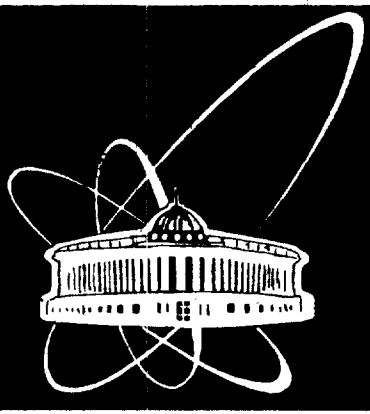

ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

CC

E11-96-494

P.G.Akishin, I.V.Puzynin, Yu.S.Smirnov

THE NEWTONIAN CONTINUATION METHOD FOR NUMERICAL STUDY OF 3D POLARON PROBLEM

Submitted to the First Workshop on Numerical Analysis and Applications, August 1996, Russe, Bulgaria

1996

1. INTRODUCTION

We consider the problem of numerical solving of the spherically-nonsymmetrical model of polaron [1] in the limit of strong coupling. Such a model of polaron describes the behavior of a non-relativistic particle (electron) in the field, created by the interaction with medium.

Let us formulate a mathematical statement of the problem. The wave function ψ and potential u satisfy the following system of partial differential equations in the space R^3 :

$$\Delta\psi(\mathbf{x}) + (u(\mathbf{x}) - v(\mathbf{x}))\psi(\mathbf{x}) - \lambda\psi(\mathbf{x}) = 0, \tag{1}$$

$$\Delta u(\mathbf{x}) + 4\pi\psi^2(\mathbf{x}) = 0, \tag{2}$$

$$\Delta v(\mathbf{x}) - c^2 v(\mathbf{x}) + 4\pi\psi^2(\mathbf{x}) = 0, \tag{3}$$

where Δ is the Laplace operator and c is the constant of coupling.

The wave function $\psi(\mathbf{x})$ satisfy the normalization condition:

$$\int_{R^3} \psi^2(\mathbf{x}) dV_{\mathbf{x}} = 1. \tag{4}$$

In spherically symmetrical case (when $\psi(\mathbf{x})$ depends on $r = |\mathbf{x}|$ only), the system (1)-(2) may be reduced to a boundary problem for the system of ordinary differential equations on semi-axis [2],[3]. This problem has been studied quite well. In paper [4] the authors consider the axi-symmetrical solutions of the polaron model. The papers [5],[7] are devoted to numerical investigations of the problem for the nonsymmetrical case.

In the present paper to approximate equations (1)-(3) we use the approach proposed in [5],[6]. To solve the nonlinear discrete problem, a parametrization of initial equations is introduced by means of the additional continuous parameter t [8]. At the initial moment $t = 0$ the problem is reduced to the sufficiently simple spectral Helmholtz problem for a ball. All eigenvalues and eigenfunctions of this problem may be easily found. After that, the solution of the original nonlinear problem (1)-(3) may be obtained if we use a movement with respect to continuous parameter t.

2. DISCRETIZATION

In this section we consider the problem of discretization of the system of equations (1)-(2). For this aim we use the Bubnov - Galerkin method [9]. Let functions $\psi(\mathbf{x})$, $u(\mathbf{x})$ and $v(\mathbf{x})$ be expanded in spherical harmonic series [5]:

$$\psi(\mathbf{x}) = \sum_{k=0}^{\infty} \sum_{l=-k}^{k} \psi_{kl}(r) Y_{kl}(\theta, \varphi), \tag{5}$$

$$u(\mathbf{x}) = \sum_{k=0}^{\infty} \sum_{l=-k}^{k} u_{kl}(r) Y_{kl}(\theta, \varphi), \qquad v(\mathbf{x}) = \sum_{k=0}^{\infty} \sum_{l=-k}^{k} v_{kl}(r) Y_{kl}(\theta, \varphi), \tag{6}$$

where Y_{kl} are spherical harmonics [10].

