Reccurent sequenses in solving the Schrödinger equation

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ABSTRACT
An explicit numerical-analytical method is demonstrated for accurate solving the Schrödinger equation in those cases when this equation reducible to a system of n coupled ordinary differential equations with singular points. Fundamental system of solutions is constructed as algebraic combinations of power series, power functions and logarithmic function in the neighbourhood of the regular singular point and as asymptotic expansions of solutions in the neighbourhood of the irregular singular point. The method is based on the calculation of recurrent sequences of constant matrices of coefficients in power series and in inverse power series in asymptotic expansions using derived recurrent relations, that makes possible to calculate solutions at any given point using only algebraic computations and elementary functions. In turn it makes possible to solve accurately the eigenvalue problem and scattering problem and to derive analytical expressions for the wavefunctions. The method is applied to calculations of energies and wavefunctions of the discrete spectrum and wave functions of the continuous spectrum of the hydrogen-like atoms and of acceptors in semiconductors.

Keywords: numerical methods, Coulomb potential, ordinary differential equations, singular points, recurrent sequences, eigenvalue problem, scattering problem

1. INTRODUCTION

We consider the Schrödinger equation

$$H\Psi(z) = E\Psi(z), \tag{1}$$

where the Hamiltonian H is a quadratic form of the momentum, in those cases when Eq. (1) is reducible to a system of n coupled ordinary differential equations with singular points. Hamiltonian H can be represented in the following form:

$$H = Ap^2 + \sum_{m=-2}^{2} B_m P_m^{(2)} + V(r), \tag{2}$$

where $\boldsymbol{p} = -i\nabla$ is a momentum operator ($\hbar = 1$), $P_m^{(2)}$ are the components of the irreducible spherical tensor operator of the second rank [1] composed of the components of the

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symmetric tensor $P_{ik} = p_i p_k - \frac{1}{3}\delta_{ik} p^2$, and A, B_m are constant $n \times n$ matrices. We suppose that $V(r)$ is the Coulomb potential. Using the expansion of the wavefunction $\Psi(z)$ in the complete basis functions of angular variables or if necessary the functions of angular and spin variables, such as functions in the *L-S* coupling scheme (see [2], and the references cited therein) it is possible to reduce (1) to a system of n coupled radial equations:

$$w \cdot r^2 \frac{d^2 R}{dr^2} + p_0 \cdot r \frac{dR}{dr} + (q_0 + q_1 \cdot r + q_2 \cdot r^2) R = 0, \tag{3}$$

where w, p_0 and q_i are constant $n \times n$ matrices, $R = (R_{L\tau})$ is an n-dimensional column-function, L is a quantum number of the orbital angular momentum operator $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$, τ is a set of some quantum numbers chosen in accordance with a Hamiltonian symmetry. Hermitian character of the Hamiltonian imposes the following conditions on the matrices of coefficients: $w = w^* > 0$ (this matrix is proportional to the inverse masses matrix), $p_0 = 4w^* - p_0^*$, $q_0 = q_0^* + 2w^* - p_0^*$, $q_{1,2} = q_{1,2}^*$.

There are two singular points of Eq. (3): the regular singular point $r = 0$ and irregular singular point $r = \infty$. Eq. (3) describes Coulomb states of a particle (or of two attractive particles, i.e. of exciton) in various systems. In case $n = 1$ these are states of a hydrogen-like atom, if $n > 1$ (3) describes states of, e.g., a shallow acceptor impurity or exciton in semiconductors in different approximations.

Using the substitution $\phi = r \cdot \begin{pmatrix} R \\ R + rR' \end{pmatrix}$ we reduce the system of n second-order equations (3) to a system of 2n first order equations:

$$r \frac{d\phi}{dr} = \alpha(r)\phi \ , \ \alpha(r) = \alpha_0 + \alpha_1 r + \alpha_2 r^2 . \tag{4}$$

It is obvious now that $r = 0$ is the regular singular point (by definition). Here

$$\alpha_0 = \begin{pmatrix} 0 & 1 \\ -Q_0 & (1 - P_0) \end{pmatrix}, \ \alpha_1 = \begin{pmatrix} 0 & 0 \\ -Q_1 & 0 \end{pmatrix}, \ \alpha_2 = \begin{pmatrix} 0 & 0 \\ -Q_2 & 0 \end{pmatrix}$$

are $2n \times 2n$ matrices, $Q_0 = w^{-1}(q_0 - p_0) + 2$, $Q_{1,2} = w^{-1} q_{1,2}$ $P_0 = w^{-1} p_0 - 1$.

The methods of construction of the fundamental system of solutions of Eq. (4) in the neighbourhood of the regular singularity $r = 0$ and solving the singular eigenvalue problem and the scattering problem, that are based on the recurrent sequences procedure were developed in [3, 2] in general case, i.e. when $\alpha(r)$ in (4) is an arbitrary holomorphic at the point $r = 0$ $N \times N$ matrix function. In the present paper we derive solutions of (3) in the neighbourhood of the irregular singularity $r = \infty$ in general case of arbitrary n using a method specifically pertinent in case of Eq. (3) (section 2), and study particular problems ($n = 1, 2$ in (4)), i.e. derive solutions of (3) and solve the eigenvalue problem and related problems both in the case when exact analytical solutions are known, that makes possible to estimate the accuracy of the method, and in cases when only numerical methods are applicable (sections 3, 4). Note that the method based on the use of recurrent sequences of constant coefficients allows us to compute the solution at any given point, using only simple algebraic computations and elementary functions, without the use of any step-by-step procedures.

