# Approximation of the scattered waves of the Schrödinger operator

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Abstract: In the paper we shall investigate an approximation of a solution of the Schrödinger equation:  $(-\Delta + q(x) - \lambda)u(x) = f(x)$  in an unbounded region  $\Omega \subset \mathbb{R}^n$  for  $\lambda$  belonging to absolute continuous spectrum of an operator  $-\Delta + q$ , where potential q is of short or long range type or oscillating one. Two steps are considered. In the first step  $\Omega$  is replaced by a finite region and generalized Sommerfeld condition is applied. In the second step the Galerkin method is used. The error estimates are given showing explicit dependence on radius of a finite region.

Key-Words: Scattered wave, Schrödinger operator, Galerkin method.

### 1 Introduction

In the paper we shall investigate an approximation of a solution of the Schrödinger equation:

$$(-\Delta + q(x) - \lambda)u(x) = f(x) \tag{1}$$

in an unbounded region  $\Omega \subset \mathbb{R}^n$  with zero Dirichlet, Robin or Neumann boundary condition on  $\partial \Omega$  or in the whole space  $\Omega = \mathbb{R}^n$ . We assume that  $\partial \Omega$  is bounded and sufficiently smooth. We also assume that the potential q is such that  $-\Delta + q$  admits a unique self-adjoint realisation in  $L^2(\Omega)$ , which we denote by H, with the domain  $D(H) \subset \{u \in H^2 : Bu = 0\}$ , where operator B defines boundary condition on  $\partial\Omega$ : Bu = u or  $Bu = \frac{\partial u}{\partial \nu} + du = 0$  (the case d = 0 is also included). The point  $\lambda$  belongs to absolute continuous spectrum of operator H [12]. The paper generalizes results obtained by Kako [8] and other authors dealing with Helmholtz problem [5,7]. In his paper Kako considered "short range" and "long range" perturbations of the Laplacian. The approximation is based on the so called "limiting absorption principle" stating that the scattered waves  $u^{\pm}$  (known as outgoing and incoming waves) satisfy radiation condition:  $D_{\lambda}^{\pm}u^{\pm} \equiv \frac{\partial u^{\pm}}{\partial r}(x) \mp i\sqrt{\lambda}u^{\pm}(x) + \frac{n-1}{2r}u^{\pm}(x) \to 0$  in some sense as radius  $r \to \infty$ . Kako introduced an analytical approximation in the finite region  $B_R = \{x : |x| < R\}$ :

$$(-\Delta + q(x) - \lambda)u_R^{\pm}(x) = f(x) \text{ in } B_R,$$
$$D_{\lambda}^{\pm}u_R^{\pm} = 0 \text{ on } S_R = \{x : |x| = R\}.$$

Then he proved [8] that  $\exists (R_n \to \infty)$  such that  $\|e_{R_n}^{\pm}\|_{L^2(S_{R_n})} \to 0$ , where  $e_R^{\pm}$  is the error between exact and approximate solutions  $e_R^{\pm} \equiv u^{\pm} - u_R^{\pm}$ , and in a very special case of "short range" perturbations for  $q(x) = O(|x|)^{-1-\delta}$  and  $\delta > (n - 1)/2$  on some fixed, bounded region  $B \subset B_R$ :  $\sup_B R_n^{\epsilon} |e_{R_n}^{\pm}| \to 0$  for some  $\epsilon > 0$ . He investigated further approximation by sequence of solutions of discrete problems obtained by means of the Bubnov-Galerkin method. There are three main aims of this paper:

- we would like to extend these results for more types of potentials. In the paper we consider also oscillating potentials, however the used method can be applied to other types of potentials under some additional conditions (see [10]),
- we want to obtain estimates for the difference  $e_R^{\pm}$  on the whole domain of analytical approximation (not only on some fixed subregion),
- we want to know how the error explicitly depends on radius R.

In order to reach our aims we do not assume any special form of the potential, but we use the "limiting absorption principle" as our main assumption. Our estimates will be expressed in weighted  $L^2$  norm because the exact solution of (1) belongs to this kind of space.

