ON THE NUMERICAL TREATMENT OF SYSTEM OF PARTIAL DIFFERENTIAL EQUATIONS CONNECTED WITH THE SCHRODINGER EQUATION AND SOME APPLICATIONS TO THE PARTICLE TRANSPORT AT THE CUBICAL LATTICED NANOSTRUCTURES

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*Abstract*

The electron transport in the materials having cubical crystal structures (gold, silver) 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. The numerical treatment of this system by means of the implicit finite difference schemes is given. The modulus of the wave function is estimated. The numerical example for the gold nanostructure is considered. For the small time interval this system is reduced to the Fredholm integral equation and then analyzed.

*Key words and phrases*: Schrodinger Equation, Finite difference schemes, Fredholm Equation.

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# 1 Introduction

Some metals in the solid state form a cubical crystal lattice, for example gold, silver, germanium [1–5]. We will consider homogeneous electron gas at this latticed structure affected by the external potential.

# 2 Statement of the problem

Let one sample of the lattice in the coordinate system $0xyz$ be $G_0 = \{0 < x < a_0, 0 < y < b_0, 0 < z < c_0\}$. For the cubic lattice $a_0 = b_0 = c_0$. For the crystal lattice it is sufficient to consider the movement of one electron [1,2,3]. Suppose that under outer force the particle moves in the direction of the axis $oz$ in the area $V = \{0 < x < a_0, 0 < y < b_0, 0 < z < n_0 c_0\}$, where $n_0 c_0$ is the length of the area $V$. The electron transport at this system could be described by Schrödinger's Equation [1–5]

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

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

$$v|_\Gamma = 0, \ \ u|_\Gamma = 0, \ \ t > 0, \tag{2}$$

$$v|_{t=0} = 0, \ \ u|_{t=0} = u_0,$$

where $\Gamma$ is the lateral boundary of the considered structure. The condition (2)reflects initial quantum states of a particle, when it is confined at the quantum box $G_0$ [1–3].

The equation (1) is equivalent to the following system of partial differential equations

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

$$v|_{t=0} = 0, \ \ u|_{t=0} = u_0,$$

$$(u=v)|_\Gamma = 0, \ \ t > 0$$

Suppose that $E - U = c(z,t)$ is a function of time and $z$ coordinate.

In the area $Q_T = V \times \{0 < t < T\}$, let us consider more general system

$$\begin{cases} \alpha\dfrac{\partial v}{\partial t} = \beta\Delta u - c(z,t)u + f_1, \\ \alpha\dfrac{\partial u}{\partial t} = -\beta\Delta v + c(z,t)v + f_2, \end{cases}$$

where $\alpha = \hbar = const$, $\beta = \frac{\hbar^2}{2m} = const$, $c$, $u_0$, $f_1$, $f_2$ are the definite continuous functions.

## 3 The finite difference schemes

The finite difference schemes for this system will be given by

$$\begin{cases} \sigma\tau^2 R_1 \overset{1}{y}_{t\bar{t}} = \beta\left(\overset{1}{y}_{x_1\bar{x}_1} + \overset{1}{y}_{x_2\bar{x}_2} + \overset{1}{y}_{x_3\bar{x}_3}\right) \\ -c_n\overset{1}{y}^n - \alpha\frac{\overset{2}{y}^n - \overset{2}{y}^{n-1}}{\tau} + f_{1n}, \\ \sigma\tau^2 R_2 \overset{2}{y}_{t\bar{t}} = -\beta\left(\overset{2}{y}_{x_1\bar{x}_1} + \overset{2}{y}_{x_2\bar{x}_2} + \overset{2}{y}_{x_3\bar{x}_3}\right) \\ +c_n\overset{2}{y}^n - \alpha\frac{\overset{1}{y}^{n+1} - \overset{1}{y}^{n-1}}{2\tau} + f_{2n}, \end{cases} \tag{4}$$

where

$$R_1 = \beta\Delta_{11}, \quad R_2 = -\beta\Delta_{22}, \quad \Delta_{ii}y = y_{x_i\bar{x}_i},$$

$$\overset{1}{y}{}^0_{ijk} = u_0,\ \overset{1}{y}{}^1_{ijk} = \overset{1}{y}_{ijk}(\tau) = 0,\ \overset{2}{y}{}^0_{ijk} = 0,$$
$$\overset{2}{y}{}^1_{ijk} = \overset{2}{y}_{ijk}(\tau) = -\frac{(c(z_k,\tau) - c(z_k,0))u_0}{\alpha},$$

