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Accurate solutions of coupled radial Schrödinger equations

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Abstract. A constructive numerical-analytical method of solving coupled Schrödinger equations is presented when a Hamiltonian is a quadratic form of the momentum and contains a matrix potential energy term, which is, in particular, a superposition of Coulomb and polynomial potentials. A technique for solving coupled radial Schrödinger equations is developed. The method is based on the matching of exact solutions, constructed as algebraic combinations of power series, power functions, and a logarithmic function in the neighbourhood of regular singularity $r = 0$, and of the asymptotic expansions of solutions in the neighbourhood of irregular singularity $r = \infty$. This method of matching allows us to calculate accurately eigenvalues with corresponding wavefunctions of a discrete spectrum, in(out)-solutions and an S-matrix for a given value of energy from a continuous spectrum, and resonance states. Wavefunctions derived are expressed in analytical form. The method is applied to solving the Schrödinger equation in the case of a matrix Hamiltonian with Coulomb potential.

1. Introduction

In some quantum mechanical problems which are considered in solid-state physics, atomic and nuclear physics, etc, Hamiltonians are differential-matrix operators. The matrix nature of a radial Hamiltonian ensues from two reasons: either (1) the initial three-dimensional Hamiltonian itself is matrix-valued (see e.g. [1–3]), or (2) the one is a scalar operator but, for lack of spherical symmetry, there originates a system of coupled radial equations (e.g. [4–6]). In this paper we present a constructive numerical-analytical approach to solving eigenvalue–eigenfunction problems for systems of coupled radial equations without resorting to any finite-difference procedure or to the variational method. The gist of this method of matching is as follows:

(1) in the neighbourhood of $r = 0$ (regular singularity) the solutions, obeying a boundary condition at $r = 0$, are represented in terms of certain algebraic combinations of power series, power functions, and logarithmic function ('left-hand' solutions);
(2) in the neighbourhood of $r = \infty$ (irregular singularity)—in terms of certain asymptotic expansions obeying a boundary condition at $r = \infty$ ('right-hand' solutions);
(3) at some intermediate point $r = \hat{r}$ these solutions are matched to form the eigenfunctions.

Matching of solutions can always be accomplished with any given accuracy by the proper choice of matching point $\hat{r}$. Formally, this can be expressed in the following way: let $X = X(\hat{r})$ denote a mathematical object to be calculated (eigenfunction, energy level, S-matrix, its poles, etc), then

$$X_{\text{exact}} = \lim X(\hat{r}) \qquad \hat{r} \to \infty.$$

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In practical calculations, for the error of X to be estimated, it is helpful to use variations of the matching point $\hat{r} \to \hat{r} + \delta\hat{r}$.

The method of matching seems to be the most effective procedure in solving one-dimensional eigenvalue–eigenfunction problems because it takes into account the analytical structure of differential-matrix operator (in our case a radial Hamiltonian) as outright as merely possible.

The remainder of this paper is organized as follows: in section 2 we give the reduction of the Schrödinger equation in $\mathbb{R}^3$ to a coupled set of radial equations; in section 3 the analytical solutions of these equations in the neighbourhood of the regular singularity $r = 0$ are constructed; in section 4 a method of derivation of the asymptotic expansions of the solutions in the neighbourhood of the irregular singularity $r = \infty$ is presented; in section 5 a method of matching is described, enabling the singular eigenvalue–eigenfunction problems to be solved; in section 6 an example of the application of this method is presented, and finally, in section 7 we summarize results and make some general statements on extensions of the method to other problems.

2. Reduction to coupled radial Schrödinger equations

We consider the Schrödinger equation

$$H\Psi(\boldsymbol{r}) = E\Psi(\boldsymbol{r}) \tag{1}$$

where the Hamiltonian H is an $N \times N$ matrix operator and Ψ is an N-component wavefunction. Hamiltonian H is supposed to be a quadratic form of the momentum. In this case H can be presented as follows:

$$H = A\boldsymbol{p}^2 + \sum_{m=-2}^{2} B_m P_m^{(2)} + V(\boldsymbol{r}) \tag{2}$$

where $\boldsymbol{p} = -\mathrm{i}\nabla$ is a momentum operator (we set here $\overline{h} = 1$), $P_m^{(2)}$ are the components of the irreducible spherical tensor operator of the second rank composed in the usual way [7] of the components of the 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. The potential energy term is supposed to be, generally speaking, an $N \times N$ matrix function of the form

$$V(\boldsymbol{r}) = \sum_{k=-1}^{v} V_k(\theta, \varphi, \boldsymbol{L}) r^k \qquad \boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$$

(the case of potential functions of much more general form is considered below, in section 7, see also remark 2 in section 5).

