Proceedings of I. Vekua Institute
of Applied Mathematics
Vol. 59-60, 2009-2010

ON THE SYSTEM OF INTEGRAL EQUATIONS CONNECTED WITH THE SCHRODINGER EQUATION

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Abstract. The particle transport in the micromaterials having crystal structure is considered from the relativistic point of view. The process is modeled by the system of partial differential equations connected with the 3D non-stationary Schrödinger equation with the appropriate initial-boundary conditions. For the small time interval this system is reduced to the Fredholm integral equation. The sufficient conditions of existence of the solution of this system is obtained.

Keywords and phrases: Boundary value problem, Schrödinger equation, integro-differential equation.

AMS subject classification (2000): 30E25; 35R10; 35Q41.

Let us consider a particle transport at the $3D$ crystal nanostructure. This structure is periodical. Let us denote one sample (period) of this structure by G_0 in the coordinate system $Oxyz$ and let the crystal area V contain n number of these samples.

Some metals in the solid state form a cubical crystal lattice, for example gold, silver, germanium [1–4]. We will consider the general case, when G_0 is a simply-connected domain of any form. For the crystal lattice it is sufficient to consider the movement of one particle [1–4]. The particle transport at this system could be described by the Schrödinger equation [1–4]

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + (E-U)\psi, \tag{1}$$

where $\hbar$ is the Plank constant, m is a mass of the electron, $E-U$ is the energy, ψ is a wave function, $\psi = u+iv$. Also the following initial-boundary conditions are satisfied:

$$v\big|_{t=0} = v_0, \;\; u\big|_{t=0} = u_0, \;\; v\big|_{\Gamma\times\{0<t<T\}} = 0, \;\; u\big|_{\Gamma\times\{0<t<T\}} = 0, \tag{2}$$

where Γ is the boundary of the considered structure, u_0, v_0 are the definite continuous functions. The condition (2) reflects initial quantum states of a particle, when it is confined at the quantum box G_0 [1–4].

The equation (1) is equivalent to the following system of partial differential equations in the area $Q_T = V\times\{0<t<T\}$:

$$\begin{cases} \alpha\dfrac{\partial v}{\partial t} = \beta\Delta u - (E-U)u \\ \alpha\dfrac{\partial u}{\partial t} = -\beta\Delta v + (E-U)v, \end{cases} \tag{3}$$

$$v\big|_{t=0} = v_0, \quad u\big|_{t=0} = u_0,$$
$$(u = v)\big|_{\Gamma\times\{0<t<T\},} = 0,$$

where $\alpha = \hbar = const$, $\beta = \frac{\hbar^2}{2m} = const$. Suppose that $E - U = c(x, y, z, t)$, then the system (3) becomes:

$$\begin{cases} \alpha \dfrac{\partial v}{\partial t} = \beta \Delta u - c(x, y, z, t)u, \\ \alpha \dfrac{\partial u}{\partial t} = -\beta \Delta v + c(x, y, z, t)v. \end{cases} \tag{4}$$

At the small time-interval $0 < t < t_1$ (t_1 is rather small), the system (4) could be written as:

$$\begin{cases} \alpha \dfrac{v - v_0}{t_1} = \beta \Delta u - cu, \\ \alpha \dfrac{u - u_0}{t_1} = -\beta \Delta v + cv. \end{cases} \tag{5}$$

Let us rewrite the system (5) in the form:

$$\begin{cases} \Delta u = \dfrac{c}{\beta} u + \dfrac{\alpha}{\beta} \dfrac{v - v_0}{t_1}, \\ \Delta v = \dfrac{c}{\beta} v - \dfrac{\alpha}{\beta} \dfrac{u - u_0}{t_1}. \end{cases} \tag{6}$$

Putting first equation of (6) into the second, the system (6) could be equivalently reduced to the following partial differential equation with respect to u_1

$$\Delta\Delta u_1 - 2\frac{c}{\beta}\Delta u_1 - \frac{2}{\beta}\left(\frac{\partial c}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial c}{\partial y}\frac{\partial u}{\partial y} + \frac{\partial c}{\partial z}\frac{\partial u}{\partial z}\right) + \left(\frac{c^2}{\beta^2} + \frac{\alpha^2}{\beta^2 t_1^2}\right) u_1 - \frac{\Delta c}{\beta} u_1$$
$$= \frac{\alpha^2}{\beta^2 t_1^2} u_0 - \frac{\alpha}{\beta t_1} \Delta v_0 + \frac{c\alpha}{\beta^2 t_1^2} v_0 \equiv f(x, y, z), \tag{7}$$

with a boundary condition $u_1\big|_\Gamma = 0$, where $u_1 = u(t_1)$.

Suppose $\Delta u_1\big|_\Gamma = 0$. Applying Poisson's formula [5,6,7] we obtain the following integro-differential equation

$$\Delta u_1 = -\frac{1}{4\pi}\int_V \left(2\frac{c}{\beta}\Delta u_1 + \frac{2}{\beta}\left(\frac{\partial c}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial c}{\partial y}\frac{\partial u}{\partial y} + \frac{\partial c}{\partial z}\frac{\partial u}{\partial z}\right) - \left(\frac{c^2}{\beta^2} + \frac{\alpha^2}{\beta^2 t_1^2}\right) u_1\right.$$
$$\left. + \frac{\Delta c}{\beta} u_1 - f(x', y', z')\right) G(x, y, z, x', y', z') dV', \tag{8}$$

where $dV' = dx'dy'dz'$, $G(x, y, z, x', y', z')$ is Green's function for the area V.