Let us rewrite (4) in the form

$$\frac{\sigma\beta}{h_1^2}\left(\overset{1}{y}{}^{n+1}_{i+1,j,k} + \overset{1}{y}{}^{n+1}_{i-1,j,k}\right) + \left(\frac{2\sigma\beta}{h_1^2} - \frac{1}{2}c_k^n\right)\overset{1}{y}{}^{n+1}_{ijk} = \phi^1_{ijk}, \tag{5}$$

$$-\frac{\sigma\beta}{h_1^2}\left(\overset{2}{y}{}^{n+1}_{i+1,j,k} + \overset{2}{y}{}^{n+1}_{i-1,j,k}\right) + \left(-\frac{2\sigma\beta}{h_1^2} + \frac{1}{2}c_k^n\right)\overset{2}{y}{}^{n+1}_{ijk} = \phi^2_{ijk}, \tag{6}$$

where

$$\phi^1_{ijk} = \frac{\beta(1-2\sigma)}{h_1^2}\left(\overset{1}{y}{}^n_{i+1,j,k} - 2\overset{1}{y}{}^n_{ijk} + \overset{2}{y}{}^n_{i-1,j,k}\right)$$
$$+\frac{\sigma\beta}{h_1^2}\left(\overset{1}{y}{}^{n-1}_{i+1,j,k} - 2\overset{1}{y}{}^{n-1}_{ijk} + \overset{2}{y}{}^{n-1}_{i-1,j,k}\right)$$
$$+\frac{\beta}{h_2^2}\left(\overset{1}{y}{}^n_{i,j+1,k} - 2\overset{1}{y}{}^n_{ijk} + \overset{1}{y}{}^n_{i,j-1,k}\right) - \frac{1}{2}c_k^n\overset{1}{y}{}^n_{ijk} - \frac{\alpha}{\tau}\left(\overset{1}{y}{}^n_{ijk} - \overset{1}{y}{}^{n-1}_{ijk}\right)$$
$$+\frac{\beta}{h_3^2}\left(\overset{1}{y}{}^n_{i,j,k+1} - 2\overset{1}{y}{}^n_{ijk} + \overset{1}{y}{}^n_{i,j,k-1}\right) + (f_1^n)_{ijk},$$
$$i,j,k = 1,2,\ldots,(N_1-1);\ \ t_n = n\tau;\ \ y^n_{ijk} = y(x_{1i}, x_{2j}, x_{3k}, t_n);$$
$$n = 1,2,\ldots,(N-1);$$
$$\phi^2_{ijk} = -\frac{\beta(1-2\sigma)}{h_1^2}\left(\overset{1}{y}{}^n_{i+1,j,k} - 2\overset{2}{y}{}^n_{ijk} + \overset{2}{y}{}^n_{i-1,j,k}\right)$$

$$-\frac{\sigma\beta}{h_1^2}\left(\overset{2}{y}{}^{n-1}_{i+1,j,k}-2\overset{2}{y}{}^{n-1}_{ijk}+\overset{2}{y}{}^{n-1}_{i-1,j,k}\right)$$

$$-\frac{\beta}{h_2^2}\left(\overset{2}{y}{}^{n}_{i+1,j,k}-2\overset{2}{y}{}^{n}_{ijk}+\overset{2}{y}{}^{n}_{i-1,j,k}\right)-\frac{\beta}{h_3^2}\left(\overset{2}{y}{}^{n}_{i,j,k+1}-2\overset{2}{y}{}^{n}_{ijk}+\overset{2}{y}{}^{n}_{i,j,k-1}\right)$$

$$+\frac{1}{2}c_k^n\overset{2}{y}{}^{n}_{ijk}-\frac{\alpha}{2\tau}\left(\overset{1}{y}{}^{n+1}_{ijk}-\overset{1}{y}{}^{n-1}_{ijk}\right)+(f_2^n)_{ijk}.$$

By (5), (6) - we will find $\overset{1}{y}{}^{n+1},\overset{2}{y}{}^{n+1}$ (alternating direction method with respect to the axis $0x_1$) [6]

$$\frac{\sigma\beta}{h_2^2}\left(\overset{1}{y}{}^{n+2}_{i,j+1,k}+\overset{1}{y}{}^{n+2}_{i,j-1,k}\right)+\left(\frac{2\sigma\beta}{h_2^2}-\frac{1}{2}c_k^{n+1}\right)\overset{1}{y}{}^{n+2}_{ijk}=\overset{1}{\phi}{}^{1}_{ijk}, \tag{7}$$

