarrow -\Delta u + |t|^2 u(t)$, defined on Schwartz nuclear spaces of rapidly decreasing functions $S(R^p)$ on p -dimensional Euclidean R^p space is considered, where Δ is Laplace operator and $|t|^2 = t_1^2 + t_2^2 + \dots + t_p^2$. We study now the equation contained this operator that is named as the Schrödinger equation and connected with suppersymmetry in quantum mechanics. In particular, suppersymmetry quantum mechanics gives possibility to find nontrivial solutions of Schrödinger equations.

In the previous paper [2] the least squares method generalized for Frechet spaces by us [3] was used for approximate calculation of the inverse of classical harmonic oscillator in S(R), i.e. for the approximate solution of the equation $-u''(t) + t^2u(t) = f(t)$, $t \in R$. The convergence and some estimates of convergence of a sequence of the approximate solutions to the exact solution was also proved.

In this paper generalized the least squares method is used for approximate calculation of the inverse of Schrodinger equation in $S(R^p)$. We give now necessary explanations about Schrodinger equation and calculation of the inverse of multidimensional harmonic oscillator on Schwartz space.

Schwartz space $S(R^p)$ of rapidly decreasing functions on p-dimensional Euclidean space R^p as usually is considered with the sequence of norms

$$\|\varphi\|_{nm} = \sup_{t \in \mathbb{R}^p} |t^i D^j \varphi(t)|, n \in N, m \in N, |i| = i_1 + \dots + i_m, |i| \le n, |j| \le m,$$

where $t^{i} = t_{1}^{i_{1}} \cdots t_{p}^{i_{p}}$, $D^{j} = \partial^{j_{1}+\cdots+j_{p}} / \partial t_{1}^{j_{1}} \cdots \partial t_{p}^{j_{p}}$, $D^{|j|} = \partial^{j_{1}+\cdots+j_{p}} / \partial t_{1}^{j_{1}} \cdots \partial t_{p}^{j_{p}}$, for arbitrary $t = (t_{1}, \cdots, t_{p})$ and multiindices (from nonnegative whole numbers) $i = (i_{1}, \cdots, i_{p}), j = (j_{1}, \cdots, j_{p})$.

The space of all orbits, orbital operator and statement of orbital equation

It is well-known that classical harmonic oscillator operator

$$Au = -\Delta u + |t|^2 u = f(t)$$
 (1)

is a symmetric and positive operator in the Hilbert space $L^2(\mathbb{R}^p)$. For such operators the Frechet space $D(\mathbb{A}^\infty) = \bigcap D(\mathbb{A}^{n-1})$ is created the topology of which is generated with the sequence of norms

$$\|u\|_{n} = \left(\|u\|^{2} + \|Au\|^{2} + \dots + \|A^{n-1}u\|^{2}\right)^{1/2}$$

= $\left(\|u\|^{2} + \|-\Delta u(t) + t^{2}u(t)\|^{2} + \dots + \|A^{n-2}(-\Delta u(t) + t^{2}u(t))\|^{2}\right)^{1/2}, n \in \mathbb{N},$ (2)

where

$$||f|| = (\int_{R^p} |f(x)|^2 dx)^{1/2}$$
 is a norm in $L^2(R^p)$ space.

The norms $\|\cdot\|_n$ are generated by a sequence of inner products

$$(f,g)_n = (f,g) + (Af,Ag) + \dots + (A^{n-1}f,A^{n-1}g).$$

The space $D(A^{\infty})$ is the space of all orbits of the operator A, because their elements has the form $orb(A, x) := \{x, Ax, \dots, A^{n-1}x, \dots\}$ and call as orbit of the operator A at the point x.