Taking into account a finite number K of terms in the expansions (5),(6) for approximations of functions $\psi(\mathbf{x}), u(\mathbf{x}), v(\mathbf{x})$, multiplying (1)-(3) by the spherical harmonics and integrating over the angle variables, we get the following approximate system of equations for the functions $\tilde{\psi}_{kl} = \psi_{kl} r$, $\tilde{u}_{kl} = u_{kl} r$, $\tilde{v}_{kl} = v_{kl} r$:

$$\tilde{\psi}''_{kl} - \frac{k(k+1)}{r^2}\tilde{\psi}_{kl} + \frac{1}{r} \sum_{k_1,l_1} \sum_{k_2,l_2} W^{ll_1l_2}_{kk_1k_2} \tilde{\psi}_{k_1l_1} \tilde{u}_{k_2l_2} = \lambda \tilde{\psi}_{kl} \tag{7}$$

$$\tilde{u}''_{kl} - \frac{k(k+1)}{r^2}\tilde{u}_{kl} + 4\pi \frac{1}{r} \sum_{k_1,l_1} \sum_{k_2,l_2} W^{ll_1l_2}_{kk_1k_2} \tilde{\psi}_{k_1l_1} \tilde{\psi}_{k_2l_2} = 0, \tag{8}$$

$$\tilde{v}''_{kl} - (c^2 + \frac{k(k+1)}{r^2})\tilde{v}_{kl} + 4\pi \frac{1}{r} \sum_{k_1,l_1} \sum_{k_2,l_2} W^{ll_1l_2}_{kk_1k_2} \tilde{\psi}_{k_1l_1} \tilde{\psi}_{k_2l_2} = 0, \tag{9}$$

$$k = 0, 1, 2, ..., K; l = 0, \pm 1, \pm 2, ..., \pm k.$$

Here coefficients $W^{l_1l_2l_3}_{k_1k_2k_3}$ equal to the integral over the unit sphere for the product of spherical harmonics:

$$W^{l_1l_2l_3}_{k_1k_2k_3} = \int_0^{2\pi} \left[\int_0^{\pi} Y_{k_1l_1}(\theta, \varphi) Y_{k_2l_2}(\theta, \varphi) Y_{k_3l_3}(\theta, \varphi) sin\theta d\theta \right] d\varphi. \tag{10}$$

The normalization condition (4) may be written in the following form:

$$\sum_{k,l} \int_0^{\infty} \tilde{\psi}^2_{k,l} dr = 1. \tag{11}$$

Let $[0, R]$ be an interval of the variation of r. We assume that R is large enough, so functions $\tilde{\psi}_{kl}(r), \tilde{u}_{kl}(r), \tilde{v}_{kl}(r)$ have a behavior, which may be approximated analytically for $r \geq R$. We choose a uniform grid of nodes for variable r : $\{r_i; i = \overline{1,N}\}\left(r_i = (i-1)h, h = \frac{R}{N-1}\right)$ to discretize the system (7)-(9). The second order accuracy finite difference scheme with respect to step h is used for the approximation of equations (7)-(9). Let the functions $\psi^i_{kl}, u^i_{kl}, v^i_{kl}$ be

$\psi^i_{kl} = \tilde{\psi}_{kl}(r_i), u^i_{kl} = \tilde{u}_{kl}(r_i), v^i_{kl} = \tilde{v}_{kl}(r_i)$. Then the discrete system of equations has the following form:

$$\frac{\psi^{i+1}_{kl} - 2\psi^i_{kl} + \psi^{i-1}_{kl}}{h^2} - \frac{k(k+1)}{r_i^2}\psi^i_{kl} + \frac{1}{r_i}\sum_{k_1,l_1}\sum_{k_2,l_2} W^{ll_1l_2}_{kk_1k_2}\psi^i_{k_1l_1}u^i_{k_2l_2} = \lambda\psi^i_{kl} \tag{12}$$

$$\frac{u^{i+1}_{kl} - 2u^i_{kl} + u^{i-1}_{kl}}{h^2} - \frac{k(k+1)}{r_i^2}u^i_{kl} + 4\pi\frac{1}{r_i}\sum_{k_1,l_1}\sum_{k_2,l_2} W^{ll_1l_2}_{kk_1k_2}\psi^i_{k_1l_1}\psi^i_{k_2l_2} = 0 \tag{13}$$

$$\frac{v^{i+1}_{kl} - 2u^i_{kl} + v^{i-1}_{kl}}{h^2} - (c^2 + \frac{k(k+1)}{r_i^2})v^i_{kl} + 4\pi\frac{1}{r_i}\sum_{k_1,l_1}\sum_{k_2,l_2} W^{rll_1l_2}_{kk_1k_2}\psi^i_{k_1l_1}\psi^i_{k_2l_2} = 0 \tag{14}$$

