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ITERATION METHOD FOR SOLVING THE SPHERICAL NON-SYMMETRICAL POLARON EQUATION (THE LUTTINGER-LU MODEL)

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1.INTRODUCTION

The problem of existence of spherically non-symmetrical polaron states is an actual one in connection with the problem of electron transfer of excitations in different condensed matters.[1]

In ref.[2] classification of possible solutions of the polaron equation (the Pecar model) is developed and some of spherically non-symmetrical solutions are found.

In this paper schemes of a numerical investigation of spherically non-symmetrical polaron states (the Luttinger-Lu model) are proposed. A description of the iteration process in order to calculate them based on modifying the continuous analogue of Newton method [5] is also given in the work, and numerical results obtained with help of this method are presented.

2.THE STATEMENT OF THE PROBLEM

The problem of finding polaron states according to the Luttinger- Lu model is formulated as a non-linear eigenvalue problem for a system of equations:

$$\begin{gathered} \Delta\psi(\vec{r}) - \lambda\psi(\vec{r}) + A(V_1(\vec{r}) - V_2(\vec{r}))\psi(\vec{r}) = 0 \\ \Delta V_1(\vec{r}) + \mid \psi(\vec{r}) \mid^2 = 0 \\ \Delta V_2(\vec{r}) - C^2 V_2(\vec{r}) + \mid \psi(\vec{r}) \mid^2 = 0 \end{gathered} \tag{1}$$

with the normalization condition

$$\int_0^\infty \mid \psi(\vec{r}) \mid^2 d\vec{r} = 1, \tag{2}$$

where Δ - a three-dimensional Laplace operator, A and C - physical parameters of the problem, λ - eigen-values, determining energy levels.

If the solution to the system (1) we present as an expansion in spherical functions $Y_{lm}(\Theta, \phi)$

$$\psi(\vec{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{\psi_{lm}(r)}{r} Y_{lm}(\Theta, \phi) .$$

$$V_i(\vec{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{V_{ilm}(r)}{r} Y_{lm}(\Theta, \phi), \qquad i = 1,2 \tag{3}$$

and substitute this expansion into system (1), multiplying from the left by $Y(\Theta,\phi)$ and integrating with respect to $d\Omega = \sin\Theta d\Theta d\Phi$, then the system of equations for expansions coefficients $\psi_l m(r)$, $V_i l m(r)$ will be as follows:

$$\psi''_{lm}(r) - \lambda\psi_{lm}(r) - \frac{l(l+1)}{r^2}\psi_{lm}(r) + \frac{A}{r}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1} Q_{lml_1m_1}(r)\psi_{l_1m_1}(r) = 0$$

$$V''_{1lm}(r) - \frac{l(l+1)}{r^2}V_{1lm}(r) + S_{lm}(r) = 0 \qquad (4)$$

$$V''_{2lm}(r) - \frac{l(l+1)}{r^2}V_{2lm}(r) - C^2V_{2lm}(r) + S_{lm}(r) = 0 \qquad l = 0,1,2,..., \qquad m = -l,...,l$$

with the normalization condition

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\int_0^{\infty}\psi^2_{lm}(r)dr = 1, \qquad (5)$$

where

$$Q_{lml_1m_1} = \sum_{l_2=0}^{\infty}\sum_{m_2=-l_2}^{l_2} W_{lml_1m_1l_2m_2}(V_{1l_2m_2}(r) - V_{2l_2m_2}(r))$$

$$S_{lm} = \frac{1}{r}\sum_{l_1=0}^{\infty}\sum_{m_1=-l_1}^{l_1}\sum_{l_2=0}^{\infty}\sum_{m_2=-l_2}^{l_2}\bar{W}_{lml_1m_1l_2m_2}\psi_{l_1m_1}(r)\psi_{l_2m_2}(r) \qquad (6)$$