The Frechet space $D(A^{\infty})$ was first defined in [4] for any symmetric operator, where $D(A^{\infty})$ was whole symbol and A^{∞} , if taken separately, meant nothing. The space $D(A^{\infty})$ of all orbits was studied by many mathematicians for various differential operators. In [5] we have defined the operator A^{∞} for all symmetric operators on the space of all orbits as follows

$$A^{\infty}\{x, Ax, \dots, A^{n-1}x, \dots\} = \{Ax, A^{2}x, \dots, A^{n}x, \dots\},$$
(3)

i.e. $A^{\infty}(\operatorname{orb}(A, x))=\operatorname{orb}(A, Ax)$. We call A^{∞} orbital operator. Due to this notation the space $D(A^{\infty})$ acquire new meaning that differs from the classical. It will be also noted that according the [5], for positive definite operator A, the orbital operator A^{∞} is topological isomorphism of the Frechet space $D(A^{\infty})$ onto itself. As well Orbital operator A^{∞} coincides algebraically to the restriction of the operator A from $L^2(R^p)$ on $D(A^{\infty})$ and coincides to the restriction of the operator A^N from the Frechet space $(L^2(R^p))^N$ on the space $D(A^{\infty})$ with considering topology. This means that the restriction of equation Au=f on $S(R^p)$ with considering topology coincides to the orbital operator equation

$$A^{\infty} u = f, i.e. A^{\infty}(\operatorname{orb}(A, x)) = \operatorname{orb}(A, f).$$
(4)

This equation has unique and stable solution. Stability is very important for numerical calculations of practical follows, harmonic problems. this assertion that classical oscillator operator From $u(t) \rightarrow -u''(t) + t^2 u(t), t \in \mathbb{R}$, defined on the Hilbert space $L^2(\mathbb{R})$ and the same operator considered on quite S(R)different each-other. Schwartz spaces are from Moreover, the equation $-u''(t) + t^2 u(t) = f(t), t \in \mathbb{R},$ in $L^2(R)$ the space is ill-posed and the equation $-u'(t) + t^2u(t) = f(t)$ $t \in R$, in the space S(R) is well-posed. As well this operator on the space $L^2(R)$ is 'nt positive definite and the operator on the space S(R) is positive definite. Analogously, the Schrodinger equation $Au = -\Delta u + |t|^2 u = f(t)$ in the space $L^2(\mathbb{R}^p)$ is ill-posed and the equation $A^{\infty}u = -\Delta u + |t|^2 u = f(t)$ in the space $S(R^p)$ is well-posed. Therefore, the operator considered in Hilbert space will be denoted through A and the "exsternally same operator" considered in the Frechet space of all orbits $D(A^{\infty})$ with considering topology will be denoted through A^{∞} Namely, the operator in equation $Au = -\Delta u + |t|^2 u = f(t)$ defined on the space $L^{2}(\mathbb{R}^{p})$ will be denoted through A and the "exsternally same operator" in equation $A^{\infty}u = -\Delta u + |t|^{2}u = f(t)$ considered in the Frechet space of all orbits $D(A^{\infty})$ with considering topology will be denoted through A^{∞} We will call this equation orbital operator equation.

Schwartz space $S(R^p)$ is isomorphic to the space $D(A^{\infty})$ of all orbits of the operator A and this isomorphism is obtained by the mapping

$$S(\mathbb{R}^p) \ni x \to \operatorname{orb}(A, x) \coloneqq \{x, Ax, \dots, A^{n-1}x, \dots\} \in D(A^\infty)$$
.

Therefore, norm (2) has the following form $||u||_n = ||\operatorname{orb}(A, u)||_n$ for $n \in N$.

This means that the spaces $D(A^{\infty})$ and $S(R^p)$ are isomorphic and these sequences of norms $\{\|\cdot\|_n\}$ and $\{\|\cdot\|_{n,m}\}$ generates the equivalent topologies. For p = 1 the equivalence of these norms is proved in [6]. From this follows also that $\|x\|_n = \|\operatorname{orb}(A, x)\|_n$ for each $x \in S(R^p)$.

Definition of approximate solution of orbital equation

In this paper the least squares method for approximate calculation of the inverse of Schrödinger equation $A^{\infty}u = -\Delta u + |t|^2 u = f(t)$ in $S(R^p)$ is used, i.e. for approximate solution of orbital equation $A^{\infty}u = f$ the generalized least squares method is used. The convergence and some estimates of convergence of a sequence of the approximate solutions to the exact solution was proved.