$$-\frac{\sigma\beta}{h_2^2}\left(\overset{1}{y}{}^{n+2}_{i,j+1,k}+\overset{2}{y}{}^{n+2}_{i,j-1,k}\right)+\left(-\frac{2\sigma\beta}{h_2^2}+\frac{1}{2}c_k^{n+1}\right)\overset{2}{y}{}^{n+2}_{ijk}=\overset{1}{\phi}{}^{2}_{ijk}, \tag{8}$$

where

$$\overset{11}{\phi}_{ijk}=\frac{\beta(1-2\sigma)}{h_2^2}\left(\overset{1}{y}{}^{n+1}_{i,j+1,k}-2\overset{1}{y}{}^{n+1}_{ijk}+\overset{1}{y}{}^{n+1}_{i,j-1,k}\right)$$

$$+\frac{\sigma\beta}{h_2^2}\left(\overset{1}{y}{}^{n}_{i,j+1,k}-2\overset{1}{y}{}^{n}_{ijk}+\overset{1}{y}{}^{n}_{i,j-1,k}\right)$$

$$+\frac{\beta}{h_1^2}\left(\overset{1}{y}{}^{n+1}_{i+1,j,k}-2\overset{1}{y}{}^{n+1}_{ijk}+\overset{1}{y}{}^{n+1}_{i-1,j,k}\right)+\frac{\beta}{h_3^2}\left(\overset{1}{y}{}^{n+1}_{i,j,k+1}-2\overset{1}{y}{}^{n+1}_{ijk}+\overset{1}{y}{}^{n+1}_{i,j,k-1}\right)$$

$$-\frac{1}{2}c_k^{n+1}\overset{1}{y}{}^{n+1}_{ijk}-\frac{\alpha}{\tau}\left(\overset{2}{y}{}^{n+1}_{ijk}-\overset{2}{y}{}^{n}_{ijk}\right)+(f_1^{n+1})_{ijk},$$

$$\overset{12}{\phi}_{ijk}=-\frac{\beta(1-2\sigma)}{h_2^2}\left(\overset{2}{y}{}^{n+1}_{i,j+1,k}-2\overset{2}{y}{}^{n+1}_{ijk}+\overset{2}{y}{}^{n+1}_{i,j-1,k}\right)$$

$$-\frac{\sigma\beta}{h_2^2}\left(\overset{2}{y}{}^{n}_{i,j+1,k}-2\overset{2}{y}{}^{n}_{ijk}+\overset{2}{y}{}^{n}_{i,j-1,k}\right)$$

$$-\frac{\beta}{h_1^2}\left(\overset{2}{y}{}^{n+1}_{i+1,j,k}-2\overset{2}{y}{}^{n+1}_{ijk}+\overset{2}{y}{}^{n+1}_{i-1,j,k}\right)-\frac{\beta}{h_3^2}\left(\overset{2}{y}{}^{n+1}_{i,j,k+1}-2\overset{2}{y}{}^{n+1}_{ijk}+\overset{2}{y}{}^{n+1}_{i,j,k-1}\right)$$

$$+\frac{1}{2}c_k^{n+1}\overset{2}{y}{}^{n+1}_{ijk}-\frac{\alpha}{\tau}\left(\overset{1}{y}{}^{n+2}_{ijk}-\overset{1}{y}{}^{n}_{ijk}\right)+(f_2^{n+1})_{ijk}.$$

By (7), (8) - we will find $\overset{1}{y}{}^{n+2},\overset{2}{y}{}^{n+2}$ (alternating direction method with respect to the axis $x_2$)

$$i,j,k=1,2,\ldots,(N_1-1);\quad n=1.$$

$$\frac{\sigma\beta}{h_3^2}\left(\overset{1}{y}{}^{n+3}_{i,j,k+1}+\overset{1}{y}{}^{n+3}_{i,j,k-1}\right)+\left(\frac{2\sigma\beta}{h_3^2}-\frac{1}{2}c_k^{n+2}\right)\overset{1}{y}{}^{n+3}_{ijk}=\overset{1}{\phi}{}^{3}_{ijk}, \tag{9}$$

$$-\frac{\sigma\beta}{h_3^2}\left(\overset{1}{y}{}^{n+3}_{i,j,k+1}+\overset{2}{y}{}^{n+3}_{i,j,k-1}\right)+\left(-\frac{2\sigma\beta}{h_3^2}+\frac{1}{2}c_k^{n+2}\right)\overset{2}{y}{}^{n+3}_{ijk}=\overset{1}{\phi}{}^{3}_{ijk}, \tag{10}$$