## 2 Preliminaries

By  $L^{2,s}$  we denote the space:

$$L^{2,s}(\Omega) := \{ u : \int_{\Omega} (1 + |x|)^{2s} |u(x)|^2 dx < \infty \}$$

with the norm:

$$\| u \|_{0,s} = \left( \int_{\Omega} (1 + |x|)^{2s} |u(x)|^2 dx \right)^{1/2}$$

for any  $s \in R$ . We use also typical notation for Sobolev space and its norm (like  $\|\cdot\|_{1,\Omega}$  or simply  $\|\cdot\|_1$  for space  $H^1(\Omega)$ ; for space  $H^0 = L^2$  we sometimes omit the subscript "0"). By B(X, Y)we denote space of linear, bounded operators from a Banach space X into a Banach space Y. The "limiting absorption principle" is our main assumption:

(**LAP**) There exist  $s_1, s_2, \sigma \in R$ , such that a function:

$$(0,1) \ni \epsilon \longrightarrow R(\lambda \pm i\epsilon) := (H - \lambda \mp i\epsilon)^{-1},$$

 $R(\lambda \pm i\epsilon) \in B(L^{2,s_1}(\Omega), L^{2,s_2}(\Omega))$  has a limit at point  $\epsilon = 0$ . For any  $f \in L^{2,s_1}(\Omega)$  the functions:

$$u^{\pm} = R^{\pm}(\lambda)f := \lim_{\varepsilon \to 0} R(\lambda \pm i\epsilon)f$$

verify the differential equation (1). Moreover there exist  $R_0 > 0$  and functions  $k_{\lambda}^{\pm} : E_{R_0} \to C$ such that, the following generalized Sommerfeld condition holds:

$$D_{\lambda}^{\pm}u^{\pm} \equiv \frac{\partial u^{\pm}}{\partial r} - k_{\lambda}^{\pm}(x)u^{\pm} \in L^{2,\sigma}(E_{R_0}),$$

where  $E_{R_0} = \{x : |x| > R_0\}$ . Finally  $\exists K > 0$  such that:

$$\| u^{\pm} \|_{0,s_2} + \| D^{\pm}_{\lambda} u^{\pm} \|_{0,\sigma} \le K \| f \|_{0,s_1}$$

The next assumption is connected with properties of function  $k_{\lambda}$  typical for any (LAP). (**K**)  $\exists c_1, c_2 > 0$  such that

1. 
$$k_{\lambda}^{+} = \overline{k_{\lambda}^{-}}$$
  
2.  $\pm Im \ k_{\lambda}^{\pm}(x) \ge c_{1}$   
3.  $|k_{\lambda}^{\pm}(x)| \le c_{2}$ 

The last assumption is related to the properties of the potential and practically does not give additional constraint on class of potential as typically (LAP) holds under similar conditions. (**Q**) (a)  $\forall R > 0 \ \forall \epsilon > 0 \ \exists c > 0 \ \forall \varphi \in H^1(B_R)$ 

$$\int_{B_R} q |\varphi|^2 \le \varepsilon \int_{B_R} |\nabla \varphi|^2 + c(\varepsilon, R) \int_{B_R} |\varphi|^2$$
  
(b)  $\forall R > 0 \exists c > 0 \ \forall \varphi \in H^1(B_R)$   
 $\|q\varphi\|_0 \le c \|\varphi\|_1.$ 

(c) 
$$\exists R_0 > 0 \ \forall R > R_0 \ \exists c > 0$$

$$||q||_{L^{\infty}(B_{R-1,R+1})} \le c,$$

where  $B_{r,R} = \{x : r < |x| < R\}.$ 

The assumpton (Q)(a) is satisfied for example under following conditions:

 $q \in L^p + L^{\infty}$ , where p > n/2 for  $n \ge 4$  and p = 2 for  $n \le 3$ . Also Stummel functions satisfy (Q)(a) [12]. Condition (Q)(b) assures that multiplication operator (by potential) is bounded in Sobolev space, while (Q)(c) means that the potential is locally bounded in some sense. To illustrate our considerations we will assume, that potential q is one of the following type: (SR) "short range":  $|q(x)| \le c(1+|x|)^{-1-\delta_s}$ 