2. SOLUTIONS IN THE NEIGHBOURHOOD OF THE IRREGULAR SINGULARITY r = ∞∞

In order to construct the fundamental system of solutions $R(r)$ of Eq. (3) in the neighbourhood of the irregular singularity $r = \infty$ we derive asymptotic expansions of the functions $f(r) = r \cdot R(r)$ at $r \to \infty$. We reduce the system of equations (3) to a system of first order equations using the substitution $\mathrm{X}(r) = \begin{pmatrix} f \\ \dfrac{df}{dr} \end{pmatrix}$:

$$\frac{d\mathrm{X}(r)}{dr} = \beta(r)\mathrm{X}(r) = \left(\beta_0 + \frac{1}{r}\beta_1 + \frac{1}{r^2}\beta_2\right)\mathrm{X}(r), \tag{5}$$

where

$$\beta_0 = \begin{pmatrix} 0 & 1 \\ -Q_2 & 0 \end{pmatrix},\ \beta_1 = \begin{pmatrix} 0 & 0 \\ -Q_1 & -P_0 \end{pmatrix},\ \beta_2 = \begin{pmatrix} 0 & 0 \\ -Q_0 & 0 \end{pmatrix}, \tag{6}$$

To analyse the structure of the $2n \times 2n$ matrix β_0 whose form determines the behaviour of the solutions of (5) at $r \to \infty$ we consider the following eigenvalue problem

$$\beta_0 \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \lambda \begin{pmatrix} \xi \\ \eta \end{pmatrix},$$

where ξ, η are n-dimensional vectors, and we obtain from (6)

$$\eta = \lambda\xi;\ -Q_2\xi = \lambda^2\xi.$$

Note that the matrix Q_2 is similar to a Hermitian matrix, i.e. its eigenvalues are real, and eigenvectors form complete system in the n-dimensional space. We suppose henceforth that there are n_+ positive and n_- negative eigenvalues of the matrix Q_2 ($n = n_+ + n_-$), and there are no multiple ones among them. Thus the matrix Q_2 is similar to the diagonal matrix $diag(\varepsilon_1,...,\varepsilon_{n_-},\varepsilon_{n_-+1},...,\varepsilon_n)$. Hence β_0 is a plain matrix, its eigenvalues are $2n$ unlike numbers: $\pm i\sqrt{\varepsilon_{n_-+1}},\ldots,\pm i\sqrt{\varepsilon_n},\pm\sqrt{-\varepsilon_1},\ldots,\pm\sqrt{-\varepsilon_{n_-}}$, and eigenvectors are of the form

$$\begin{pmatrix} \xi^{(k)} \\ (-\varepsilon_k)^{1/2}\xi^{(k)} \end{pmatrix}, \begin{pmatrix} \xi^{(k)} \\ -(-\varepsilon_k)^{1/2}\xi^{(k)} \end{pmatrix},\ k = 1,\ldots,n.$$

Obviously these eigenvectors form complete system in the n-dimensional space.

We perform the following substitution:

$$\mathrm{X} = T_\infty \mathrm{Z}\ ,\ T_\infty^{-1}\beta_k T_\infty = \mathrm{B}_k\ ,\ k = 0, 1.2, \tag{7}$$

where

$$\mathrm{B}_0 = diag[(-\varepsilon_1)^{1/2},\ldots,(-\varepsilon_{n_-})^{1/2},i\varepsilon_{n_-+1}^{1/2},\ldots,i\varepsilon_n^{1/2},-(-\varepsilon_1)^{1/2},\ldots,-(-\varepsilon_{n_-})^{1/2},-i\varepsilon_{n_-+1}^{1/2},\ldots,-i\varepsilon_n^{1/2}]\,.$$

Then Eq. (5) assumes the form

$$\frac{dZ}{dr} = \left(B_0 + \frac{B_1}{r} + \frac{B_2}{r^2} \right) Z. \tag{8}$$

The asymptotic expansion of solutions of Eq. (8) $Z(r)$ at $r \to \infty$ is of the form (see [4]):

$$Z(r) \approx \left(\sum_{k=0}^{\infty} \frac{R_k}{r^k} \exp\left(D_0 r + D_1 \ln r + \sum_{p=2}^{\infty} D_k \frac{r^{1-p}}{1-p} \right) \right) C. \tag{9}$$

C in Eq. (9) is an arbitrary 2n-dimensional vector, R_k and D_k are $2n \times 2n$ matrices, and the following relations are valid: 1) $R_0 = \hat{1}$; 2) $D_0 = B_0$; 3) $(R_k)_{\alpha\alpha} \equiv 0, k \geq 1, \alpha = 1, \ldots, 2n$; 4) $D_k = diag, k \geq 0$. Constant matrices R_k, D_k, $k \geq 1$ (recurrent sequences) satisfy the following recurrent relations:

$$B_0 R_k - R_k B_0 = D_k + \sum_{l=1}^{k-1} \left(R_l D_{k-l} - B_{k-l} R_l \right) - B_k + (1-k) R_{k-1}. \tag{10}$$

It is easy to compute all required components $(R_k)_{\alpha\beta}$, $\alpha \neq \beta$, and $(D_k)_{\alpha\alpha}$ using the fact that B_o is a diagonal matrix with unlike eigenvalues.