where

$$\begin{aligned}
\overset{13}{\phi}_{ijk} &= \frac{\beta(1-2\sigma)}{h_3^2}\left(\overset{1}{y}{}^{n+2}_{i,j,k+1}+2\overset{1}{y}{}^{n+2}_{ijk}+\overset{1}{y}{}^{n+2}_{i,j,k-1}\right)\\
&+\frac{\sigma\beta}{h_2^3}\left(\overset{1}{y}{}^{n+1}_{i,j,k+1}-2\overset{1}{y}{}^{n+1}_{ijk}+\overset{1}{y}{}^{n+1}_{i,j,k-1}\right)\\
&+\frac{\beta}{h_2^1}\left(\overset{1}{y}{}^{n+2}_{i+1,j,k}-2\overset{1}{y}{}^{n+2}_{ijk}+\overset{1}{y}{}^{n+2}_{i-1,j,k}\right)\\
&+\frac{\beta}{h_2^2}\left(\overset{1}{y}{}^{n+2}_{i,j+1,k}-2\overset{1}{y}{}^{n+2}_{ijk}+\overset{1}{y}{}^{n+2}_{i,j-1,k}\right)\\
&-\frac{1}{2}c_k^{n+2}\,\overset{1}{y}{}^{n+2}_{ijk}-\frac{\alpha}{\tau}\left(\overset{2}{y}{}^{n+2}_{ijk}-\overset{2}{y}{}^{n+1}_{ijk}\right)+(f_1^{n+2})_{ijk},\\
\overset{14}{\phi}_{ijk} &= -\frac{\beta(1-2\sigma)}{h_3^2}\left(\overset{2}{y}{}^{n+2}_{i,j,k+1}-2\overset{2}{y}{}^{n+2}_{ijk}+\overset{2}{y}{}^{n+2}_{i,j,k-1}\right)\\
&-\frac{\sigma\beta}{h_3^2}\left(\overset{2}{y}{}^{n+1}_{i,j,k+1}-2\overset{2}{y}{}^{n+1}_{ijk}+\overset{2}{y}{}^{n+1}_{i,j,k-1}\right)\\
&-\frac{\beta}{h_1^2}\left(\overset{2}{y}{}^{n+2}_{i+1,j,k}-2\overset{2}{y}{}^{n+2}_{ijk}+\overset{2}{y}{}^{n+2}_{i-1,j,k}\right)\\
&-\frac{\beta}{h_2^2}\left(\overset{2}{y}{}^{n+2}_{i,j+1,k}-2\overset{2}{y}{}^{n+2}_{ijk}+\overset{2}{y}{}^{n+2}_{i,j-1,k}\right)\\
&+\frac{1}{2}c_k^{n+2}\overset{2}{y}{}^{n+2}_{ijk}-\frac{\alpha}{2\tau}\left(\overset{1}{y}{}^{n+3}_{ijk}-\overset{1}{y}{}^{n+1}_{ijk}\right)+(f_2^{n+2})_{ijk}.
\end{aligned}$$

By (9), (10) - we will find $\overset{1}{y}{}^{n+3},\overset{2}{y}{}^{n+3}$ (alternating direction method with respect to the axis $0x_3$)

$$i,j,k=1,2,\ldots,(N_1-1);\;\; n=1.$$

i.e. at the first step the scheme will be done for $n=1$, and we find $(\overset{1}{y}{}^2,\overset{2}{y}{}^2),(\overset{1}{y}{}^3,\overset{2}{y}{}^3)(\overset{1}{y}{}^4,\overset{2}{y}{}^4)$ at the second step $n=2$ we find $(\overset{1}{y}{}^5,\overset{2}{y}{}^5)$, $(\overset{1}{y}{}^6,\overset{2}{y}{}^6)$ and $(\overset{1}{y}{}^7,\overset{2}{y}{}^7)$ . This circle will continue until $n=(N-3)$ .

The accuracy of these schemes is $O(\tau+h^2)$,where $\tau$ and $h$ are steps along time and axis $h=(h_1,h_2,h_3)$, and investigated in analogy with [7].