$k = 0, 1, 2, ...K; l = 0, \pm1, \pm2, ..., \pm k; i = \overline{2, N-1}$. For $r_1 = 0$ we have the following left-hand boundary conditions: $\psi^1_{kl} = 0, u^1_{kl} = 0, v^1_{kl} = 0$. Taking into account exponential vanishing of the function ψ_{kl} on infinity, we get the right-hand boundary condition for ψ^i_{kl}:

$$\frac{\psi^N_{kl} - \psi^{N-2}_{kl}}{2h} = (-\sqrt{\lambda} + \frac{k}{r_{N-1}})\psi^{N-1}_{kl}. \tag{15}$$

Analogously, for u^i_{kl} and v^i_{kl} we have

$$\frac{u^N_{kl} - u^{N-2}_{kl}}{2h} = \frac{k}{r_{N-1}}u^{N-1}_{kl}, \qquad \frac{v^N_{kl} - v^{N-2}_{kl}}{2h} = (-c + \frac{k}{r_{N-1}})v^{N-1}_{kl}. \tag{16}$$

By using some numerical approximation for (11) the normalization conditions may be written in the form:

$$\sum_{k,l}\sum_{i=1}^{N}\alpha_i(\psi^i_{kl})^2 = 1, \tag{17}$$

where α_i are the coefficients of the quadrature formula for calculation of integrals.

To find the approximate solutions of the original problem (1)-(3), it is necessary to solve the nonlinear system of algebraic equations (12)-(17) for the unknown variables $\{\psi^i_{kl}, u^i_{kl}, v^i_{kl}, i = \overline{1, N}\}$ and the spectral parameter λ.

3. THE METHOD FOR SOLVING THE NONLINEAR DISCRETE SYSTEMS

Let $\vec{\Psi}_i$ be the vector with the components ψ^i_{kl}, $\vec{U}_i$ and $\vec{V}_i$ be the vectors with the components u^i_{kl} and v^i_{kl} correspondingly. Analogously we define the vectors corresponding to the nonlinear terms (double sums) in the equations (12) and (13), as $\vec{F}_i = \vec{F}_i(\vec{\Psi}_i, \vec{U}_i), \vec{G}_i = \vec{G}_i(\vec{\Psi}_i, \vec{\Psi}_i)$. Then the system (12)-(14) can be written in the form:

$$\frac{\vec{\Psi}_{i+1} - 2\vec{\Psi}_i + \vec{\Psi}_{i-1}}{h^2} + [D_i]\vec{\Psi}_i + \vec{F}_i(\vec{\Psi}_i, \vec{U}_i) = \lambda\vec{\Psi}_i. \tag{18}$$

$$\frac{\vec{U}_{i+1} - 2\vec{U}_i + \vec{U}_{i-1}}{h^2} + [D_i]\vec{U}_i + \vec{G}_i(\vec{\Psi}_i, \vec{\Psi}_i) = 0. \tag{19}$$

$$\frac{\vec{V}_{i+1} - 2\vec{V}_i + \vec{V}_{i-1}}{h^2} - c^2\vec{V}_i + [D_i]\vec{V}_i + \vec{G}_i(\vec{\Psi}_i, \vec{\Psi}_i) = 0, \tag{20}$$

where $i = \overline{2, N-1}$; the matrices $[D_i]$ are diagonal matrices with coefficients on the main diagonal depending on the number k of the correspondent harmonic. The normalization condition (17) may be written in new variables as