Let *E* be a Frechet space with the generated of nondecreasing sequence of norms. For any continuous operator $T: E \to E$ we define the function $\sigma_T: N \to N$ that characterizes the continuity of *T* as follows [3]:

$$\sigma_T(n) = \inf \{ \sigma \in N; \sup \{ \|Tx\|_n; \|x\|_{\sigma} \le 1 \} < \infty \}.$$

The operator is called tame, if $\sigma_T(n) = n+l$ for some integer $l \ge 0$. The operator is called tamely invertible, if $\sigma'(n) = n+l$ for some integer $l \ge 0$, where $\sigma'(n)$ is the function that characterizes the continuity of inverce operator T^{-1} .

For the metrization of the metrizable locally convex spaces E we will use the metric constructed by D.Zarnadze [6]. This metric essentially is used for coordination of parallel computations. Let $\{||.||_n\}$ be an nondecreasing sequence of Hilbertian norms on E, then

$$d(x, y) = \begin{cases} \|x - y\|_{1}, & \text{if} & \|x - y\|_{1} \ge 1, \\ 2^{-n+1}, & \text{if} & \|x - y\|_{n} \le 2^{-n+1} & \text{and} & \|x - y\|_{n+1} \ge 2^{-n+1}, n \in N, \\ \|x - y\|_{n+1}, & \text{if} & 2^{-n} \le \|x - y\|_{n+1} < 2^{-n+1}, n \in N, \\ 0, & \text{if} & x - y = 0 \end{cases}$$
(5)

is a metric on *E* with the quasinorm d(x, y) = |x - y|. This metric has closed absolutely convex balls $K_r = \{x \in E; d(x, y) \le r\} = rV_n$, where $V_n = \{x \in E, ||x||_n \le 1\}$ and

$$r \in I_n = \begin{cases} [1, \infty[, \text{ if } n = 1, \\ [2^{-n+1}, 2^{-n+2}[, \text{ if } n \ge 2. \end{cases}$$

The Minkowski functional $q_r(\cdot)$ of the balls K_r has the following form $q_r(x) = r^{-1} ||x||_n$, $r \in I_n$.

As a basic sequence in the Schwartz space $S(R^p)$ we consider $H_j(t)$ functions [7], that has following form $H_j(t) = \prod_{i=1}^p H_j(t_i)$, where $H_j(t_i) = (2^j j!)^{-1/2} (-1)^j \pi^{-1/4} \exp(t_i^2/2) (d/dt_i)^{(j)} \exp(-t_i^2)$ $(j \ge 1)$ are

Hermits functions. The sequence $\{H_j^{\sim}(t)\}$ forms a basis in $L^2(\mathbb{R}^p)$ ([7], p.391). It is not hard to verify, that $A^{\infty}(H_j(t_1) \cdot H_j(t_2) \cdots H_j(t_p)) = p(2j+1)H_j(t_1) \cdot H_j(t_2) \cdots H_j(t_p)(j \ge 1)$. From this follows that $\{H_j^{\sim}(t)\}$ forms a basis in nuclear space $S(\mathbb{R}^p)$ too. It is also proved that subspace $A^{\infty}(H_j^{\sim}(t))$ admits an orthogonal complement in the Schwartz space $S(\mathbb{R}^p)$. Let $\{H_j^{\sim}(t)\}$ be a sequence of Hermitian functions and G_m be a subspace of $S(\mathbb{R}^p)$, spanned by $H_1^{\sim}(t), \ldots, H_m^{\sim}(t)$. It is easy to prove that this sequence $\{H_j^{\sim}(t)\}$ is $A^{\infty} -$ complete in $S(\mathbb{R}^p)$, i.e. for any $\varepsilon > 0$ and $g \in S(\mathbb{R}^p)$ there exists $n_0 = n_0(g, \varepsilon)$ such that $\overline{\bigcup_{m=1}^{\infty} A^{\infty}(G_m)} = E$.