$$W_{lml_1m_1l_2m_2} = \int d\Omega Y^*_{lm}Y_{l_1m_1}Y_{l_2m_2}$$

$$\bar{W}_{lml_1m_1l_2m_2} = \int d\Omega Y^*_{lm}Y_{l_1m_1}Y^*_{l_2m_2}$$

The desired solutions of the system satisfy the boundary conditions:

$$\psi_{lm}(r)_{r\to 0} \to A_{1lm}r^{l+1}$$

$$\psi_{lm}(r)_{r\to\infty} \to A_{2lm}e^{-\sqrt{\lambda}r}$$

$$V_{1lm}(r)_{r\to 0} \to B_{1lm}r^{l+1} \qquad (7)$$

$$V_{1lm}(r)_{r\to\infty} \to B_{2lm}r^{-l}$$

$$V_{2lm}(r)_{r\to 0} \to C_{1lm}r^{l+1}$$

$$V_{2lm}(r)_{r\to\infty} \to C_{2lm}r^{-Cr},$$

where $A_{1lm}, A_{2lm}, B_{1lm}, B_{2lm}, C_{1lm}, C_{2lm}$ are constants.

The numerical solving of the problem (4)-(6) with boundary conditions (7) is performed on the finite interval $0 \le r \le R_m$ with a limitation of a number of members in expansion (3) by the number L_m for $\psi(\vec{r})$ and $L_v = 2L_m$ for $V_i(r), i = 1,2$.

The case of spherically symmetrical solutions $\psi(r,\theta,\phi) \Rightarrow \psi(r)$, corresponding to $L_m = 0$, has received the most study. In this case the problem (4)-(6) is reduced to the solving of the system of three non-linear differential equations. This problem was studied by a number of authors (see, for instance, ref.[4]).

In this paper a more complicate case $\psi(r,\theta,\phi) \Rightarrow \psi(r,\theta)$ is considered. Here in expansion (3) the function $Y_{lm}(\theta,\phi)$ must be replaced by $Y_{l0} = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta)$, where P_l- Legendre polinoms, $l = 0,1,...,L_m$.

Using more suitable designations and taking into account the states above limitations, the system (4)-(6) can be written in the form

$$\psi''_l(r) - \lambda\psi_l(r) - \frac{l(l+1)}{r^2}\psi_l(r) + \frac{A}{r}\sum_{l_1=0}^{L_m} Q_{ll_1}(r)\psi_{l_1}(r) = 0 \qquad ,l = 0,1,...,L_m, \quad (8)$$

$$V''_{1l}(r) - \frac{l(l+1)}{r^2}V_{1l}(r) + S_l(r) = 0 \qquad (9)$$

$$V''_{2l}(r) - \frac{l(l+1)}{r^2}V_{2l}(r) - C^2V_{2l}(r) + S_l(r) = 0 \qquad ,l = 0,1,...,L_v,$$

with the normalization condition

$$\sum_{l=0}^{L_m}\int_0^{R_m}\psi^2_l(r)dr = 1, \qquad (10)$$

where

$$Q_{ll_1}(r) = \sum_{l_2=0}^{L_v} W_{ll_1l_2}(V_{1l_2}(r) - V_{2l_2}(r)) \qquad (11)$$

$$S_l(r) = \sum_{l_1=0}^{L_m}\sum_{l_2=0}^{L_m} W_{ll_1l_2}\psi_{l_1}(r)\psi_{l_2}(r) \qquad (12)$$

$$W_{ll_1l_2}(r) = 2\pi\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{2l_1+1}{4\pi}}\sqrt{\frac{2l_2+1}{4\pi}}\int_{-1}^{+1}P_l(x)P_{l_1}(x)P_{l_2}(x)dx. \qquad (13)$$