$$\sum_{i=1}^{N} \alpha_i |\vec{\Psi}_i|^2 - 1 = 0. \tag{21}$$

The left-hand boundary conditions reduce to the following equations:

$$\vec{\Psi}_1 = 0, \qquad \vec{U}_1 = 0, \qquad \vec{V}_1 = 0. \tag{22}$$

Analogously, we rewrite the right-hand boundary conditions:

$$\frac{\vec{U}_N - \vec{U}_{N-2}}{2h} = [B_1]\vec{U}_{N-1}, \qquad \frac{\vec{V}_N - \vec{V}_{N-2}}{2h} = (-c[E] + [B_2])\vec{V}_{N-1}, \tag{23}$$

$$\frac{\vec{\Psi}_N - \vec{\Psi}_{N-2}}{2h} = (-\sqrt{\lambda}[E] + [B_2])\vec{\Psi}_{N-1}, \tag{24}$$

where $[E]$ is an identity matrix, $[B_1]$, $[B_2]$ are diagonal matrices.

Let us consider an auxiliary problem. We can write the right boundary condition for the wave functions in the following form:

$$\vec{\Psi}_N = 0. \tag{25}$$

Then the system of equations (18)-(23),(25) also approximates the problem (7)-(11), but with the lesser accuracy. To solve the nonlinear problem (18)-(23),(25), we use the continuation method from [8]. In equations (18)-(20) we introduce a parameter $t, (t \in [0, 1])$ by the following way:

$$\vec{F}_i(t) = t\vec{F}_i(\vec{\Psi}_i, \vec{U}_i), \qquad \vec{G}_i(t) = t\vec{G}_i(\vec{\Psi}_i, \vec{\Psi}_i).$$

After this substitution the system (18)-(20) may be transformed to the following system of equations:

$$\frac{\vec{\Psi}_{i+1} - 2\vec{\Psi}_i + \vec{\Psi}_{i-1}}{h^2} + D_i\vec{\Psi}_i + t\vec{F}_i(\vec{\Psi}_i, \vec{U}_i) = \lambda\vec{\Psi}_i \tag{26}$$

$$\frac{\vec{U}_{i+1} - 2\vec{U}_i + \vec{U}_{i-1}}{h^2} + D_i\vec{U}_i + t\vec{G}_i(\vec{\Psi}_i, \vec{\Psi}_i) = 0, \tag{27}$$

$$\frac{\vec{V}_{i+1} - 2\vec{V}_i + \vec{V}_{i-1}}{h^2} - c^2\vec{V}_i + D_i\vec{V}_i + t\vec{G}_i(\vec{\Psi}_i, \vec{\Psi}_i) = 0, \tag{28}$$

with boundary conditions (22)-(23),(25). In this case the solutions $\vec{\Psi}_i, \vec{U}_i, \lambda$ of the problem (21)-(23),(25)-(28) will be the functions of the parameter t ($t \in [0,1]$). Obviously, for $t = 1$ we have the original system of equations (18)-(23),(25), and for $t = 0$ we obtain the sufficiently simple non-connected linear spectral problem for each harmonic separately.

To find the values of functions $\vec{U}(t), \vec{V}(t), \vec{\Psi}(t), \lambda(t)$ at the moment $t = 0$ for the fixed orbital momentum k_0, we solve the one-dimensional spectral problem for one equation only:

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} - \frac{k_0(k_0+1)}{r_i^2} y_i = \lambda y_i, i = \overline{2, N-1} \tag{29}$$

with boundary and normalization conditions

$$y_1 = 0, \qquad y_N = 0; \qquad \sum_{i=1}^{N} \alpha_i y_i^2 = 1. \tag{30}$$

Let $\{y_i^*\}, \lambda_i^*$ be a solution of the problem (29)-(30). For the fixed number $l_0 : -k_0 \le l_0 \le k_0$ we assume

$$\psi_{kl}^i(t)|_{t=0} = \begin{cases} y_i^*/\sqrt{2}, & l = l_0, k = k_0 \\ y_i^*/\sqrt{2}, & l = -l_0, k = k_0 \\ 0, & l \neq l_0 \\ 0, & k \neq k_0. \end{cases} \tag{31}$$