(LR) "long range":  $|q(x)| \leq c(1+|x|)$ (LR) "long range":  $|q(x)| \leq c(1+|x|)^{-\delta_l}$  and

$$\left|\frac{\partial q}{\partial r}(x)\right| \le c(1+|x|)^{-1-\delta_l}$$

(OSC) "oscillating": 
$$|q(x)| \le c$$
,  
 $\left|\frac{\partial q}{\partial r}(x)\right| \le c(1+|x|)^{-1}$  and for some  $a > 0$   
 $\left|\frac{\partial^2 q}{\partial r^2}(x) + aq(x)\right| \le c(1+|x|)^{-1-\delta_o}.$ 

Then the limiting absorption principle is valid in the space  $B(L^{2,s}, L^{2,-s})$  for some s > 1/2 (s depends on  $\delta$ ) [6,9,11]. The radiation condition is satisfied with the following functions  $k_{\lambda}$ : (SR) and (LR)  $k_{\lambda}^{\pm} = \pm i\sqrt{\lambda} - \frac{n-1}{2\pi}$ 

(OSC) 
$$k_{\lambda}^{\pm} = \pm i \sqrt{\lambda - wq(x)} - \frac{n-1}{2r} + \frac{w\partial_r q}{4(\lambda - wq)}$$
  
where  $w = \frac{4\lambda}{4\lambda - q}$ .

At the end of this section we formulate simple lemma.

**Lemma 1**  $\forall f \in L^{2,s}(\Omega) \exists (r_n \to \infty) \text{ such that,}$ 

$$r_n^{2s+1} \int_{S_{r_n}} |f|^2 dS_{r_n} \to 0.$$

#### 3 Analytical approximation

The analytical approximation problem is defined as follows:

Find 
$$u \in H^2(\Omega_R)$$
  $(\Omega_R = \Omega \cap B_R)$  such that:

$$(-\Delta + q(x) - \lambda)u_R^{\pm}(x) = f(x) \text{ in } \Omega_R, \qquad (2)$$
$$Bu_R^{\pm}(x) = 0 \text{ on } \partial\Omega,$$
$$D_{\lambda}^{\pm}u_R^{\pm} = 0 \text{ on } S_R.$$

It can be shown that (2) has unique solution under conditions (LAP), (K) and (Q) [8,10]. Let  $e_R^{\pm} = u^{\pm} - u_R^{\pm}$  be the error between original solution of (1) and analytical approximation of (2).

**Theorem 1** Let the assumption (LAP), (K) and (Q) be satisfied. Then  $\exists (R_n \to \infty)$ 

$$R_n^{\sigma+1/2} \| e_{R_n}^{\pm} \|_{L^2(S_{R_n})} \to 0.$$

<u>Proof.</u> The error  $e_R(x)$  verifies the following equations (we omit the subscript  $\pm$ ):

 $(-\Delta + q - \lambda)e_R = 0$  in  $\Omega_R$  $Be_R = 0$  on  $\partial\Omega$ 

 $D_{\lambda}e_R = D_{\lambda}u$  on  $S_R$ .

Multiplying the first equation by  $\overline{e}_R$ , integrating it and taking imaginary part, from (K) and Schwartz's inequality we get:

$$\|e_R\|_{L^2(S_R)} \le c \|D_\lambda u\|_{L^2(S_R)}.$$
 (3)

Hence the result is an obvious consequence of the assumption (LAP) and Lemma 1.