Taking into account asymptotic properties of solutions (7), the boundary conditions for the finite interval $0 \le r \le R_m$ can be written as follows:

$$\psi_{1A}(0)\psi'_l(0) - \psi'_{1A}(0)\psi_l(0) = 0$$

$$\psi_{2A}(R_m)\psi'_l(R_m) - \psi'_{2A}(R_m)\psi_l(R_m) = 0 \qquad (14)$$

$$V_{i1A}(0)V'_{il}(0) - V'_{i1A}(0)V_{il}(0) = 0$$

$$V_{i2A}(R_m)V'_{il}(R_m) - V'_{i2A}(R_m)V_{il}(R_m) = 0, \qquad (15)$$

where

$$\psi_{1A} = A_{1l} r^{l+1}, \psi_{2A} = A_{2l} e^{-\sqrt{\lambda} r},$$
$$V_{11A} = B_{1l} r^{l+1}, V_{12A} = B_{2l} r^{-l},$$
$$V_{21A} = C_{1l} r^{l+1}, V_{22A} = C_{2l} e^{-Cr},$$

A_{il}, B_{il}, C_{il} are constants, $i = 1, 2$.

3.A DESCRIPTION OF THE ITERATION METHOD

The problem (8)-(15) can be numerically solved by means of the continuous analogue of the Newton method /5/. In this case the system of $(L_m + 2L_v + 3)$ nonlinear differential equations should be solved. However, in this paper a more simple method for solving this problem is proposed. A similar approach was applied in /4/ for calculating spherically symmetrical solutions. The solving of the system of the $(L_m + 2L_v + 3)$ nonlinear differential equations is reduced to the sequential solving of the eigenvalue problem for $(L_m + 1)$ linear differential equations and to the solving of $2(L_v + 1)$ boundary problems for linear differential equations.

An algorithm of this iteration process is as follows.

By taking some set $\{\lambda^{(0)}, \psi_l^{(0)}(r), l = 0, 1, .., L_m\}$ (the initial approach), using formula (12) we calculate coefficients $S_l(r)$ for the system (9). Solving (9) with boundary conditions (15), $V_{1l}^{(0)}(r)$ and $V_{2l}^{(0)}(r)$ are found. Then, using (11), effective potentials $Q_{ll_1}^{(0)}(r)$ are calculated. Later, if solving the eigenvalue problem for the system (8) with boundary conditions (14), normalization condition (10) and the obtained potentials $Q_{ll_1}^{(0)}(r)$, new set $\{\lambda^{(1)}, \psi_l^{(1)}(r), l = 0, 1, ...L_m\}$ can be obtained. These functions, in their turn, are used for calculating $V_{1l}^{(1)}(r), V_{2l}^{(1)}(r)$ and effective potentials $Q_{ll_1}^{(1)}(r)$ during the next iteration. This process must be continued until eigen-values and eigen-functions $\{\lambda^{(k)}, \psi_l^{(k)}(r), l = 0, 1, ...L_m\}$, functions $V_{il}^{(k)}(r), i = 1, 2, l = 0, 1, ..., L_v$, obtained after two sequential iterations, would coincided with each other with given accuracy ϵ, that is, until the condition $\delta \le \epsilon$ will be performed, where

$$\delta = \max\{| \lambda^{(k+1)} - \lambda^{(k)} |, \max_{r_j \in [0, R_m]} \{ \max_{l \in [0,1,...,L_v], i=1,2} | V_{il}^{(k+1)}(r_j) - V_{il}^{(k)}(r_j) |,$$

$$\max_{l \in [0,1,...,L_m]} | \psi_l^{(k+1)}(r_j) - \psi_l^{(k)}(r_j) | \}\} \qquad (16)$$

The eigenvalue problem (8),(10),(14) for the system of differential linear equations is solved by means of the continuous analogue of the Newton method. Solutions of boundary problems (9),(15) are calculated by 'run'. For approximation of equations (8)-(9) difference schemes of the accuracy order $O(h^2)$ are used. In most cases the calculations are performed for $R_m = 50$ and 100.