3. THE CASE OF A HYDROGEN-LIKE ATOM

The following radial equation (Eq. (3), $n = 1$) is considered,

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{L(L+1)}{r^2} + \frac{2\alpha}{r} + E \right\} R_L(r) = 0 \tag{11}$$

where L is the quantum number of the orbital angular momentum, α is an integer ($\alpha = 1$ corresponds to the Coulomb attraction in a hydrogen atom), $R_L(r)$ is a Coulomb radial wavefunction, E is the energy. Generally speaking, distances and the energy are measured in the units of $a = \hbar^2 \kappa / (me^2)$ (effective Bohr radius) and $Ry = me^4 / (2\hbar^2 \kappa^2)$ (effective Rydberg constant) respectively, where e – electron charge, m – electron effective mass or reduced mass in case of two attractive particles (exciton), κ – static dielectric constant.

Note that this equation describes the states of a hydrogen atom or hydrogen-like donor impurities in the direct-gap semiconductors.

3.1. FUNDAMENTAL SYSTEM OF SOLUTIONS

The neighbourhood of the regular singular point $r = 0$.

The regular solution of Eq. (11) is of the form

$$R_L^R(r) = \sum_{n=L}^{\infty} a_n r^n, \tag{12}$$

where coefficients a_n satisfy the following recurrent relation

$$a_L = C, a_n = -\frac{2a_{n-1} + Ea_{n-2}}{(n-L)(n+L+1)}, n > L. \tag{13}$$

a_L is an arbitrary constant C that is determined by normalization.

The second, irregular solution of Eq. (11) assumes the form:

$$R_L^I(r) = \sum_{n=-L-1}^{\infty} b_n r^n + \ln r R_L^R(r). \tag{14}$$

Here $R_L^R(r)$ is the solution (12) with a coefficient a_L :

$$a_L = -\frac{2b_{L-1} + Eb_{L-2}}{2L+1}.$$

Coefficients b_n satisfy the recurrent relation:

$$b_{-L-1} = D, b_L = 0, b_n = -\frac{2b_{n-1} + Eb_{n-2} + (2n+1)a_n}{(n-L)(n+L+1)}, \tag{15}$$

Coefficient b_L is an arbitrary number and we set $b_L = 0$ that results in the proportionality of a_l and D. The value D is determined by normalization.

As follows from the results of [3], power series in (12), (14) converges uniformly in the whole interval $(0, \infty)$ and $R_L^R(r), R_L^I(r)$ are linear-independent solutions of Eq. (3). It is clear that to calculate radial wavefunctions with any given accuracy at an arbitrary point $\hat{r}, 0 < \hat{r} < \infty$, it is sufficient to take into account only a finite number N in the power series. The value of N is limited only by the computer resources and round-off errors in the process of computations.

The neighbourhood of the irregular singular singular point $r = \infty$.

As it follows from the results of section 3, the asymptotic expansions of the function $f_L(r) = r \cdot R_L(r)$ and its derivative at $r \to \infty$ are as follows

$$F_L \sim \left(1 + \sum_{n=1} \frac{(P_n)_{12}}{r^n}\right) \omega_i, \ \frac{dF_L}{dr} \sim \lambda \left(1 - \sum_{n=1} \frac{(P_n)_{12}}{r^n}\right) \omega_i, \ \lambda = \sqrt{-E} \tag{16}$$

$$\omega_i = C_i \exp\left((B_0)_i r + (B_1)_i \ln r - \sum_{n=2} \frac{(B_n)_i}{(n-1)r^{n-1}}\right), i = 1, 2 \tag{17}$$

Matrix recurrent sequences P_n and B_n are determined by the following recurrent relations

$$A_0 P_n - P_n B_0 = P_0 B_n - \sum_{s=0}^{n-1} A_{n-s} P_s + \sum_{s=1}^{p-1} P_s B_{n-s} - (n-1) P_{n-1}, n \geq 1. \tag{18}$$

Matrices B_n are diagonal $(B_n)_{ik} = (B_n)_i \delta_{ik}$, $B_0 = A_0$, $(P_0)_{ik} = \delta_{ik}$, $(P_n)_{ii} = 0$, $n \geq 1$, and

$$A_0 = \lambda \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ A_1 = \frac{\alpha}{\lambda} \begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix}, \ A_2 = \frac{L(L+1)}{2\lambda} \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}.$$