We will seek an approximate solution of orbital equation $A^{\infty}u = f$ in the form

$$u_m(t) = \sum_{j=1}^m \alpha_j H_j^{\sim}(t) \in G_m,$$

which minimizes the discrepancy $J_n(g) = ||Ag - f||_n$, where *n* is given by $\inf \{|Ag - f|; g \in G_m\} \in I_n$.

Existence and uniqueness of approximate solution of orbital equation

By means of the injectivity of the operator A approximate solution $u_m \in G_m$ for $A^{\infty}u = f$ can be constructed for each $m \in N$ and it is defined in a unique manner. Really, we prove that there exist u_m such that

$$\inf \{ \|A^{\infty}g - f\|_n; g \in G_m \} = r = J_n(u_m).$$

We remark that positive function $J_n(g)$ attains its minimum on G_m at some point u_m only if its square $J_n^2(g)$ attains its minimum on G_m at this point. But as is well known ([8], p.57), $J_n^2(g)$ attains its minimum on G_m at the function $u_m(t) = \sum_{j=1}^m \alpha_j^m H_j^{\sim}(t)$ with coefficients that satisfy the system of equations

$$\sum_{j=1}^{m} \alpha_j (A^{\infty} H_j^{\tilde{}}(t), A^{\infty} H_k^{\tilde{}}(t))_n = (f, A^{\infty} H_k^{\tilde{}}(t))_n, \ k = 1, 2, \cdots, m.$$
(6)

Because A is one-to-one it follows that the function $A^{\infty}H_1^{\sim}(t)$, ..., $A^{\infty}H_m^{\sim}(t)$ are linearly independent for any $m \in M$. It is well-known that necessary and sufficient conditions for the linear independence of the system $\{(A^{\infty}H_j^{\sim}(t))\}_{j=1}^m$ is that the Gramm determinant does not vanish: $\det(A^{\infty}H_1^{\sim}(t), A^{\infty}H_k^{\sim}(t))_n \neq 0$, when n = n(m). Hence, the determinant of the system $\{A^{\infty}H_1^{\sim}(t)\}_{i=1}^m$ is not zero, and (6) has an unique solution for any $m \in N$. From Theorem that s proved in [3] follows the following

Theorem 1. Let *E* be Frechet space the topology of which is defined with the nondecreasing sequence of Hilbertian norms $\{ \|u\|_n \}, T: E \to E,$, injective operator, u_0 be the exact solution of the operator

equation Tu = f. If $\{H_i\}$ be a T-complete basic sequence and there exists continuous inverse operator T^{-1} ,

then the sequence of approximate solutions $\{u_m\}$, constructed using the method of least squares, converges to u_0 in *E*. Moreover, the following estimates hold

a) For every n and m

$$\|u_0 - u_m\|_n \leq C_n \|T u_0 - T u_m\|_{\sigma'(n)},$$

where $\sigma'(n)$ is the function that characterize the continuity of the operator T^{-1} .

b) For every n there exists $m_0 = m_0(n)$ such that for every $m > m_0$

 $||u_0 - u_m||_n \le C_n |f - Tu_m|.$

From this follows the following

Theorem 2. Let $A: D(A^{\infty}) \to D(A^{\infty})$ be harm $A^{\infty}: D(A^{\infty}) \to D(A^{\infty})$ be harmonic oscilator operator and the topology of the space $S(R^p)$ is defined with the sequence of Hilbertian norms $\{\|\cdot\|_n\}$ where $\|u\|_n = (\|u\|^2 + \|Au\|^2 + \dots + \|A^{n-1}u\|^2)^{1/2}$. Let u_0 be the exact solution of orbital equation $A^{\infty}u = f$, then the sequence of approximate solutions constructed using the method of least squares converges to u_0 in $S(R^p)$. Moreover, the following estimates hold:

a) For every n and m

 $||u_0 - u_m||_n \le ||A^{\infty}u_0 - A^{\infty}u_m||_n,$

- b) For every *n* there exists $m_0 = m_0(n)$ such that for every $m > m_0$
- $||u_0 u_m||_n \le |f A^{\infty}u_m|.$