We represent N-column wavefunction $\Psi(\boldsymbol{r})$ in the following form:

$$\Psi(\boldsymbol{r}) = \sum_{l=0}^{\infty} \sum_{\tau=1} \Xi_{l\tau}(\theta, \varphi) R_{l\tau}(r) \tag{3}$$

where $R_{l\tau}(r)$ are radial wavefunctions, l is the quantum number of the orbital angular momentum operator $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$, τ is a set of quantum numbers of some operators chosen in accordance with a Hamiltonian symmetry; $\Xi_{l\tau}(\theta, \varphi)$ is a complete orthonormalized set of the N-components functions of the space $L^2(S^2)^N$, and

$$\boldsymbol{L}^2 \Xi_{l\tau}(\theta, \varphi) = l(l+1)\Xi_{l\tau}(\theta, \varphi).$$

'Multiplying' equation (1) from the left by $\int_{S^2} \mathrm{d}\Omega\, \Xi^*_{l'\tau'}(\theta,\varphi)$ (the asterisk means the Hermitian conjugation) we obtain the following system of an infinite number of coupled radial equations:

$$\left(\mathcal{W}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \mathcal{A}r^{-1}\frac{\mathrm{d}}{\mathrm{d}r} + \sum_{k=-2}^{v}\mathcal{B}_k r^k\right)R(r) = 0 \tag{4}$$

where $\mathcal{W}$, $\mathcal{A}$, and $\mathcal{B}_k$ are constant $\infty \times \infty$ matrices, $R = (R_{l\tau})$ is a ∞-dimensional column-function.

In the case of a sufficiently high symmetry of the Hamiltonian, the infinite system (4) is reduced to the infinite set, with each element of this set being a finite-dimensional coupled system of ordinary differential equations (the simplest example is the radial equations for a hydrogen atom, see also section 6). In cases when it is impossible to reduce equation (4) to finite-order systems using the symmetry arguments, one truncates this infinite system using the consideration of the accuracy, i.e. the invariability of results (in limits of given accuracy) with the increase of a number of equations in the truncated system (see e.g. [8]). So the problem of solving equation (4) is reduced to that of solving a system of n coupled radial equations of the following form (henceforth we use functions $F(r) = rR(r)$ instead of $R(r)$):

$$\left(r^2 w\frac{\mathrm{d}^2}{\mathrm{d}r^2} + r p_0\frac{\mathrm{d}}{\mathrm{d}r} + \sum_{k=0}^{M} q_k r^k\right)F(r) = 0 \qquad r > 0 \tag{5}$$

where $M = \max\{0, v\} + 2$, $F(r)$ is the n-component radial function and w, p_0, and q_k are constant $n \times n$ matrices. The matrix $q_2 = q_2(E)$, where E is the energy. The hermiticity of the Hamiltonian imposes the following conditions on these matrices: $w = w^* > 0$ and this matrix is proportional to the inverse masses matrix; $p_0 = -p_0^*$; $q_0 = q_0^* + p_0^*$; $q_k = q_k^*$, $k \geqslant 1$. Besides, there are some boundary conditions imposed on the solutions at $r = 0, \infty$ (see section 5).

3. Solutions. Neighbourhood of the regular singularity $r = 0$

Let us reduce the n-component equation of the second order (5) to the $2n$-component equation of the first order for the function $\chi(r) = \binom{F(r)}{r\,\mathrm{d}F/\mathrm{d}r}$:

$$\left(r\frac{\mathrm{d}}{\mathrm{d}r} - \sum_{k=0}^{M}\alpha_k\right)\chi(r) = 0 \tag{6}$$

where

$$\alpha_0 = \begin{pmatrix} 0 & 1 \\ -w^{-1}q_0 & (1 - w^{-1}p_0) \end{pmatrix} \qquad \alpha_k = \begin{pmatrix} 0 & 0 \\ -w^{-1}q_k & 0 \end{pmatrix} \qquad k \geqslant 1.$$

The Jordan structure of the leading matrix α_0 determines the structure of solutions of equation (6) (and hence of the radial Schrödinger equation (5)) and their behaviour in the neighbourhood of the regular singular point $r = 0$ (see [9]). In appendix A we show that in the case of Hamiltonians of the form (2), matrix α_0 in the corresponding radial equation (6) is diagonalizable, its eigenvalues are integers and we explicitly find these eigenvalues.