3.2. THE MATCHING OF THE SOLUTIONS. EIGENVALUE PROBLEM

The conventional eigenvalue problem for Eq. (11) is in the following: one should find such value of the energy E: $E < 0$ (eigenvalue) that the solution $R_L(r)$ is finite at $r = 0$

and $R_L(r) \to 0$ at $r \to \infty$, one should find also the wavefunction corresponding to this value of E and normalized by the condition (eigenfunction):

$$\int_0^\infty R_L^2(r) r^2 \, dr = 1 \tag{19}$$

To solve the problem it is necessary to perform matching at some intermediate point $r = \hat{r}$, $0 < \hat{r} < \infty$ of a function $f_L(r) = rR_L^R(r)$ (R_L^R is the regular at $r = 0$ solution (12)) and its derivative (the "left" solution) with a "right" solution that tends to zero as $r \to \infty$ and its derivative (defined by (16) – (18) with $i = 2$). We designate by $\Phi_0(E)$ a column composed of the values that take the "left" solution and its derivative when $a_L = 1$ (13) at the point $r = \hat{r}$ at some given E, and by $\Omega_0(E)$ - a column composed of the "right" solution and its derivative when $C_2 = 1$. We define a matrix

$$A(E) = \left(\Phi_0(E), -\Omega_0(E)\right).$$

To complete the matching it is necessary to ensure compliance with the following equation:

$$A(E)\chi(E) = 0, \; \chi(E) = \begin{pmatrix} a_1(E) \\ C_2(E) \end{pmatrix}. \tag{20}$$

Thus the procedure of calculating some eigenvalue $E = E_0$ is reduced to the numerical solution of the equation

$$\det A(E) = 0 \tag{21}$$

Then, after finding the eigenvalue E_0 and using (20), (19) one determines values of constants $C_2(E_0)$ and $a_l(E_0)$ and thus completely determines eigenfunction and its derivative on $(0, \infty)$.

In order to estimate the accuracy of the computations the energies and wavefunctions of a few lowest bound states of a hydrogen atom were calculated. In this case exact analytical solutions of the problem are well-known (see e.g. [5], [6]). Eigen energies equal: $E_n = -\frac{1}{n^2}, n = 1,..$ Eigenfunctions (radial wavefunctions) of two lowest states with $L = 0$ are of the form: $R_{10} = 2e^{-r}$, $R_{20} = \frac{1}{\sqrt{2}} e^{-r/2}(1 - r/2)$ (the first index is the principal quantum number n, the second is L). Calculated values are close to exact ones with high accuracy. In particular, in case of above mentioned states 14 significant digits in calculated eigenvalues and 12 in the eigenfunctions coincide with the exact ones.

Eigenvalue problem in the case of a finite interval.

In this case the eigenvalue problem for Eq. (11) on a finite interval $r \in [0, r_0]$ is in the following: one should find such value of the energy E that the solution $R_L(r)$ is finite

at $r = 0$ and $R_L(r = r_0) = 0$, one should find also the wavefunction corresponding to this value of E and normalized by the condition:

$$\int_0^{r_0} R_L^2(r) r^2 \, dr = 1 \tag{22}$$

Note that the problem (in the simplest model) about states of a hydrogen-like donor impurity, located in the center of a semiconductor spherical quantum dot of the radius r_0 (see e.g. [7]) is reduced to this one.

The problem should be solved numerically since analytical solutions can be found only in the cases when the value r_0 coincides with the position of a node of some wavefunction of the problem at the semi-infinite interval [7]. In the present case the problem of finding of eigenvalues is reduced to the numerical solving of the equation

$$R_{nL}^R(r = r_0, E) = 0, \tag{23}$$

where $R_{nL}^R(r, E)$ is the regular solution (12). Note that index n in this notation corresponds to the one in the notation of the solution of the problem at semi-infinite interval (i.e. when $r_0 \to \infty$). For definiteness we set $a_L = 1$ in (12). After finding some eigenvalue $E = E_0$ and implementation of integration (22) one has an expression (12) with $a_L = 1/\sqrt{Q}$ for a normalized solution, where

$$Q = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{a_n a_m}{(n + m + 3)} r_0^{n+m+3}. \tag{24}$$

Some results of calculations are demonstrated in Table 1. Here indices in the notation of the energy $E = E_{nl}$ correspond to those in the notation $R_{nl}(r)$.

Table 1: The dependence of the energies of the lowest three Coulomb states of the radius r_0

r_0	$E_{1,0}$	$E_{2,0}$	$E_{2,1}$
∞	–1	–0.25	–0.25
15	–0.9999999998	–0.2490	–0.2495
10	–0.999998	–0.2256	–0.2377
9	–0.999991	–0.2057	–0.2275
8	–0.99995	–0.1695	–0.2089
7	–0.9997	–0.1025	–0.1750
6	–0.9986	0.0255	–0.1111
5	–0.9928	0.2825	0.01520
4	–0.9665	0.8405	0.2871
3	–0.8479	2.223	0.9625
2	–0.2500	6.655	3.152
1, 8	0.06510	8.622	4.131
1, 6	0.5426	11.42	5.530
1, 4	1.294	15.59	7.614
1, 2	2.539	22.12	10.89
1	4.748	33.14	16.45

In particular it can be seen from the table that at finite r_0 energy level is no longer corresponds to the number n (principal quantum number): accidental (Coulomb) degeneracy of the states with $n = 2$, $L = 0, 1$ is removed.