This case corresponds to the real initial approximation for determing the solutions which are even functions with respect to angle φ. The case corresponding to the odd initial approximation can be written by the following way:

$$\psi_{kl}^i(t)|_{t=0} = \begin{cases} y_i^*/\sqrt{2}, & l = l_0, k = k_0 \\ -y_i^*/\sqrt{2}, & l = -l_0, k = k_0 \\ 0, & l \neq l_0 \\ 0, & k \neq k_0. \end{cases} \tag{32}$$

Accordingly for the spectral parameter we have $\lambda(t) = \lambda^*$ for $t = 0$.

So, for every $t \in [0,1]$ we have obtained the nonlinear boundary problem. Let $\{t_j; j = \overline{0, M}\}(t_0 = 0, t_M = 1)$ be some partition of the interval [0 ,1]. To find the solutions $\psi_{kl}(t_j)$, $u_{kl}(t_j)$, $v_{kl}(t_j)$, $\lambda(t_j)$ of the problem (29)-(30) in the point t_j the Newton method is used. Supposing the difference $|t_j - t_{j+1}|$ is small enough, we have the good initial approximation from previous step t_{j-1} for Newtonian iterative procedure.

Let $\vec{\Psi}_i^m$ be the vector of components ψ_{kl}^i on $m-$th step of Newtonian iterative process. Analogously let $\vec{U}_i^m$ and $\vec{V}_i^m$ be the vectors with components u_{kl}^i and v_{kl}^i. Then we have the following boundary problem for the vectors of corrections $\delta\vec{\Psi}_i^m = \vec{\Psi}_i^{m+1} - \vec{\Psi}_i^m, \delta\vec{U}_i^m = \vec{U}_i^{m+1} - \vec{U}_i^m, \delta\vec{V}_i^m = \vec{V}_i^{m+1} - \vec{V}_i^m$:

$$\frac{\delta\vec{\Psi}_{i+1}^m - 2\delta\vec{\Psi}_i^m + \delta\vec{\Psi}_{i-1}^m}{h^2} + [D_i]\delta\vec{\Psi}_i^m + [A_{11}](\vec{u}_i^m)\delta\vec{\Psi}_i^m + [A_{12}](\vec{\Psi}_i^m)\delta\vec{U}_i^m - \lambda_m\delta\vec{\Psi}_i^m +$$

$$+\delta\lambda_m\vec{\Psi}_i^m = -\left(\frac{\vec{\Psi}_{i-1}^m - 2\vec{\Psi}_i^m + \vec{\Psi}_{i+1}^m}{h^2} + [D_i]\vec{\Psi}_i^m + \vec{F}_i(\vec{\Psi}_i^m, \vec{U}_i^m) - \lambda_m\vec{\Psi}_i^m\right),$$

$$\frac{\delta\vec{U}_{i+1}^m - 2\delta\vec{U}_i^m + \delta\vec{U}_{i-1}^m}{h^2} + [D_i]\delta\vec{U}_i^m + [A_{21}](\vec{U}_i^m)\delta\vec{U}_i^m + [A_{22}](\vec{U}_i^m)\delta\vec{U}_i^m =$$

$$= -\left(\frac{\vec{U}_{i-1}^m - 2\vec{U}_i^m + \vec{U}_{i+1}^m}{h^2} + [D_i]\vec{U}_i^m + \vec{G}_i(\vec{\Psi}_i^m, \vec{\Psi}_i^m)\right),$$

$$\frac{\delta\vec{V}_{i+1}^m - 2\delta\vec{V}_i^m + \delta\vec{V}_{i-1}^m}{h^2} + ([D_i] - c^2[E])\delta\vec{V}_i^m + [A_{31}](\vec{V}_i^m)\delta\vec{V}_i^m + [A_{32}](\vec{V}_i^m)\delta\vec{V}_i^m =$$

$$= -\left(\frac{\vec{V}_{i-1}^m - 2\vec{V}_i^m + \vec{V}_{i+1}^m}{h^2} + ([D_i] - c^2[E])\vec{V}_i^m + \vec{G}_i(\vec{\Psi}_i^m, \vec{\Psi}_i^m)\right),$$