A number of the iterations depends on a quality of initial approximations. Having sufficiently good initial approximations $\{\lambda^{(0)}, \psi_l^{(0)}(r), l = 0, 1, .., L_m\}$, when a initial

residual $\Delta^{(0)} \simeq 10^{-1} - 10^{-2}$, where

$$\Delta^{(0)} = \max_i \Delta_i^0,$$

$$\Delta_1^{(0)} = \max_l | \psi''^{(0)}_l(r) - \lambda^{(0)} \psi_l^{(0)}(r) - \frac{l(l+1)}{r^2} \psi_l^{(0)}(r) + \frac{A}{r} \sum_{l_1=0}^{L_m} Q_{l\, l_1}(r) \psi_{l_1}^{(0)}(r) |$$

$$\Delta_2^{(0)} = \max_l | V''_{1l}(r)^{(0)} - \frac{l(l+1)}{r^2} V_{1l}^{(0)}(r) + S_l(r) = 0 |$$

$$\Delta_3^{(0)} = \max_l | V''_{2l}(r)^{(0)} - \frac{l(l+1)}{r^2} V_{2l}^{(0)}(r) - c^2 V_{2l}(r) + S_l(r) = 0 |$$

the accuracy may be $\delta \simeq 10^{-4} - 10^{-5}$ in $8 - 10$ iterations in the average. In doing so $\Delta^{(k)} \simeq 10^{-7} - 10^{-10}$. The calculations were sequentially performed for $L_m = 0, 1, 2, 3, 4, 5$. The results obtained for the each mean of L_m, were used as an initial approach for $L_m + 1$. When constructing the initial approximations $\tilde{\psi}_l^{(0)}, L_m = 1$ a device of the "mouse" type (Genius Driver Mouse) was used.

The constants A and C are selected in accordance with the existing spherically symmetrical solutions, obtained in /4/.

$$c = \frac{\sqrt{2}\mu}{\sqrt{1-\mu}}, \mu = 0.45858, A = 8\sqrt{2}\pi\alpha, \alpha = 2.$$

For the eigen-values and the eigen-functions of the (8),(10),(14) to be received, the program packet SLIPH4 /6/ for $L_m = 0$, the program packet SLIPS2 /7/ for $L_m = 1$ and the program packet START for $L_m = 1, 2, ..., 5$ (the description is prepared for publication by Yu.S.Smirnov) are used.

The computations were performed on VAX 8350 and PC/AT 286/386 computers.

4.NUMERICAL RESULTS

By calculations, performed with the help of the method described in sec.3 the set of solutions $\vec{\psi} = \{\psi_l, l = 0, 1, 2, ...L_m\}$ of problem (8)-(15) are found. The singularity of this solutions is that some of components $\psi_l = 0$. Obtained solutions can be separated into the next groups:

1. Spherically symmetrical solutions, in which only function $\psi_0 \neq 0$. The solutions of this group coincide with the results of /4/.
2. Non-zero functions are ψ_l for even means of l $(l = 0, 2, 4)$.
3. Non-zero functions are ψ_l for odd means of l $(l = 1, 3, 5)$.