Now we give variational formulation of our problem. Further on we assume that Robin condition on  $\partial\Omega$  is imposed. Dirichlet and Neumann conditions can be treated in the same way. Firstly we define a space:

$$V_R = \begin{cases} \{u \in H^1(\Omega_R) : u = 0 \mid_{\partial\Omega}\} & \text{if } Bu = u \\ H^1(\Omega_R) & \text{otherwise} \end{cases}$$

and bilinear forms  $a_R, b_R : V_R \times V_R \to C$ :

$$a_R^{\pm}(u,v) = \int\limits_{\Omega_R} (\nabla u \nabla \overline{v} + c_0 u \overline{v}) + \int\limits_{\partial\Omega} du \overline{v} - \int\limits_{S_R} k_\lambda u \overline{v}$$

where the constant  $c_0$  is taken in such a way that the form  $a_R^{\pm}$  in  $V_R$ -elliptic i.e.  $|a_R(u, u)| \ge m ||u||_1^2$  for some m > 0 (for a choice of  $c_0$  see [10]).

$$b_R(u,v) = \int_{\Omega_R} (q - \lambda - c_0) u\overline{v}$$

The form  $b_R$  in virtue of (Q) is bounded in  $V_R$ . Then the functions  $u^{\pm}$ ,  $u_R^{\pm}$ ,  $e_R^{\pm}$  satisfy the following equations respectively:

$$a_{R}^{\pm}(u^{\pm}, v) + b_{R}(u^{\pm}, v) = (f, v) + \int_{S_{R}} D_{\lambda}^{\pm} u^{\pm} \overline{v} \quad (4)$$

$$a_R^{\pm}(u_R^{\pm}, v) + b_R(u_R^{\pm}, v) = (f, v)$$
 (5)

$$a_R^{\pm}(e_R^{\pm}, v) + b_R(e_R^{\pm}, v) = \int_{S_R} D_{\lambda}^{\pm} u^{\pm} \overline{v} \qquad (6)$$

for any  $v \in V_R$ .

Our main theorem can be formulated as follows:

**Theorem 2** Let the assumptions (LAP), (K) and (Q) be satisfied with (LAP) holding in the space  $B(L^{2,s}, L^{2,-s})$  (s > 0). If  $f \in L^{2,s}$  then the following estimate is valid:

$$|e_R^{\pm}||_{0,-s} \le (c_1 + \frac{c_2}{R^{\sigma}}) ||D_{\lambda}^{\pm}u||_{L^2(S_R)}$$

for some constants  $c_1, c_2 > 0$  and  $R > R_0 > 0$ .

<u>Proof</u> (sketch). Let us begin with the well known formula (we consider the + case):

$$\|e_R^+\|_{0,-s} = \sup_{g \in C_0^\infty} \frac{|(e_R^+,g)|}{\|g\|_{0,s}}$$

Using (LAP) we can assume, that  $g = (-\Delta + q - \lambda)u^-$ . Integrating by parts we get from (4,5,6)

$$\begin{split} \|e_{R}^{+}\|_{0,-s} &= \sup_{g} \frac{|(e_{R}^{+}, (-\Delta + q - \lambda)u^{-}))|}{\|g\|_{0,s}} = \\ &= \sup_{g} \frac{|\int_{S_{R}} D_{\lambda}^{+}u^{+}u^{-} - \int_{S_{R}} e_{R}^{+} \overline{D_{\lambda}^{-}u^{-}}|}{\|g\|_{0,s}} \leq \\ &\leq \sup_{g} \frac{\|D_{\lambda}^{+}u^{+}\|_{S_{R}}\|u^{-}\|_{S_{R}}}{\|g\|_{0,s}} + \\ &+ \sup_{g} \frac{\|e_{R}^{+}\|_{S_{R}}\|D_{\lambda}^{-}u^{-}\|_{S_{R}}}{\|g\|_{0,s}} \end{split}$$

From previous theorem it follows that

$$\|e_{R}^{+}\|_{S_{R}} \leq c \|D_{\lambda}^{+}u^{+}\|_{S_{R}} \sup_{g} \left(\frac{\|u^{-}\|_{S_{R}}}{\|g\|_{0,s}} + \frac{\|D_{\lambda}^{-}u^{-}\|_{S_{R}}}{\|g\|_{0,s}}\right)$$