Using Green's formulas after simple transformations (8) implies [5,6,7]

$$\Delta u_1 = -\frac{1}{4\pi}\int_V u_1 \frac{\Delta c}{\beta} G dV' \tag{9}$$

$$+\frac{1}{4\pi}\int_V u_1 \frac{2}{\beta}\left(\frac{\partial c}{\partial x}\frac{\partial G}{\partial x} + \frac{\partial c}{\partial y}\frac{\partial G}{\partial y} + \frac{\partial c}{\partial z}\frac{\partial G}{\partial z}\right) dV'$$

$$+\frac{1}{4\pi}\int_V u_1 \left(\frac{c^2}{\beta^2} + \frac{\alpha^2}{\beta^2 t_1^2}\right) G dV' - \frac{1}{4\pi}\int_V f(x',y',z')G(x,y,z,x',y',z')dV'.$$

Once again, applying Poisson's formula from (9) we obtain

$$u_1 = \frac{1}{16\pi^2}\int_V u_1 K_0(x,y,z,x',y',z')dV' \tag{10}$$

$$+\frac{1}{16\pi^2}\int_V\int_V f(x',y',z')G(x,y,z,x',y',z')G(x'',y'',z'',x',y',z')dV'dV'',$$

where

$$K_0(x,y,z,x',y',z') = \int_V (G(x,y,z,x'',y'',z'')G(x'',y'',z'',x',y',z')$$

$$+\left(\frac{\partial c}{\partial x}\frac{\partial G}{\partial x} + \frac{\partial c}{\partial y}\frac{\partial G}{\partial y} + \frac{\partial c}{\partial z}\frac{\partial G}{\partial z}\right) G(x'',y'',z'',x',y',z')$$

$$+\left(\frac{c^2}{\beta^2} + \frac{\alpha^2}{\beta^2 t_1^2}\right) G(x,y,z,x'',y''z'')G(x''y'',z'',x',y',z'))dV'',$$

where $dV'' = dx''dy''dz''$.

(10) is the Fredholm equation with a weakly singular kernel and we can use the Fredholm theory [5,6,7].

For the small parameters applying Banach theorem [7] one obtains the following sufficient condition for the existence of the solution of this equation.

Theorem. *If*

$$\frac{1}{16(\pi)^2}\int_V K_0(x,y,z,x',y',z')dV' << 1,$$

then there exists a unique solution of the equation (10) and this solution is given by the series f_n, where f_0 is the second (known) term of (10) and

$$f_n = f_0 + \frac{1}{16(\pi)^2}\int_V K_0(x,y,z,x',y',z')f_{n-1}dV'.$$

Note 1. If G_0 and V are parallelepipeds, then Green's function G is representable by the Fourier series and consequently we can obtain the solution of the equation (10) by means of Fourier series.

Note 2. If $c > 0$ is a function only of time then we can obtain more simple equations than (10).

Let us rewrite the system (6) in the form:

$$\begin{cases} \Delta u - \dfrac{c}{\beta} u = \dfrac{\alpha}{\beta} \dfrac{v - v_0}{t_1}, \\ \Delta v - \dfrac{c}{\beta} v = -\dfrac{\alpha}{\beta} \dfrac{u - u_0}{t_1}. \end{cases} \tag{11}$$

If we admit, that right hand sides of this equations are known, we obtain [6,7,8]:

$$v = \frac{1}{4\pi} \int_V \left\{ \frac{\alpha}{\beta} \frac{u - u_0}{t_1} \right\} \frac{e^{-kr}}{r} dV', \tag{12}$$

$$u = -\frac{1}{4\pi} \int_V \left\{ \frac{\alpha}{\beta} \frac{v - v_0}{t_1} \right\} \frac{e^{-kr}}{r} dV', \tag{13}$$

where $r^2 = (x - x')^2 + (y - y')^2 + (z - z')^2$, $dV' = dx'dy'dz'$, $k^2 = \dfrac{c}{\beta}$.

Putting (12) into (13) and taking into account the boundary condition [5,6,7], after simple transformations we obtain the following integral equation

$$u = -\frac{1}{(4\pi)^2} \frac{\alpha^2}{\beta^2 t_1^2} \int_V (u - u_0) K(x, y, z, x', y', z') dV' + \frac{1}{(4\pi)^2} \int_V \frac{v_0}{t_1} \frac{e^{-kr}}{r} dV', \tag{14}$$

where

$$K(x, y, z, x', y', z') = \int_V \frac{e^{-kr'}}{r'} \frac{e^{-kr}}{r} dV'',$$

$$(r')^2 = (x'' - x')^2 + (y'' - y')^2 + (z'' - z')^2, \quad dV'' = dx''dy''dz''.$$

(14) is the Fredholm equation with a weakly singular kernel.

The Banach theorem implies the following sufficient condition for the existence of the solution of this equation.

If

$$\frac{1}{(4\pi)^2} \left\{ \frac{\alpha^2}{\beta^2 t_1^2} \right\} < \frac{1}{M},$$

$$\int_V K(x, y, z, x', y', z') dV' < M,$$

then there exists a unique solution of the equation (14) and consequently of the system (11).

Acknowledgement. The designated project has been fulfilled by financial support of the Georgia Rustaveli Foundation (Grant#GNSF/ST08/3-

395). Any idea in this publication is possessed by the author and may not represent the opinion of the Foundation itself.

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Received 29.01.2010; revised 18.07.2010; accepted 20.10.2010.

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