Let:

$$d \equiv 2n$$
$$A_0 = T_0^{-1}\alpha_0 T_0 = \mathrm{diag}(\sigma_1, \ldots, \sigma_{2n}) \qquad \sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_{2n} = \sigma_d$$
$$A_k = T_0^{-1}\alpha_k T_0 \qquad k = 1, \ldots, M$$
$$y = T_0^{-1}\chi.$$

Then

$$r\frac{\mathrm{d}y}{\mathrm{d}r} = \left(A_0 + \sum_{k=1}^{M} A_k r^k\right) y. \tag{7}$$

Let us denote the values of σ_k which are not equal to each other by λ_p and their multiplicities by d_p, $p = 0, \ldots, g$, $\sum_p d_p = d$, i.e.

$$A_0 = \mathrm{diag}(\underbrace{\lambda_0, \ldots, \lambda_0}_{d_0}, \ldots, \underbrace{\lambda_g, \ldots, \lambda_g}_{d_g}).$$

Our goal is to construct all $2n$ linearly independent solutions of equation (7) corresponding to the values of λ_p.

Let $u(r)$ be d-component vector functions of the following form:

$$u(r) = r^{\lambda} \sum_{k=0}^{\infty} u_k r^k$$

where $\{u_k\}$ are d-component constant vectors. It is not difficult to show (see [9]) that if the function

$$y^{(s)}(r) = u^{(s)} + s(\ln r)u^{(s-1)}(r) + \cdots + (\ln r)^s u^{(0)}(r) \equiv \sum_{p=0}^{s} \binom{s}{p} (\ln r)^p u^{(s-p)}(r)$$

is a solution of equation (7), then the following functions are also solutions of (7) (here the index in brackets labels functions and does not designate some derivative):

$$y^{(k)}(r) = \sum_{p=0}^{k} \binom{k}{p} (\ln r)^p u^{(k-p)}(r) \qquad s \geqslant k \geqslant 0.$$

It is convenient for further considerations to introduce a linear operator $\mathcal{L}_s$, $s \geqslant 0$ which acts by definition in the following way:

$$\mathcal{L}_s\{(\ln r)^p u(r)\} = \frac{(s+1)}{(p+1)} (\ln r)^{p+1} u(r). \tag{8}$$

Then

$$y^{(s)}(r) = u^{(s)}(r) + \mathcal{L}_{s-1} y^{(s-1)}(r).$$

Designating by $y^{(s,i)}(r)$, $i = 1, \ldots, d_s$ solutions of equation (7) corresponding to an eigenvalue λ_s, we seek them in the form

$$y^{(s,i)}(r) = u^{(s,i)}(r) + \sum_{p=0}^{s-1} \mathcal{L}_p \sum_{j=1}^{d_p} u^{(p,j)}(r) C_{p,j}^{s,i} \qquad s = 0, \ldots, g \tag{9}$$

where

$$u^{(s,i)}(r) = r^{\lambda_g} \sum_{k=0}^{\infty} u_k^{(s,i)} r^k \qquad u_k^{(s,i)} \equiv 0 \qquad k < \lambda_s - \lambda_g$$

with unknown vectors $u_k^{(s,i)}$ and coefficients $C_{p,j}^{s,i}$ which are to be determined. Relations (9) can be presented in a matrix form, namely