where $[A_{\ell n}]$, $\ell = \overline{1,3}$, $n = \overline{1,2}$ are the matrices corresponding to differential operators for functions $\vec{F}_i$ and $\vec{G}_i$ from (18)-(20). After that, the boundary conditions can be written in the following form:

$$\delta\vec{\Psi}_0^m = 0, \delta\vec{\Psi}_N^m = 0; \qquad \delta\vec{U}_0^m = 0, \delta\vec{U}_N^m = 0; \qquad \delta\vec{V}_0^m = 0, \delta\vec{V}_N^m = 0.$$

To find the correction $\delta\lambda_m$ for spectral parameter, we have the equation:

$$(\delta\vec{\Psi}^m, \vec{\Psi}^m) = 0.$$

To solve this boundary problem, we apply the matrix sweep method [11]. The found solutions $\{\vec{\Psi}_i^*(t_M), \vec{U}_i^*(t_M)\,\vec{V}_i^*(t_M)\}, \lambda^*(t_M)$ are used as the initial approximations for Newtonian iterative process to solve the problem (18)-(23) with the non-zero boundary conditions (24). Initial approximations $\{y_i^*\}, \lambda^*$ for $t = 0$ have been found by using the procedure from [12].

4. THE RESULTS OF NUMERICAL SIMULATION

On the base of the proposed techniques the FORTRAN code to calculate the three-dimensional egenvalues and eigenfunctions for the polaron model has been created. These programs allow one to find as spherically-symmetrical and axi-symmetrical solutions as essentially three-dimensional solutions.

Now we define some classification of solutions. Let the class of solutions $\Omega_{k_0 l_0}$ correspond to the solutions obtained from initial guesses with $k = k_0, l = l_0$ in (31),(32). It should be noted that from iteration process we have functions ψ_{kl}, u_{kl} equal to 0 for $k < k_0$. So the class Ω_{00} includes the spherically-symmetrical solutions of the polaron problem. The case with $l_0 = 0$ corresponds to the axial symmetry of the problem. In Table 1 the summary of the obtained results for polaron model in the limit of strong coupling ($c = \infty$) and the comparison with results from [5] are shown. From this Table we see that the fast convergence of solutions in respect to the number of harmonics takes place near the ground state, but there is a dynamics of the numerical results for the low part of spectrum. In order to obtain the reliable results in this case it is necessary to increase the dimension of the solving discrete problem. In Table 2

Table 1. The calculated eigenvalues λ in dependence on the number of harmonics $K = k_0$

Eigenvalue	**Class**	$K = 1$	$K = 3$	$K = 5$	**results from [5]**
λ_0	Ω_{00}	0.08139	-	-	0.0814
λ_1	Ω_{00}	0.01540	-	-	0.0154
λ_2	Ω_{00}	0.00626	-	-	0.0062
λ_3	Ω_{00}	0.00337	-	-	-
λ_0	Ω_{10}	0.02705	0.03392	0.03443	0.0343
λ_1	Ω_{10}	0.00880	0.00833	0.01327	0.0126
λ_2	Ω_{10}	0.00432	0.00407	0.00415	-
λ_3	Ω_{10}	0.00255	0.00263	0.00276	-
λ_0	Ω_{21}	-	0.01490	0.01642	0.0159
λ_1	Ω_{21}	-	0.00618	0.00573	-
λ_2	Ω_{21}	-	0.00342	-	-