Table

	LM=0		LM=1			LM=2				LM=3					LM=4						LM=5						
	f0	λ	f0	f1	λ	f0	f1	f2	λ	f0	f1	f2	f3	λ	f0	f1	f2	f3	f4	λ	f0	f1	f2	f3	f4	f5	λ
nz	0	1.421	0	-	1.421	0	-	-	1.421	0	-	-	-	1.421	0	-	-	-	-	1.421	0	-	-	-	-	-	1.421
N	1.		1.			1.				1.					1.						1.						
nz	-		-	0	.791	-	0	-	.791	-	0	-	0	.816	-	0	-	0	-	.816	-	0	-	0	-	0	.817
N				1.			1.				.97		.03			.97		.03				.970		.028		.002	
nz						1	-	0	.455	1	-	0	-	.455	1	-	0	-	0	.455	1	-	0	-	0	-	.455
N						.79		.21		.79		.21			.789		.206		.003		.789		.206		.003		
nz	1	.443	1	-	.443	1	-	-	.443	1	-	-	-	.443	1	-	-	-	-	.443	1	-	-	-	-	-	.443
N	1.		1.			1.				1.					1.						1.						
nz			-	1	.303	-	1	-	.303	-	1	-	1	.362	-	1	-	1	-	.362	-	1	-	1	-	1	.388
N				1.			1.				.78		.22			.78		.22				.73		.21		.06	
nz						2	-	1	.208	2	-	1	-	.206	2	-	1	-	1	.208	2	-	1	-	1	-	.208
N						.76		.24		.76		.24			.64		.32		.04		.64		.32		.04		
nz	2	.194	2	-	.194	2	-	-	.194	2	-	-	-	.194	2	-	-	-	-	.194	2	-	-	-	-	-	.194
N	1.		1.			1.				1.					1.						1.						
nz			-	2	.156	-	2	-	.156	-	2	-	2	.193	-	2	-	2	-	.193	-	2	-	2	-	2	.217
N				1.			1.				.68		.32			.68		.32				.55		.32		.13	
nz			—		(*)	3	-	2	.136	3	-	2	-	.136													
N						.36		.64		.36		.64															
nz						3	-	2	.114	3	-	2	-	.114	3	-	2	-	2	.116	3	-	2	-	2	-	.116
N						.68		.32		.68		.32			.66		.31		.05		.66		.31		.03		
nz	3	.106	3	-	.106	3	-	-	.106	3	-	-	-	.106	3	-	-	-	-	.106	3	-	-	-	-	-	.106
N	1.		1.			1.				1.					1.						1.						
nz				3	.081	-	3	-	.081																		
N				1.			1.																				