$$Y^s(r) = U^s(r) + \sum_{p=0}^{s-1} \mathcal{L}_p Y^p(r) C_p^s \tag{10}$$

$$U^s(r) = r^{\lambda_g} \sum_{k=0}^{\infty} U_k^s r^k \tag{11}$$

where $Y^s(r)$ and $U^s(r)$ are $d \times d_s$ matrix functions, C_p^s, $0 \leqslant p < s$ and U_k^s are $d_p \times d_s$ and $d \times d_s$ constant matrices, respectively. Note that using the definition of the operator $\mathcal{L}_p$ we can obtain an expression for the functions $Y^s(r)$ containing only functions $U^p(r)$, $0 \leqslant p \leqslant s$ and matrices C_q^p. Really, as follows from (10)

$$Y^s(r) = U^s(r) + \sum_{p=1}^{s} \sum_{k=1}^{p} \tilde{\sum_{q_i}} \mathcal{L}_{q_k} \mathcal{L}_{q_{k-1}} \dots \mathcal{L}_{q_2} \mathcal{L}_{q_1} U^{s-p}(r) C_{q_1}^{q_2} \dots C_{q_{k-1}}^{q_k} C_{q_k}^{s} \tag{12}$$

where the sum with the 'tilde' means the summation over such $q_1, \dots, q_k$ that $s - p = q_1 < q_2 < \dots < q_k \leqslant s - 1$, and at $s = 0$ we have $Y^0(r) = U^0(r)$. Finally, using the definition (8) we obtain

$$Y^s(r) = U^s(r) + \sum_{p=1}^{s} U^{s-p}(r) \sum_{k=1}^{p} \tilde{\sum_{q_i}} \frac{(q_k + 1)(q_{k-1} + 1) \dots (q_1 + 1)}{k!} (\ln r)^k \times C_{q_1}^{q_2} \dots C_{q_{k-1}}^{q_k} C_{q_k}^{s}. \tag{13}$$

Substituting (13) into equation (7) we obtain the following recurrence relations:

$$(k + \lambda_g - A_0) U_k^p = \sum_{l=1}^{\min(k,M)} A_l U_{k-l}^p - \sum_{q=1}^{p} (p + 1 - q) U_k^{p-q} C_{p-q}^p \tag{14}$$

where $k = \lambda_p - \lambda_g, \dots, N$. As follows from the results of [9], power series in the expression (11) for the functions $U^r(r)$ converges uniformly in the whole interval $(0, \infty)$ and each column of the $d \times d_s$-dimensional matrix function $Y^s(r)$ is a linear-independent solution $y(r)$ of equation (7).

Thus 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 of terms in the power series in (11). The value of N is limited only by the computer resources and round-off errors in the process of computations.

The procedure of the calculation of constant matrices U_k^p and C_s^p, which completes the calculation of the solutions $Y^s(r)$, is described in appendix B.

It is obvious that $(d_0 + \dots + d_g)$ solutions $Y^0(r), \dots Y^g(r)$ of the equation (7) thus obtained are linearly independent and the $2n$-order matrix of the solutions and derivatives of equation (5) assumes the following form (1_k is the unit $k \times k$-matrix):

$$\Phi(r) = \begin{pmatrix} 1_n & 0 \\ 0 & r^{-1} 1_n \end{pmatrix} T_0 (Y^0(r) \dots Y^g(r)).$$

4. Construction of solutions in the neighbourhood of an irregular singularity at $r = \infty$

In this section we describe a method enabling us to construct solutions of coupled radial Schrödinger equations (5) in the form of asymptotic expansions in the neighbourhood of an irregular singularity at $r = \infty$. We consider equation (5) for the function $F = rR$, supposing that the number $M > 0$ is even (without loss of generality, since in the opposite case one can make a substitution $r \to r^2$).

In order to derive asymptotic expansions of the solutions we reduce equation (5) to the first-order equations of the form

$$\frac{\mathrm{d}}{\mathrm{d}r} g^{\pm} \sim r^{\frac{M}{2}-1} (B_0^{\pm} + B_1^{\pm}/r + B_2^{\pm}/r^2 + \cdots) g^{\pm} \qquad r \to \infty \tag{15}$$

where $g(r) = T_\infty^{-1} F(r)$, and matrices $B_k^{\pm}$ and T_∞ should be found.