As it was mentioned above the exact analytical solution can be found in the case when the value of r_0 coincides with the position of a node of some wavefunction of the problem at the semi-infinite interval. It can be seen from the table that at $r_0 = 2$ the computed lowest eigenvalue (ground state energy) equals $E_{10} = -0.25$ (with high accuracy, i.e. 12 zeroes after 5). To this value corresponds the solution $R_{21}(r) = Ce^{-r/2}(1 - r/2)$ of the problem at the semi-infinite interval, which has a node at $r = 2$. It means that this function is the eigenfunction of the problem on the finite interval which is normalized according to (22) if we set $C = 1/\sqrt{Q}$, where $Q = 2 - 14e^{-2}$. One can estimate the accuracy of the method in particular comparing the value of Q computed using Eq. (24): $Q = 0.105306034687423$, and using exact formula: $Q = 2 - 14e^{-2} = 0.105306034687422$. 14 significant digits in computed values of the eigenfunction coincide with the exact ones at all $0 < r < 2$.

Eigenvalue problem in the case of the hard core potential with a Coulomb tail.

Models that use the hard core potential are considered in various applications, and methods of solving problems of quantum mechanics in the presence of this potential are of special interest (see e.g. [8]). A model of the hard core potential with a Coulomb tail may be useful to describe the shallow states of the bound multiexciton complexes in semiconductors.

The following eigenvalue problem for Eq. (11) is considered: one should find such value of the energy E: $E < 0$ that the solution $R_L(r) = 0$ at $r \le r_{HC}$ (r_{HC} is a radius of the hard core potential) and $R_L(r) \to 0$ at $r \to \infty$, one should find also the wavefunction corresponding to this eigenvalue and normalized by the condition:

$$\int_{r_{HC}}^{\infty} R_L^2(r) r^2 \, dr = 1. \tag{25}$$

To solve this problem it is necessary to find the coefficient $M = M(E)$ in a linear combination of regular (12) and irregular (14) solutions for which the following condition is satisfied:

$$R_L(r = r_{HC}) = R_L^R(r = r_{HC}) + M(E) R_L^I(r = r_{HC}) = 0. \tag{26}$$

Then it is necessary to perform matching of a function $f_L(r) = rR_L(r)$, where $R_L(r)$ is the "left" solution, and its derivative with the "right" solution and its derivative (see (20)) at some intermediate point $r = \hat{r}$, $r_{HC} < \hat{r} < \infty$, then calculate an eigenvalue by the numerical solution of Eq. (21) and find the wavefunction, given the condition (25).

Some results of the calculations are presented in Figures 1 and 2.

4. COULOMB HOLE STATES

Coulomb hole states, such as the states of shallow acceptors or excitons in semiconductors with degenerate valence bands, are described by the Luttinger Hamiltonian [9]. Within the so-called spherical approximation [10] Luttinger Hamiltonian can be written as [10, 11]

$$H = p^2 - \mu\left(P^{(2)} \cdot J^{(2)}\right) + \frac{2}{r}. \tag{27}$$

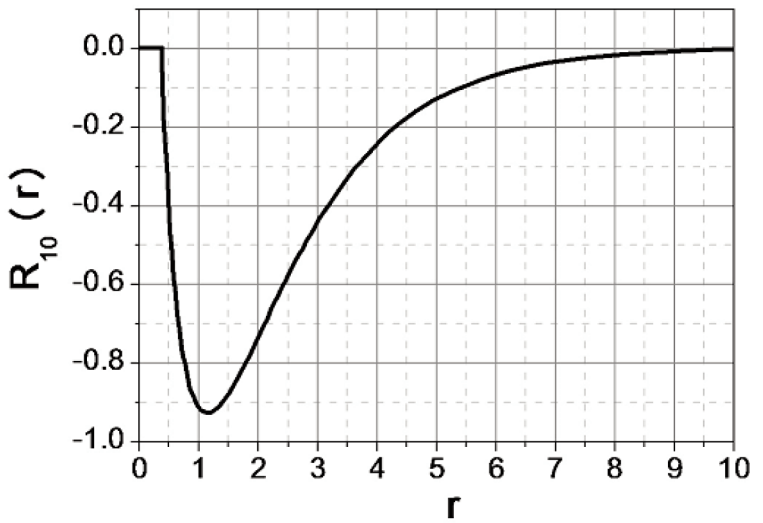

Figure 1: The wavefunction of the ground state in the case of the radius of the hard core potential $r_{HC} = 0.4$ ($L = 0$, $E = -0.5320$)

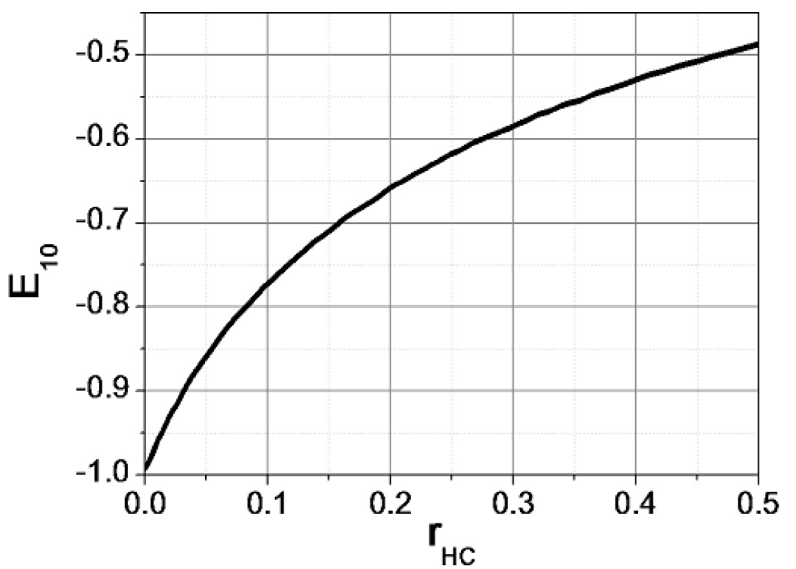

Figure 2: Dependence of the ground state energy of the radius of the hard core potential