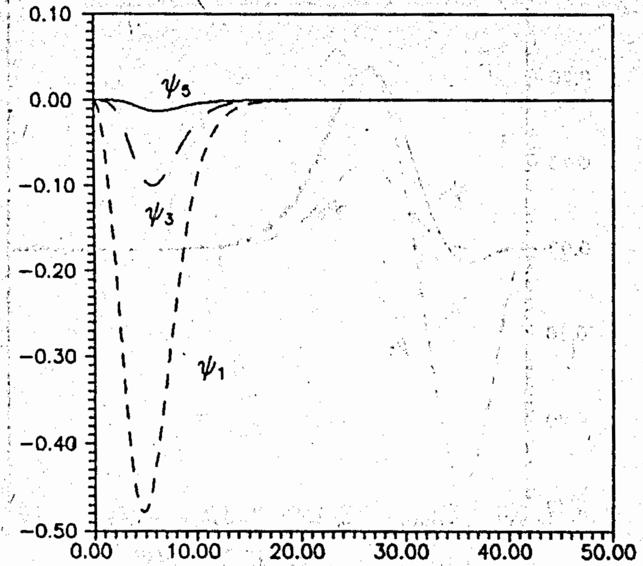

Fig 1, λ=0.817

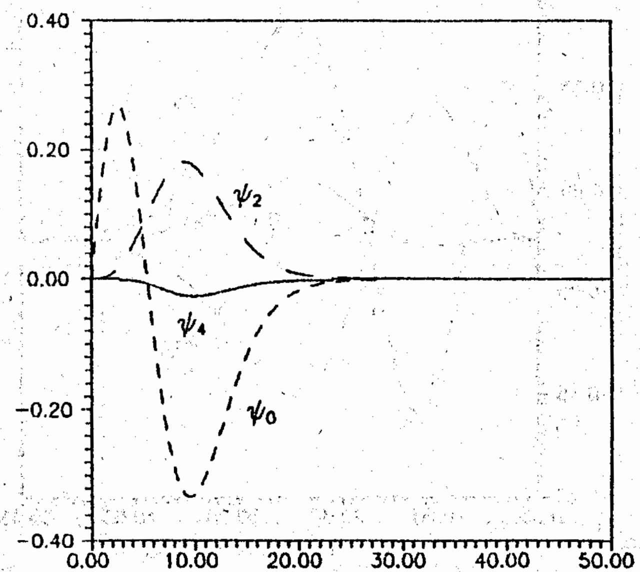

Fig 2, λ=0.455

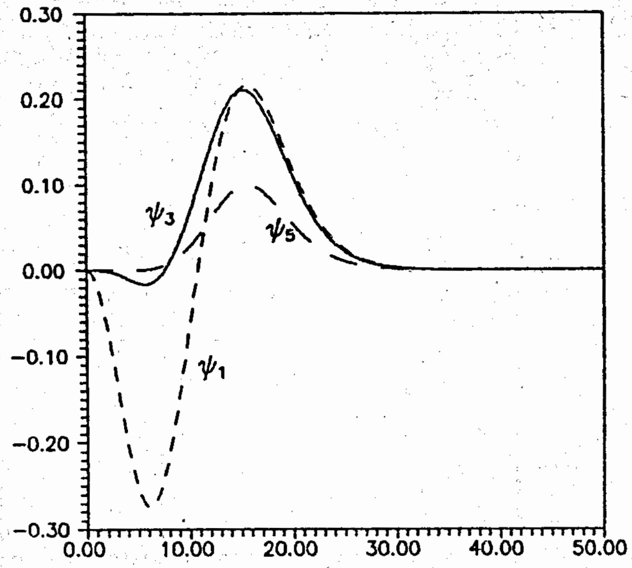

Fig 3, λ=0.388

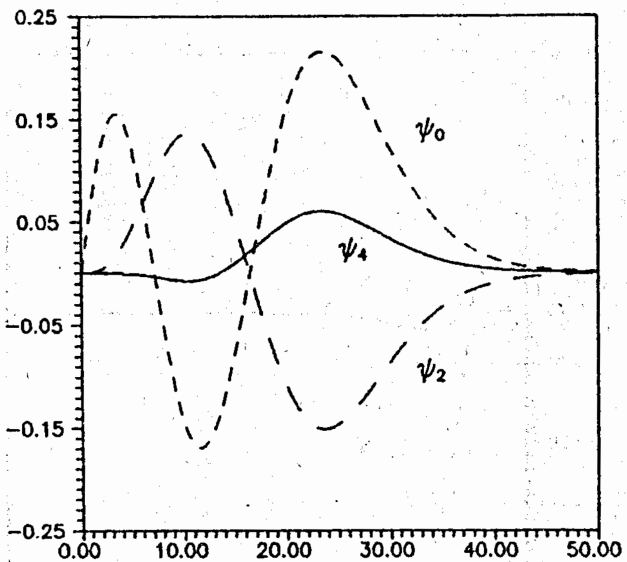

Fig 4, λ=0.208

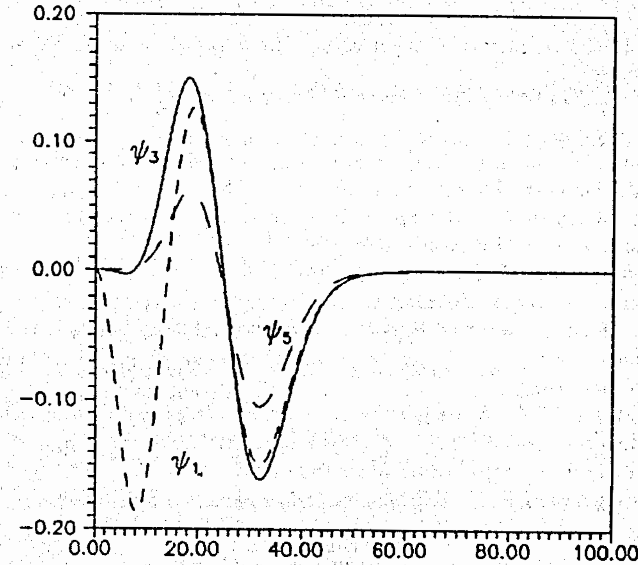

Fig 5, λ=0.217

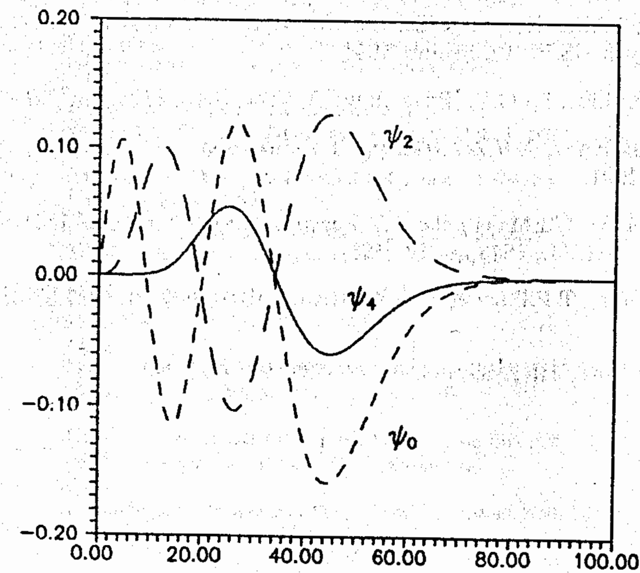

Fig 6, λ=0.116

In the table the spectrum of eigen-values,and number of zeros N_z and norms of functions $N = \int_0^{R_m} \psi_l^2 dr$ are represented for $L_m = 0,1,2,3,4,5$. Functions with $N = 0$ are denoted by minus.

As it is obvious from the table, at increasing the mean of l the norm of non-zero components ψ_l decreases for the most solutions. This allows to suppose, that using valid selected means of L_m, the approximation of solutions of the problem (4)-(7) with a high accuracy can be obtained.

In addition,for $L_m = 2,3$ the solution noted by (*) in which the norm of ψ_0 less than the norm of ψ_2, is calculated.

Another conformity reflected in the table is a correlation between the norm of ψ_l and its number of zeros. 'Dumping' of norms of ψ_l is slowing if the number of zeros in solutions is increasing.

At the figures 1,2,3,4,5,6 the graphs of non-zero components ψ_l of the spherically non-symmetrical solutions for $L_m = 6$ are represented. At the each figures the number l of function ψ_l and the eigen-value λ are indicated.

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Амирханов И.В. и др. E11-92-205
Итерационный метод вычисления
сферически-несимметричных решений
поляронной проблемы (модель Латтинжера — Лу)