Let us introduce the differential-matrix operator:

$$\mathcal{D} \equiv \frac{\mathrm{d}^2}{\mathrm{d}r^2} + r^{-1}P(r)\frac{\mathrm{d}}{\mathrm{d}r} + r^{-2}Q(r)$$

where in the case of equation (5)

$$P(r) = w^{-1}p_0 = \text{const} \equiv P_0$$
$$Q(r) = w^{-1}(q_0 + q_{-1}r + \cdots + q_M r^M) \equiv Q_0 + \cdots + Q_M r^M.$$

We present it in the following form (factorization of the operator $\mathcal{D}$ [10]):

$$\mathcal{D} = \left[\frac{\mathrm{d}}{\mathrm{d}r} - \alpha(r)\right]\left[\frac{\mathrm{d}}{\mathrm{d}r} - \beta(r)\right]$$

where $\alpha(r)$, $\beta(r)$ are some $n \times n$ matrix functions to be found. It is easy to see that the following relations hold:

$$\frac{Q(r)}{r^2} = \alpha(r)\beta(r) - \frac{\mathrm{d}}{\mathrm{d}r}\beta(r)$$
$$\frac{P(r)}{r} = -[\alpha(r) + \beta(r)].$$

The matrix equation of the Riccati type for the function $\beta(r)$ follows from these equations, namely:

$$\frac{\mathrm{d}\beta}{\mathrm{d}r} + \left(\beta + \frac{P}{r}\right)\beta + \frac{Q}{r^2} = 0. \tag{16}$$

It is obvious that any solution of the equation

$$\frac{\mathrm{d}F(r)}{\mathrm{d}r} = \beta(r)F(r)$$

is a solution of equation (5). At first we find from equation (16) the asymptotic expansion of the function $\beta(r)$ as $r \to \infty$:

$$\beta(r) \sim r^{\frac{M}{2}-1}(\beta_0 + \beta_1/r + \beta_2/r^2 + \cdots). \tag{17}$$

Substitution of the expansion (17) in equation (16) yields recurrence relations for matrices β_k:

$$\sum_{l=0}^{k} \beta_l\beta_{k-l} + Q_{M-k} + (P_0 + M - 1 - k)\beta_{k-M/2} = 0 \qquad k = 0, 1, \ldots. \tag{18}$$

Henceforth we suppose that all real eigenvalues of the matrix Q_M are *nonzero* and *different*. Now we can determine such matrix T_∞ that

$$T_\infty^{-1}Q_M T_\infty = \mathrm{diag}(\varepsilon_1, \ldots, \varepsilon_n)$$
$$\varepsilon_1 < \varepsilon_2 < \cdots < \varepsilon_n \qquad \varepsilon_1, \ldots, \varepsilon_{n_-} < 0 \qquad \varepsilon_{n_-+1}, \ldots, \varepsilon_n > 0.$$

In order to resolve equation (18) with respect to β_k it is convenient to make the following substitution:

$$\beta_k \to B_k = T_\infty^{-1}\beta_k T_\infty \qquad Q_k \to \tilde{Q}_k = T_\infty^{-1}Q_k T_\infty \qquad P_0 \to \tilde{P}_0 = T_\infty^{-1}P_0 T_\infty.$$

Then, at $k = 0$ we obtain from equation (18)

$$B_0^2 = -\tilde{Q}_M = \mathrm{diag}(-\varepsilon_1, \ldots, -\varepsilon_n)$$

and we have two solutions for the matrix B_0 which we mark by the superscripts '+' or '−':

$$B_0^{\pm} = \pm\mathrm{diag}[(-\varepsilon_1)^{1/2}, \ldots, (-\varepsilon_n)^{1/2})]. \tag{19}$$

It is clear that there are n_- real and $n - n_-$ purely imaginary eigenvalues on the diagonal of the matrix $B_0^{\pm}$.