Here $\hbar \boldsymbol{p}$ is the momentum operator; P^2 and J^2 are irreducible spherical tensor operators of the second rank [1] derived from the components of $\boldsymbol{p}$ and vector $\boldsymbol{J}$ representing the pseudospin angular momentum with $J = \frac{3}{2}$; $\mu = (6\gamma_3 + 4\gamma_2)/5\gamma_1$, where γ_i are empirical constants – Luttinger parameters of the valence band [9]; the energy and distances are measured in units of $R_a = m_0 e^4 / 2\hbar^2 \kappa^2 \gamma_1$ and $a = \hbar^2 \kappa \gamma_1 / m_0 e^2$ respectively, m_0 is the mass

of a free electron, $\varkappa$ is the static dielectric constant. Hamiltonian (28) is spherically symmetric in the coupled orbital and spin spaces and the total angular momentum $\boldsymbol{F} = \boldsymbol{L} + \boldsymbol{J}$ is a constant of motion. Wavefunctions can be written as [11]:

$$\Psi = r^{-1}\left\{(\beta f_h + f_l)\left|LJFF_z\right\rangle + (f_h - \beta f_l)\left|L+2, JFF_z\right\rangle\right\},$$

where $|LJFF_Z\rangle$ are functions in the *L-J* coupling scheme [1, 10], $\beta = 3^{L-F+1}\left(\dfrac{F+3/2}{F-1/2}\right)^{1/2}$.

The functions $f_h(r)$, $f_l(r)$ are expressed using the components of a solution of Eq. (3) $R = \begin{pmatrix} R_L \\ R_{L+2} \end{pmatrix} : f_h = (1+\beta^2)^{-1} r\cdot(\beta R_L + R_{L+2}), f_l = (1+\beta^2) r\cdot(R_L - \beta R_{L+2})$. Eq. (3) is reduced to a set of systems of equations of the same form ($n = 2$), with $f = \begin{pmatrix} f_h \\ f_l \end{pmatrix}$ instead of R, with diagonal matrices w, q_1, q_2: w = diag $(1 - \mu, 1 + \mu)$, $q_1 = 2$, $q_2 =$ E and with an anti-diagonal. matrix p_0. Explicit expressions for the matrices p_0 and q_0 in (3) are presented in [11]. Each system of equations (3) and each state corresponds to a certain value of the total angular momentum F (half-integer) and parity $P = (-1)^L$. Note that in the present case Eq. (3) describes a coupling of states of two particles with different masses, i.e. $1/(1 - \mu)$ (heavy hole) and $1/(1 - \mu)$ (light hole), by the Coulomb potential.

Two regular at $r = 0$ exact solutions of (3) ("left" solutions) are of the form

$$f^{(1)} = r^{\rho_1}\sum_{k=0}^{\infty} f_k^{(1)} r^k, \quad f^{(2)} = r^{\rho_2}\sum_{k=0}^{\infty} f_k^{(2)} r^k + K f^{(1)} \ln r, \tag{28}$$

where $\rho_1 = L + 3$, $\rho_2 = L + 1$ and recurrent sequences f_k^i and a constant K are found from the recurrent relations:

$$\begin{cases} \Gamma_0(\rho_1) f_0^{(1)} = 0 \\ \Gamma_k(\rho_1) f_k^{(1)} + q_1 f_{k-1}^{(1)} + q_2 f_{k-2}^{(1)} = 0 \end{cases}, \mathrm{k} = 1, 2, \ldots \ (fn = 0, n < 0)$$

$$\begin{cases} \Gamma_0(\rho_2) f_0^2 = 0 \\ \Gamma_1(\rho_2) f_1^{(2)} + q_1 f_0^2 = 0 \\ \Gamma_k(\rho_2) f_k^{(2)} + q_1 f_{k-1}^{(2)} + q_2 f_{k-2}^{(2)} + K[2(\rho_2 + k) + p_0 - 1] f_{k-\rho_1+\rho_2}^{(1)} = 0 \end{cases}, k = 2, 3, \ldots \tag{29}$$

Here $\Gamma_k(\rho)$ is a sequence of the matrices:

$$\Gamma_k(\rho) = (k+\rho)(k+\rho-1) + p_0(k+\rho) + q_0, k = 0, 1, \ldots$$

For completeness, we present also the expression for the two remaining irregular solutions of the fundamental system of solutions:

$$f^{(3)} = r^{\rho_3}\sum_{k=0}^{\infty} f_k^{(3)} r^k + f^{(2)} \ln r - K f^{(1)} \frac{\ln^2 r}{2},$$

$$f^{(4)} = r^{\rho_4} \sum_{k=0}^{\infty} f_k^{(4)} r^k + f^{(3)} \ln r - f^{(2)} \frac{\ln^2 r}{2} + K f^{(1)} \frac{\ln^3 r}{6} \cdot$$