## 4 Numerical examples

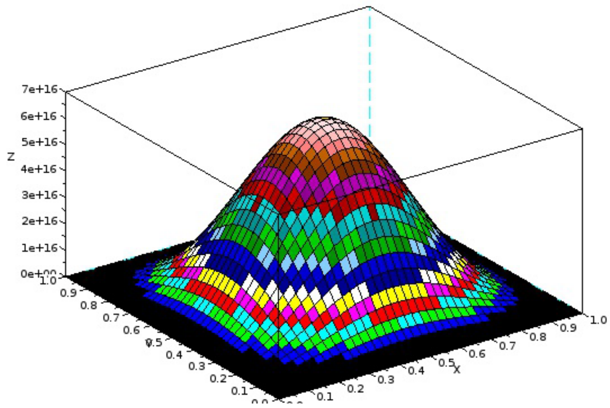
Below the numerical examples are given for 3 nm length golden nanostructure (The dimension of one sample of gold crystal is about 0.5 nm [3–5]). The case when $E-U=c(z,t)$ is a linear function of time and z, $E-U=E_1(1-\gamma zt)$,($\gamma$ is the definite constant), and

$$u_0=\frac{\sqrt{8}}{a_0b_0c_0}\sin\frac{\pi x}{a_0}\sin\frac{\pi y}{b_0}\sin\frac{\pi z}{c_0};\ a_0=b_0=c_0=0.5nm;$$

$E_1$ is a minimal energy and $u_0$ is the corresponding wave function [1-5]. At the Fig. 1 and Fig. 2 the graphs of $u_1^2+\nu_1^2$ for the different initial conditions and data

$$\frac{E_1}{\hbar}=3.454\cdot 10^3;\quad \frac{\hbar}{2m}=0.358\cdot 10^3;$$

are given



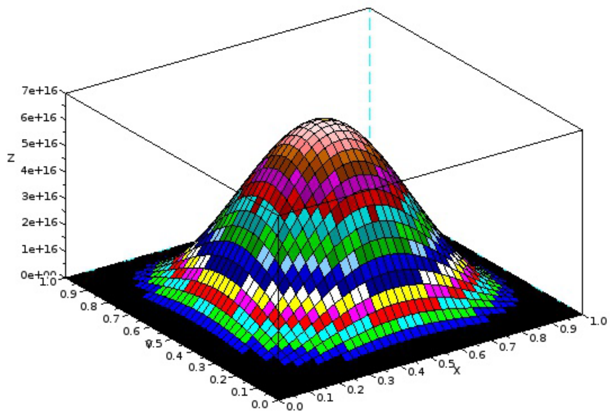




Fig 2. $T=1;\ z=1,5;\ \ \gamma$=20/3;

**Note 1.** We have constructed the schemes for the case $E-U=c(z,t)$, but in the same way as above we can construct the similar schemes for more general case $E-U=c(x,y,z,t)$.

**Note 2.** At the small time-interval $0<t<t_1$ ($t_1$ is rather small), the system (3) could be written as

$$\begin{cases} \alpha\dfrac{v}{t_1}=\beta\Delta u-cu \\ \alpha\dfrac{u-u_0}{t_1}=-\beta\Delta v+cv, \end{cases} \tag{11}$$

If $c$ is a function of time $c=c(t)$, the system (11) could be reduced to the following Partial Differential equation

$$\Delta\Delta u_1-2\frac{c}{\beta}\Delta u_1=\left(-\frac{c^2}{\beta^2}-\frac{\alpha^2}{\beta^2t_1^2}\right)u_1+\frac{\alpha^2}{\beta^2t_1^2}u_0; \tag{12}$$

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

If right hand side of the equation (12) is known and $\Delta u_1|_\Gamma=0$, then it can be reduced to the following integro-differential equation [8,9]

$$\Delta u_1=\frac{1}{4\pi}\int_V\left\{\left(\frac{c^2}{\beta^2}+\frac{\alpha^2}{\beta^2t_1^2}\right)u_1-u_0\frac{\alpha^2}{\beta^2t_1^2}\right\}\frac{e^{-kr}}{r}dV', \tag{13}$$

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

Taking into the account the boundary condition and using Poisson's formula [8,9] from (13), after simple transformations we obtain the following integral equation

$$u_1=-\frac{1}{(4\pi)^2}\int_V\left\{\left(\frac{c^2}{\beta^2}+\frac{\alpha^2}{\beta^2t_1^2}\right)u_1-u_0\frac{\alpha^2}{\beta^2t_1^2}\right\}K(x,y,z,x',y',z')dV', \tag{14}$$

where

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

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

$G(x,y,z,x",y",z")$ is a Green's function for $V$.

Consequently for the equation (12) the Fredholm theory is applicable [8,9]. Banach theory implies

**Conclusion**

If

$$\frac{1}{(4\pi)^2}\left\{\frac{c^2}{\beta^2}+\frac{\alpha^2}{\beta^2t_1^2}\right\}\int_V K(x,y,z,x',y',z')dV'<M<1,$$

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

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