Taking imaginary part in (4) for  $v = u^{-}$  we get:

$$\|u^{-}\|_{S_{R}}^{2} \le c(\|D_{\lambda}^{-}u^{-}\|_{S_{R}}\|u^{-}\|_{S_{R}} + |(g, u^{-})|)$$

which gives  $||u^-||_{S_R} \le c(||D_{\lambda}^- u^-||_{S_R} + ||g||_{0,s}).$ In this manner we obtain:

$$\|e_R\|_{0,-s} \le c \|D_{\lambda}^- u^+\|_{S_R} \cdot \\ \cdot \sup_g \frac{\|D_{\lambda}^- u^-\|_{S_R} + \|g\|_{0,s}}{\|g\|_{0,s}}$$

where constant c does not depend on R. From trace theorem it can be concluded that (see [10]):

$$\|D_{\lambda}^{-}u^{-}\|_{S_{R}} \le c \|u^{-}\|_{2,B_{R-1/2,R+1/2}}$$

where again constant c is independent of R. From a priori estimates [10] for some T > 1/2 (independent of R) we have:

$$\|D_{\lambda}^{-}u^{-}\|_{S_{R}} \le c(\|g\|_{0,B_{R-T,R+T}} + \|u^{-}\|_{0,B_{R-T,R+T}})$$

In order to estimate the norm  $||u^-||_{0,B_{R-T,R+T}}$ we will integrate (3) with respect to r over (R-T, R+T). Hence from (LAP) we obtain:

$$\|u^{-}\|_{0,B_{R-T,R+T}}^{2} \le (c_{1} + \frac{c_{2}}{R^{2\sigma}}) \|g\|_{0,s}^{2}$$

This implies the desired result.

It should be stressed that all the constants can be calculated explicitly. As a consequence of the theorem we can easily get the following corollaries:

**Corollary 1** For the oscillating potential  $\exists (R_n \to \infty)$ :

$$R_n^{2s-3/4} \| e_{R_n}^{\pm} \|_{0,-s} \to 0.$$

**Corollary 2** For the potential q with compact support the following inequality holds:

$$\|e_R^{\pm}\|_{0,-s} \le \frac{c}{R^2}.$$

<u>Proof</u>. This is consequence of theorem 2 and well known inequality [8]:

$$|D_{\lambda}^{\pm}u^{\pm}| \le \frac{c}{(1+R)^{(n+3)/2}}$$

The second corollary is particularly useful in practical cases. Theorem 2 makes it also possible to obtain estimates for resolvent operators:

**Lemma 2** Let the assumptions of theorem 2 be fulfilled. Then for sufficiently large R the following estimate is valid:

$$\| (H_R^{\pm} - \lambda)^{-1} \|_{B(L^{2,s}, V_R^{-s})} \le (c_1 + \frac{c_2}{R^{2\sigma}}).$$

where  $H_R^{\pm} = -\Delta + q$  with domain  $D(H_R^{\pm} = \{u \in H^2(\Omega_R) : Bu = 0, D_{\lambda}^{\pm}u = 0\}$  and  $V_R^s$  denotes the space  $V_R$  with the norm:

$$||u||_{1,s} = \sqrt{\int_{\Omega_R} (|u|^2 + \sum_i |\frac{\partial u}{\partial x_i}|^2)(1+|x|)^{2s}}.$$

<u>Proof.</u> Estimate for resolvent in the space  $\overline{B(L^{2,s}, L^{2,-s})}$  can be proved from estimates for  $D_{\lambda}^{\pm}u^{\pm}$  obtained in the proof of Theorem 2. In order to get such inequality in the  $B(L^{2,s}, V_R^{-s})$  additional *a priori* estimates are needed:

$$||u_R||_{1,-s} \le c(||u_R||_{0,-s} + ||f||_0).$$

We omit this proof (see [10]).

**Corollary 3** Under the assumptions of theorem 2 the following estimate holds:

$$\|e_R^{\pm}\|_{1,-s} \le (c_1 + \frac{c_2}{R^{\sigma}}) \|D_{\lambda}^{\pm}u\|_{L^2(S_R)}$$

for some constants  $c_1, c_2 > 0$  and  $R > R_0 > 0$ .

<u>Proof</u>. This is consequence of previous lemma and theorem 2.