To derive all "right" solutions, i.e. asymptotic expansions of solutions at $r \to \infty$ we use the method of Section 2 and reduce (3) to a system of 4 first-order equations (8) using the substitution

$$\begin{pmatrix} f \\ \dfrac{df}{dr} \end{pmatrix} = S \cdot Z, \text{ where } S = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ \lambda_h & -\lambda_h & 0 & 0 \\ 0 & 0 & \lambda_l & -\lambda_l \end{pmatrix}, \lambda_{h,l} = \left(\frac{-E}{1 \mp \mu} \right)^{1/2} \tag{30}$$

B_0 in (8) is a diagonal matrix: $B_0 = \text{diag}\,(\lambda_h, -\lambda_h, \lambda_l, -\lambda_l)$, and the asymptotic expansion of Z is

$$Z(r) \sim \sum_{k=0}^{\infty} \frac{R_k}{r^k} \exp\left(B_0 r + D_1 \ln r + \sum_{k=2}^{\infty} D_k \frac{r^{k-1}}{1-k} \right) \cdot C. \tag{31}$$

Here C is an arbitrary column of 4 constant elements. Recurrent sequences R_k and D_k are given by the recurrent relations (10).

Derived expressions (28–31) determine "left" solutions of Eq. (3) and all four "right" solutions. As follows from the results of [3], power series in the expressions for $f^{(1)}, f^{(2)}, f^{(3)}$ and $f^{(4)}$ converges uniformly in the whole interval $(0, \infty)$ and these solutions form a fundamental matrix of solutions of Eq. (3).

In order to solve the eigenvalue problem it is necessary to perform matching at some intermediate point $r = \hat{r}, 0 < \hat{r} < \infty$ of a linear combination of two regular "left" solutions (28) and their derivatives with a linear combination of two "right" solutions that tend to zero as $r \to \infty$ and their derivatives, i.e. those solutions (30), (31) that correspond to the eigenvalues $-\lambda_h$ and $-\lambda_l$ of the matrix B_0. Using the condition of non-trivial consistency of the resulting system of linear homogeneous algebraic equations we find the energy levels (see (21)). Then we compute the normalized wavefunctions as in subsection 3.2. In this case the normalization condition has the form: $(\beta^2 + 1) \int_{r=0}^{\infty} (f_h^2 + f_l^2)\, dr = 1$.

In order to calculate wavefunctions of the continuous spectrum of the Hamiltonian (27) it is necessary to match a linear combination of two regular "left" solutions (28) (and the derivatives) with a linear combination of four "right" solutions (30), (31) ($E > 0$ in this case) at some intermediate point $r = \hat{r}, 0 < \hat{r} < \infty$. We choose two linear combinations of "right" solutions that give the heavy-hole and the light-hole radial in-solutions, whose asymptotic behaviour at $r \to \infty$ are

$$f_h(r) \sim \frac{i^{-L}}{2ik_h} \begin{pmatrix} (-1)^{L+1} e^{-ik_h r} + S_{hh} e^{ik_h r} \\ \left(\dfrac{(1-\mu)k_h}{(1+\mu)k_l} \right)^{\frac{1}{2}} S_{lh} e^{ik_l r} \end{pmatrix}, \; f_l(r) \sim \frac{i^{-L}}{2ik_l} \begin{pmatrix} \left(\dfrac{(1+\mu)k_l}{(1-\mu)k_h} \right)^{\frac{1}{2}} S_{hl} e^{ik_h r} \\ (-1)^{L+1} e^{-ik_l r} + S_{ll} e^{ik_l r} \end{pmatrix} \tag{32}$$

(we have omitted the logarithmic phase in exponents for brevity). Here $k_{h,l} = (E/(1 \mp \mu))^{1/2}$, $S_{\alpha,\beta}$ are elements of the partial S-matrix corresponding to a given value F of the total angular momentum and parity P. This matrix is symmetric and unitary.

In the present study the method is used to calculate energy and wavefunction of the ground state (F = 3/2, P = 1) and the wavefunctions of states of the continuous spectrum (with F = 1/2, 3/2, 5/2 and P = –1) as functions of the energy $E > 0$ for different values of μ, i.e. for a shallow acceptor impurity in different semiconductors. The dipole optical transitions of a hole from the ground state of an acceptor are allowed only to these states of the continuous spectrum and thus it is possible to calculate the spectra of the photoionization cross-section of shallow acceptors in semiconductors. The choice of the wavefunctions of the continuous spectrum, asymptotic behaviour of which is described by (32) and corresponds to the scattering problem, makes it possible to calculate the partial photoionization cross sections that correspond to "creation" of separately a heavy and light hole in the valence band. Using the calculated values of energies and wave functions, as well as the explicit expression for the photoionization cross section of a shallow acceptor, see [11], we calculated the spectra of the photoionization cross section for shallow acceptors in various semiconductors (i.e. for different values of μ). Results of calculations are presented in Figures 3 and 4. In the caption of Figure 3 E_{GS} is the calculated values of the energy of the ground state (values of material parameters see in [10]). The value μ = 0.236 corresponds to the direct exciton in GaAs. Note that as is evident from Figures 3 and 4 for values of μ close to 1, i.e., for large values of the effective mass of the heavy hole, spectrum of photoionization cross section differs greatly from this spectrum for hydrogen-like atom (μ = 0).