For every m

$$|u_0 - u_m| \leq |f - A^{\infty} u_m|.$$

Proof. The Hermitian function H_j is eigen function for the operator A with the eigen number 2j+1. Therefore

$$(AH_{j}, H_{j})_{n} = (2j+1)(H_{j}, H_{j})_{n} \ge (H_{j}, H_{j})_{n}.$$
(7)

It is well known, that the set of hermitian functions are dence in S(R) [6]. Therefore $(A^{\infty}f, A^{\infty}f)_n \ge (f, f)_n$ for arbitrary $f \in S(R)$. While $(Af, f) \le ||Af||_n ||f||_n$, from (7) follows that $||f||_n \le ||Af||_n$. In this case $C_n = 1$ that follows From the inequality $(A^{\infty}f, f)_n \ge (f, f)_n$, $n \in N$ and this theorem follows from Theorem 1.

The inequality $(A^{\infty}f, A^{\infty}f)_n \ge (f, f)_n$ means time invertibility of the orbital operator A^{∞} . As well the centrality (strongly optimality) of this algorithm is proved.

As well method for calculation of discrepancy $r = |Au_m - f|$ with respect to the quasinorm of metric (5) on $S(R^p)$ is given.

Example

As an example the following equation is considered $Au(t) = -u''(t) + t^2u(t) = \exp(-t^2)\sin t, \quad t \in \mathbb{R}, \ u \in S(\mathbb{R}).$ We calculate the discrepancy

$$\|Au_{m} - f\|_{n} = \left(\|Au_{m} - f\|^{2} + \|A(Au_{m} - f)\|^{2} + \dots + \|A^{n-1}(Au_{m} - f)\|^{2} \right)^{1/2},$$

where
$$u_{m}(t) = \sum_{j=1}^{m} (2j+1)^{-1} (f, H_{j}) H_{j}(t),$$
$$H_{j}(t) = (2^{j} j!)^{-1/2} (-1)^{j} \pi^{-1/4} \exp(t^{2}/2) (d/dt)^{(j)} \exp(-t^{2}) \quad (j \ge 1).$$

We have $Au_m(t) = \sum_{j=1}^m (f, H_j) H_j(t)$ and

$$A^{k} u_{m}(t) = \sum_{j=1}^{m} (2j+1)^{k-1} (f, H_{j}) H_{j}(t)$$

$$\|Au_{m} - f\|_{n}^{2} = \|Au_{m} - f\|^{2} + \|A(Au_{m} - f)\|^{2} + \dots + \|A^{n-1} (Au_{m} - f)\|^{2} =$$

$$= \|Au_{m} - f\|^{2} + \|\sum_{j=1}^{m} (2j+1)(f, H_{j}) H_{j}(t) - Af\|^{2} + \dots + \|\sum_{j=1}^{m} (2j+1)^{n-1} (f, H_{j}) H_{j}(t) - A^{n-1} f\|^{2}$$

The calculation results

Prof. M.D.Kublashvili receive the following results:

- 1. When n = 2, then $r \in [2^{-2+1}, 2^{-2+2}] = [1/2, 1]$ and for m = 5 the quantity r = 0,775... This means that $|Au_5 f| = ||Au_5 f||_2 = r = 0,775...$
- 2. When n = 3, then $r \in [2^{-3+1}, 2^{-3+2}] = [1/4, 1/2]$ and for m = 7 the quantity r = 0,342... This means that $|Au_7 f| = ||Au_7 f||_3 = r = 0,342...$

When $n \ge 4$ it was arise necessity of parallel computing. Prof. P. Tsereteli continued now calculation of this quantities on claster. The algorithm (procedure) for direct calculation of quasinorm is also described.

Conducted numerical experiments confirm the received theoretical results.

M.D.Kublashvili was given also calculation of numerical solution for Schrodinger equation, connected with movement of sea wave.

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