Рассматривается итерационный метод вычисления сферически-несимметричных состояний полярона в рамках модели Латтинжера—Лу. Исходное уравнение полярона в частных производных при разложении решения по сферическим функциям $Y_{lm}(\theta, \varphi)$, $m = 0$, $l = 0, 1, 2, \ldots$ сводится к задаче на собственные значения для системы из $3(l+1)$ нелинейных обыкновенных дифференциальных уравнений. Ее решение, согласно предлагаемому методу, заменяется последовательным решением задач на собственные значения для системы $(l+1)$ линейных дифференциальных уравнений, осуществляемым на основе непрерывного аналога метода Ньютона, и решением $2(l+1)$ краевых задач для линейных дифференциальных уравнений. Представлены результаты счета для случаев $l = 0, 1, 2, 3, 4, 5$.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

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Перевод Аристарховой М.В.

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Iteration Method for Solving the Spherical
Non-Symmetric Polaron Equation (the Luttinger — Lu Model)

An iteration method for calculating the spherically non-symmetric polaron states in the framework of the Luttinger — Lu model is considered. The initial polaron partial differential equation by expansion of the solution in spherical functions $Y_{lm}(\theta, \varphi)$, $(l = 0, 1, 2, \ldots; m = 0)$ is reduced to the eigenvalue problem for a system of $3(l+1)$ nonlinear ordinary equations. The method proposed reduces the solving of the problem to the sequential solving of eigenvalue problems for the system of $l+1$ linear differential equations being performed on the base of the continuous analog of Newton's method and to the solving the $(l+1)$ pair of boundary problems for linear differential equations. The results of the calculations for $l = 0, 1, 2, 3, 4, 5$ are presented.

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

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