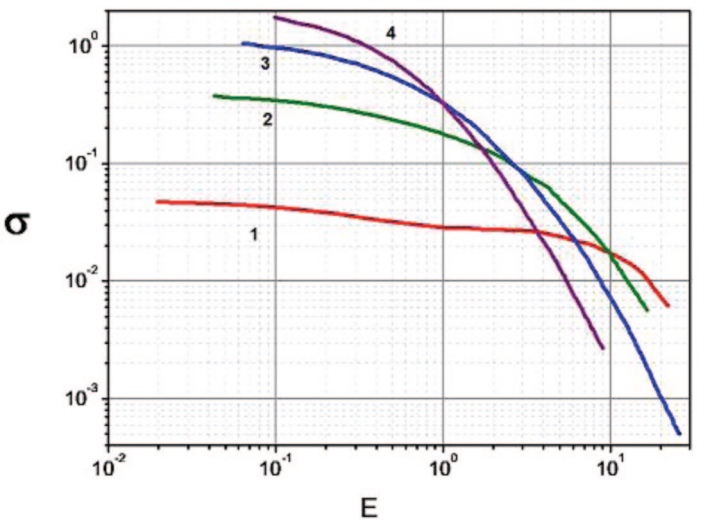

Figure 3: Spectra of the photoionization cross section of shallow acceptors in semiconductors. σ is in units of $\sigma_0 = \frac{4\pi e^2}{3\hbar c k^{1/2}} a^2$. 1 – μ = 0.907 (InAs, E_{GS} = –5.098), 2 – μ = 0.766 (Ge, E_{GS} = –2.264), 3 – μ = 0.6 (ZnTe, E_{GS} = –1.503), 4 – μ = 0.236 (E_{GS} = –1.053).

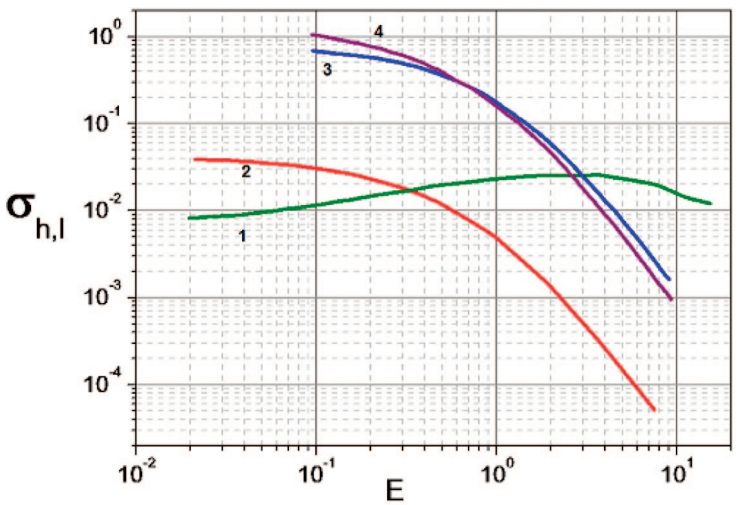

Figure 4: Partial spectra of the photoionization cross section. 1 – σ_1, 2 – σ_h (μ = 0.907); 3 – σ_1, 4 – σ_h(μ = 0.236). Units are the same as in Figure 3.

5. CONCLUSIONS

A numerical-analytical method with some applications were demonstrated for accurate solving the Schrödinger equation in those cases when it is reducible to a system of n coupled ordinary differential equations with singular points. Fundamental system of solutions is constructed as algebraic combinations of power series, power functions and logarithmic function in the neighbourhood of the regular singularity ("left" exact solutions), and as asymptotic expansions of solutions in the neighbourhood of the irregular singularity ("right" solutions). In the framework of the method, in order to solve the eigenvalue problem and the scattering problem it is necessary to perform matching of a proper linear combination of "left" solutions and their derivatives with a proper linear combination of "right" solutions and their derivatives at some intermediate point $r = \hat{r}$, $0 < \hat{r} < \infty$. The method is based on the calculation of recurrent sequences of the constant matrices of coefficients in the power series and in the inverse power series in the asymptotic expansions using derived recurrent relations, that makes possible to calculate solutions at any point r, $0 < r < \infty$ using only the simple algebraic computations without usage of any conventional step-by-step or variational procedures. In turn, it makes possible to solve accurately both the eigenvalue problem and the scattering problem and to derive analytical expressions for the wavefunctions. The method is used for calculations of states of the discrete spectrum of a hydrogen-like atom and of a shallow acceptor impurity in semiconductors, states of the continuous spectrum of an acceptor in the statement corresponding to the scattering problem, and the spectra of the photoionization cross section of shallow acceptors in various semiconductors. In conclusion we note that, as is obvious, use of recurrent sequences of coefficients in the power series makes it possible to efficiently and accurately solve the Schrödinger equation in cases where it is reduced to the ODE without regular singular point (see, e.g., [12]–[15]).

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