Table 2. Eigenvalues λ in dependence on the value of the constant of coupling c

Eigenvalue	**Class**	$C = 0.1$	$C = 1.0$	$C = 10.0$	$C = \infty$
λ_0	Ω_{00}	0.0347194	0.0769554	0.0813419	0.0813949
λ_1	Ω_{00}	0.0127952	0.0153239	0.0153978	0.0153986
λ_2	Ω_{00}	0.0058969	0.0062565	0.0062632	0.0062638
λ_0	Ω_{10}	0.0215822	0.0333973	0.0339144	0.0339199
λ_1	Ω_{10}	0.0078265	0.0083211	0.0083275	0.0083276
λ_2	Ω_{10}	0.0039902	0.0040679	0.0040688	0.0040688
λ_3	Ω_{10}	0.0026181	0.0026338	0.0026339	0.0026339
λ_0	Ω_{21}	0.0126877	0.0148575	0.0148967	0.0148970
λ_1	Ω_{21}	0.0059044	0.0061771	0.00618088	0.00618088
λ_2	Ω_{21}	0.0033554	0.0034145	0.0034152	0.0034152

the numerical results in dependence on the constant of coupling c for different classes Ω_{kl} are given. From this Table one can see the fast convergence of the solutions for large value c to the solutions in limit of strong coupling.

This investigation has been supported by the Russian Foundation for Fundamental Research, grant N 94 – 01 – 01119.

References

[1] Pekar S.I. Issledovania po elektronnoi teorii kristallov, Moscow, Gostekhizdat, 1951 (in Russian).

[2] Amirkhanov I.V. et.al. Report of Science Investigation Biological Center of USSR Science Academy , Pushchino, 1988.

[3] Amirkhanov I.V. et.al. Report of Science Investigation Biological Center of USSR Science Academy , Pushchino, 1990.

[4] Amirkhanov I.V.,Zemlyanaya E.V.,Puzynina T.P. JINR Report, P-11-91-139, Dubna, 1991.

[5] Gabdullin R.R. Report of Science Investigation Biological Center of USSR Science Academy, Pushchino, 1991.

[6] Amirkhanov I.V.,Puzynin I.V.,Puzynina T.P.,Zemlyanaya E.V. Preprint of JINR, E-11-92-205, Dubna, 1992.

[7] Gabdullin R.R. - DAN Rossii, 1993, v.333, 1, .23 (in Russian).

[8] Ortega J.M., Rheinboldt W.C. Iterative solution of nonlinear equations in several variables, Academic Press, New York and London, 1970.

[9] Fletcher C.A.J. Computational Galerkin Methods, Springer-Verlag, New York, Berlin, Heidelberg, Tokyo, 1984.

[10] Korn G.,Korn T.. Mathematical handbook for scientists and engineer, McGraw-Hill book comp., New York, Toronto, London, 1961.

[11] Samarsky A.A. Teorija raznosthykh skhem, Moscow, Nauka, 1977 (in Russian).

[12] Akishin P.G.,Puzynin I.V. JINR Report, 5-10992, Dubna, 1977.

Received by Publishing Department
on December 27, 1996.

Акишин П.Г., Пузынин И.В., Смирнов Ю.С. Е11-96-494

Метод ньютоновского продолжения для численного решения трехмерной задачи полярона

Предложен численный метод для решения трехмерной нелинейной задачи сферически-несимметричного полярона с конечной константой связи. Для аппроксимации решения использовано разложение по сферическим гармоникам. Для решения нелинейной задачи реализована ньютоновская итерационная схема с добавочной параметризацией исходного уравнения. На основе предложенной методики создан комплекс ФОРТРАН-программ для вычисления собственных значений и собственных функций. Обсуждаются результаты численного моделирования.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна, 1996

Akishin P.G., Puzynin I.V., Smirnov Yu.S. E11-96-494

The Newtonian Continuation Method for Numerical Study of 3D Polaron Problem

The numerical approach for study of the 3D-nonlinear problem for the spherically-nonsymmetric polaron is considered. Expansions in spherical harmonics are used for the approximation of the solution. The iterative Newton's scheme with an additional parametrization of the initial equation for the solving of the nonlinear problem is proposed. The results of numerical modelling are discussed. The comparison of the obtained eigenvalues with the known ones confirms the efficiency of the elaborated algorithms.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna, 1996

Макет Т.Е.Попеко

Подписано в печать 30.01.97
Формат 60 × 90/16. Офсетная печать. Уч.-изд.листов 1,04
Тираж 360. Заказ 49678. Цена 1248 р.

Издательский отдел Объединенного института ядерных исследований
Дубна Московской области