#### 4 Discrete approximation

In this section we apply the Galerkin method to the analytical approximation problem. Further on we treat the + case only and omit this subscript. We use the following assumption:

(**P**) Let  $(V_h)$  be a set of closed subspace of  $V_R$ , such that the  $a_R$ -projection  $P_h : V_R \to V_h$  defined by the formula:

$$a_R(P_hu, v_h) = a_R(u, v_h) \; \forall v_h \in V_h$$

tends strongly to identity as  $h \to 0$ , i.e.

$$\forall u \in V_R \lim_{h \to 0} \|u - P_h u\|_1 = 0.$$

The condition is satisfied, for example, when  $V_h$  is a set of piecewise linear continuous functions on uniformly regular triangulations of  $\Omega_R$  - as in finite element method (FEM). It is obvious that [4]:

1.  $||P_h|| \le C$ 2.  $\inf_{v_h \in V_h} ||u - v_h||_1 \le ||u - P_h u||_1$  and  $||u - P_h u||_1 \le c \inf_{v_h \in V_h} ||u - v_h||_1$  The discrete approximation leads then to the problem:

Find  $u_{R,h} \in V_h$  such that  $\forall v_h \in V_h$  holds:

$$a_R(u_{R,h}, v_h) + b_R(u_{R,h}, v_h) = (f, v_h)$$
(7)

Then it can be shown that the following theorem is true [10]:

**Theorem 3** Let the asymptions (LAP), (Q), (K)and (P) be fulfilled and  $u_R$  be the solution of analytical approximation problem. Then for sufficiently small h variational problem (7) has a unique solution  $u_{R,h}$  and the following estimate is valid:

$$\inf_{v_h \in V_h} \|u_R - v_h\|_1 \le \|u_R - u_{R,h}\|_1 \le \le c(R) \inf_{v_h \in V_h} \|u_R - v_h\|_1$$

In this theorem constant c depends on radius R. In the rest of this section we shall give a similar theorem but with constant c independent of R. For the sake of convenience we reformulate our problem in such a way that the solution could be estimated in the norm without the weight. Putting  $u_R = \chi w_R$ , where  $\chi$  is a positive  $C^2$ -function such that:

$$\chi(x) = \begin{cases} 1 & \text{for } |x| \le R_0\\ (1+|x|)^s & \text{for } |x| \ge R_0+1 \end{cases}$$

the analytical approximation problem takes the following form:

$$(-\Delta + q(x) - \lambda - \frac{\Delta\chi}{\chi})w_R - \frac{2\nabla\chi\cdot\nabla w_R}{\chi} = \frac{f}{\chi} \equiv g,$$
$$\mathcal{D}_{\lambda}w_R \equiv \frac{\partial w_R}{\partial r} - (k_{\lambda} - \frac{s}{1+|x|})w_R = 0 \text{ on } S_R,$$
$$Bw_R = 0 \text{ on } \partial\Omega \tag{8}$$

It is obvious that  $\exists c_1, c_2 > 0$  (independent of R) such that:

$$c_1 \| w_R \|_1 \le \| u_R \|_{1,-s} \le c_2 \| w_R \|_1$$

Let us define accordingly two bilinear forms  $a_R, b_R : V_R \times V_R \to C$ :

$$\begin{aligned} \mathbf{a}_{R}(w,v) &= \int_{\Omega_{R}} (\nabla w \nabla \overline{v} - \frac{\Delta \chi}{\chi} w \overline{v} - \frac{2 \nabla \chi \cdot \nabla w}{\chi} \overline{v}) \\ &+ \int_{\Omega_{R}} c_{0} w \overline{v} - \int_{S_{R}} k_{\lambda} w \overline{v} + \int_{\partial \Omega} dw \overline{v} \end{aligned}$$

$$\mathbf{b}(w,v) = \int_{\Omega_R} (q - \lambda - c_0) w \overline{v}$$

with appropriate choice of  $c_0$ . Then both forms are bounded and form  $a_R$  is coercive. Analytical approximation problem can be formu-

lated as follows:

Find  $w_R \in V_R$  such that  $\forall v \in V_R$ 

$$a_R(w_R, v) + b_R(w_R, v) = \int_{\Omega_R} g\overline{v} \qquad (9)$$

Let us also define an operator  $\mathcal{A}_R := -(\Delta w + \frac{\Delta \chi}{\chi}w + \frac{2\nabla \chi \cdot \nabla w}{\chi}) + c_0 w$  with the domain:

$$D(\mathcal{A}_R) = \{ w \in H^2(\Omega_R) : Bw = 0, \mathcal{D}_\lambda w = 0 \}$$

Instead of (P) we introduce the following assumption (typical for FEM [4]): (**ES**)

$$\forall u \in D(\mathcal{A}_R) \inf_{v_h} \|u - v_h\|_1 \le ch \|\mathcal{A}_R u\|_0$$

If conditions (LAP) and (K) are satisfied, then (ES) implies analogous inequality for dual operator  $\mathcal{A}_{R}^{*}$ :

$$\forall u \in D(\mathcal{A}_R^*) \inf_{v_h} \|u - v_h\|_1 \le ch \|\mathcal{A}_R^* u\|_0.$$

The discrete approximation can be rewritten as follows:

Find  $w_{R,h} \in Vh$  such that  $\forall v_h \in V_h$ :

$$\mathbf{a}_{R}(w_{R,h}, v_{h}) + \mathbf{b}_{R}(w_{R,h}, v_{h}) = \int_{\Omega_{R}} v\overline{v} \qquad (10)$$

Existence and uniqueness of solution of (10) easily follows from (8,9) and previous considerations.

**Theorem 4** Let the asumptions (LAP), (Q), (K)and (ES) be satisfied with (LAP) holding in  $B(L^{2,s}, L^{2,-s}), (s > 0)$ . Let  $w_{R,h}$  and u be the solutions of discrete approximation and original respectively. Then for sufficiently small h the following inequality holds:

$$\|w - w_{R,h}\|_{1} \leq \frac{1}{c_{3} - c_{4}hR^{2s}} (c_{1} \inf_{v_{h}} \|w - v_{h}\|_{1} + c_{2}(1 + hR^{2s}) \|D_{\lambda}u\|_{S_{R}})$$

where  $w = \frac{u}{\chi}$  and constants  $c_1, c_2, c_3, c_4$  are independent of R.

<u>Proof</u> (sketch). Let us notice that  $\forall v \in V_R$  the function w satisfies:

$$\mathbf{a}_R(w,v) + \mathbf{b}_R(w,v) = (g,v) + (\mathcal{D}_\lambda w, v)_{L^2(S_R)}$$

Then from coercivness of  $a_R$ , (Q) and theorem 2, after some manipulations we can get:

$$c_{1} \| w - w_{R,h} \|_{1}^{2} \leq c_{2} [(\| w - v_{h} \|_{1} + \| \mathcal{D}_{\lambda} w \|_{0,S_{R}}) \cdot \| w - w_{R,h} \|_{1} + \| \mathcal{D}_{\lambda} w \|_{0,S_{R}} \| w - v_{h} \|_{1} + (1 + R^{-2\sigma}) \| D_{\lambda} u \|_{0,S_{R}}^{2} + \| w - w_{R,h} \|_{0}]$$

The last term can be estimated by Aubin-Nietzche trick and corollary 3 as follows (for details see [10]):

$$\|w - w_{R,h}\|_{0} \leq c(\|D_{\lambda}u\|_{0,S_{R}} + \|w - w_{R,h}\|_{1})F_{\omega}$$
  
where  $F_{\omega} = \sup_{\phi \in L^{2}} \frac{\inf_{v_{h}} \|\omega_{R,h} - v_{h}\|_{1}}{\|\phi\|_{0}}$  and  $\omega_{R,h}$  is a

solution of a dual problem i.e.  $\forall v \in V_R$ 

$$\mathbf{a}_R(v,\omega_{R,h}) + \mathbf{b}_R(v,\omega_{R,h}) = (\phi, v)$$

Now making use of resolvent estimates (lemma 2) and assumption (ES) we can get:  $F_{\omega} \leq ch(1+R^{-2\sigma})R^{2s} \leq chR^{2s}$ . Hence for sufficiently small h we get:

$$(c_{1} - c_{2}hR^{2s}) \| w - w_{R,h} \|_{1}^{2} \leq c_{3}(\| w - v_{h} \|_{1} + \| D_{\lambda}u \|_{0,S_{R}}) \| w - w_{R,h} \|_{1} + c_{4} \| D_{\lambda}u \|_{0,S_{R}} \| w - v_{h} \|_{1} + c_{5}(1 + h^{2}R^{2s}) \| D_{\lambda}u \|_{0,S_{R}}^{2}.$$

After solving this inequality we get the result.

## 5 Conclusions

In the paper some estimates for approximation of the scattered waves of Schrödinger equations by means of generalized Sommerfeld condition have been proven. It should be stressed that presented methodology allows for obtaining analoguous results for much wider class of potentials under similar conditions [10]. In particular it concerns exploding potential as "limiting absorption principle" also holds for such potentials [2,3]. In order to deal with this the assumptions (K2) and (Q)(c) should be modified in such a way, that the constants are replaced by functions depending on radius. Then all theorems remain valid with more complex expressions in the estimates. For practical reasons it may be convenient to introduce the function  $\rho$  of  $C^2$  class such that:

$$\rho(x) = \int_{R_0}^{t} k_{\lambda}(t\omega) dt \text{ for } |x| \ge R_0,$$

<u>.</u>

$$\rho(x) \equiv 1 \text{ on } S_{R_0} \text{ and } |\rho| > c > 0,$$

where spherical coordinates are used in the integral. Then  $\frac{\partial \rho}{\partial r} = -k_{\lambda}\rho$  for  $|x| > R_0$ . Putting  $v_R = \rho u_R$  we get  $D_{\lambda}u_R = \frac{\partial v_R}{r\partial r}$ . This procedure can be applied for sufficiently smooth  $k_{\lambda}$  and eliminates integral over  $S_R$ , which simplifies numerical realisation.

*References:* 

- S. Agmon, Spectral properties of Schrödinger operators and scattering theory, Ann. Sc. Norm. Sup. 2, 1975, pp. 151-218
- M. Ben Artzi, A limiting absorption principle for Schrödinger operators with spherically symmetric exploding potentials, *Israel J.Math* 40, 1981, pp. 259-274
- 3. M. Ben Artzi, Resolvent estimates for a certain class of Schrödinger operators with exploding potentials, *J.Diff.Eq.* 52, 1984, pp. 327-341
- 4. P. G. Ciarlet, *The Finite Element Method* for Elliptic Problems, Nort-Holland, 1978
- C. I. Goldstein, The Finite Element Method with Non-iniform Mesh Sizes Applied to the Exterior Helmhlotz Problem, *Num. Math.* 38, 1982 pp. 61-82
- T. Ikebe, Y. Saito, Limiting absorption principle and absolute continuity for Schrödinger operators, J.Math. Kyoto 12, 1972, pp.513-542
- Jiang Song, Li Kai-Tai, The coupling of FEM and boundary method for 2dimensional Helmholtz equation on an exterior domain, *J. Comput. Math* 5, 1987, pp.21-37
- T. Kako, Approximation of the Scattered States by Means of the Radiation Boundary Conditions, *Math. Meth. in the Appl. Sci.* 3, 1981, pp. 506-515
- K. Mochizuki, J. Uchiyama, Radiation conditions and spectral theory for 2body Schrödinger operators with oscillating long-range potentials, *J. Math. Kyoto* 18, 1978, pp. 377-407; 19, 1979 pp. 47-70; 21, 1981, 605-618
- S. Potempski, Approximation of the solution of Schrödinger equations for some types of potentials, Ph.D.Thesis (in Polish), University of Warsaw, 1990
- 11. Y. Saito, Spectral Representation for Schrödinger operators with Long Range Potentials, Springer-Verlag, 1979
- 12. M. Schechter, Spectra of partial differential operators, North-Holland, 1986