Choosing one of two signs of the root in (19), it is easy to calculate all matrices $B_k^{\pm}$, $k = 1, 2, \ldots$ from relations (18), namely

$$(B_k^{\pm})_{ij} = \frac{1}{[(B_0^{\pm})_{ii} + (B_0^{\pm})_{jj}]}\left[\tilde{Q}_{M-k} + (\tilde{P}_0 + M - 1 - k)B_{k-M/2}^{\pm} + \sum_{l=1}^{k-1} B_l^{\pm} B_{k-l}^{\pm}\right]_{ij}. \tag{20}$$

Now we have equation (15) for the function $g(r) = T_\infty^{-1}F(r)$, where the number $q+1 \equiv M/2$ is the rank of the singular point $r = \infty$ of equation (15), and explicit expressions (20) for matrices $(B_k^{\pm})_{ij}$ in it. Then, using results of [11], we derive asymptotic expansion of the fundamental $n \times n$ matrix $G^{\pm}(r)$ of solutions of the equation (15) as $r \to \infty$:

$$G^{\pm}(r) \sim (R_0^{\pm} + R_1^{\pm}/r + R_2^{\pm}/r^2 + \cdots) \times \exp\left[\sum_{j=0}^{q} D_j^{\pm}\frac{r^{q-j+1}}{q-j+1} + D_{q+1}^{\pm}\ln r\right.$$
$$\left. - D_{q+2}^{\pm}/r - D_{q+3}^{\pm}/2r^2 - D_{q+4}^{\pm}/3r^3 - \cdots\right]. \tag{21}$$

Each column of the matrix function $G^{\pm}(r)$ is a linear-independent solution $g^{\pm}(r)$ of the equation (15). Matrices $R_k^{\pm}$ and $D_k^{\pm}$, $k = 0, 1, 2, \ldots$, satisfy the following recurrence relations [11]:

$$D_0 R_k - R_k B_0 = \begin{cases} 0, & k = 0 \\ \displaystyle\sum_{l=0}^{k-1}(R_l B_{k-l} - D_{k-l}R_l) - (k-q-1)R_{k-q-1} & k = 1, 2, \ldots. \end{cases}$$

It is convenient to choose the following conditions:

$$D_0^{\pm} = B_0^{\pm} \qquad R_0^{\pm} = 1 \qquad D_k^{\pm} = \text{diag} \qquad (R_k^{\pm})_{ii} = 0 \qquad k = 1, 2, \ldots$$

then, for the diagonal matrices $D_k^{\pm}$ and matrices $R_k^{\pm}$ with diagonal elements which equal zero, we have

$$(D_k^{\pm})_{ii} = \left(B_k^{\pm} + \sum_{l=1}^{k-1} B_{k-l}^{\pm} R_l^{\pm}\right) \qquad k = 1, 2, \ldots \tag{22}$$

in particular, $(D_1^{\pm})_{ii} = (B_1^{\pm})_{ii}$ and

$$(R_k^{\pm})_{ij} = \frac{1}{[(B_0^{\pm})_{ii} - (B_0^{\pm})_{jj}]}\left[\sum_{l=0}^{k-1}(R_l^{\pm}D_{k-l}^{\pm} - B_{k-l}^{\pm}R_l^{\pm}) - (k-q-1)R_{k-q-1}^{\pm}\right]_{ij}$$
$$i \neq j \qquad k = 1, 2, \ldots. \tag{23}$$

Thus, using (21)–(23) we determine the fundamental $n \times 2n$ matrix of solutions of coupled radial Schrödinger equations (5) in the neighbourhood of the irregular singularity $r = \infty$:

$$T_\infty \cdot (G^{+}(r), G^{-}(r)).$$

Finally, the fundamental $2n \times 2n$ matrix of solutions of equation (5) and their derivatives (we obtain derivatives from the 'truncated' formula (15), multiplied from the left by the matrix T_∞) assumes the following form as $r \to \infty$:

$$\Phi_\infty(r) \sim (\Omega_\infty(r), \Omega_+(r), \Omega_0(r), \Omega_-(r)).$$

Here each column of Φ_∞ is composed of the functions and derivatives $\binom{F}{\mathrm{d}F/\mathrm{d}r}$ and we designate by Ω_∞, Ω_+, Ω_0, and Ω_- submatrices of the dimensions $2n \times n_-$, $2n \times n_+$, $2n \times n_-$ and $2n \times n_+$,

respectively ($n_- + n_+ = n$), whose columns contain the following factors:

$$\exp\left[\frac{r^{q+1}}{q+1}(+|\varepsilon_1|^{1/2}+\cdots\right],\ldots \qquad \exp\left[\frac{r^{q+1}}{q+1}(+|\varepsilon_{n_-}|^{1/2}+\cdots\right]$$
$$\exp\left[\frac{r^{q+1}}{q+1}(+\mathrm{i}|\varepsilon_{n_-+1}|^{1/2}+\cdots\right],\ldots \qquad \exp\left[\frac{r^{q+1}}{q+1}(+\mathrm{i}|\varepsilon_{n}|^{1/2}+\cdots\right]$$
$$\exp\left[\frac{r^{q+1}}{q+1}(-|\varepsilon_1|^{1/2}+\cdots\right],\ldots \qquad \exp\left[\frac{r^{q+1}}{q+1}(-|\varepsilon_{n_-}|^{1/2}+\cdots\right]$$
$$\exp\left[\frac{r^{q+1}}{q+1}(-\mathrm{i}|\varepsilon_{n_-+1}|^{1/2}+\cdots\right],\ldots \qquad \exp\left[\frac{r^{q+1}}{q+1}(-\mathrm{i}|\varepsilon_{n}|^{1/2}+\cdots\right].$$

The detailed structure of the submatrices is evident (see (21)).

Note that if matrices w, $p_0, q_0, \ldots, q_M$ are real (usually this is the case in applications) then it is easy to construct a real fundamental matrix $\Phi_\infty^{\mathrm{real}}(r)$ of solutions and derivatives. It has the following form as $r \to \infty$:

$$\Phi_\infty^{\mathrm{real}}(r) \sim (\mathrm{Re}\,\Omega_\infty(r), \mathrm{Re}\,\Omega_+(r), \mathrm{Re}\,\Omega_0(r), \mathrm{Im}\Omega_+(r)).$$

5. Matching of solutions. Singular eigenvalue problem

In this section we describe a method of matching of 'left-hand' and 'right-hand' solutions enabling a solution of singular eigenvalue problems for the systems of coupled radial Schrödinger equations.

Let us consider equation (5) for radial wavefunctions $F(r)$ with the following boundary conditions imposed:

($*$) $F(r) \to 0$ as $r \to 0$ (the conditions for $F(r)$ to be bounded as $r \to 0$ are also possible, see e.g. [12, 13]) and:
(a) as $r \to \infty$, $|F(r)|$ decreases faster than any function of the form $r^{-\rho}$, $\rho > 0$ or:
(b) as $r \to \infty$, $F(r)$ is bounded.

Let us designate by the D-set of the problem the set of all values of E, at which a nontrivial solution $F(r) = F(r; E)$ of equation (5) exists satisfying boundary conditions ($*$) and (a). In turn, we designate by the DC-set the set of all values of E at which a nontrivial solution $F(r; E)$ of equation (5) exists, satisfying conditions ($*$) and (b). At last we define the C-set: C-set$=$ DC-set$\backslash D$-set. In applications D- and C-sets are in fact the discrete and continuous spectra, respectively. By the term 'discrete spectrum' we mean isolated eigenvalues from the point spectrum. A somewhat different structure is implied by this term in the theory of operators [14]. Note, that these definitions are convenient from the computational point of view, but they are not mathematically rigorous (see e.g. [12]).

Remark 1. *Continuous spectrum is absent when $M > 2$, $\det q_M \neq 0$. More general boundary conditions are allowed at $r = \infty$, but we assume, as usually is the case in physical applications, that $q_M < 0$ at $M > 2$.*

Solving of the eigenvalue problem is based on the matching of local solutions, which were determined in the neighbourhoods of singular points $r = 0, \infty$.

Linearly independent 'left-hand' solutions of equation (5) and their derivatives compose some $2n \times 2n$ matrix $\Phi(r)$ at a point r. Solutions which behave correctly correspond to the first n_0 columns of $\Phi(r)$ (in fact, $n_0 = n$ but we write down n_0 for the sake of generality) and we denote this submatrix of the dimension $2n \times n_0$ by $\Phi_0(r)$. Suppose then that we have

computed with desired accuracy the series in the 'left-hand' solutions $\Phi_0(r)$ at some point $\hat{r} \in (0, \infty)$, and let $\hat{\Phi}_0 \equiv \Phi_0(\hat{r})$.

Linearly independent 'right-hand' solutions and their derivatives compose at a point r a $2n \times 2n$ matrix $\Phi_\infty(r)$ which has the following form as $r \to \infty$:

$$\Phi_\infty \sim (\Omega_\infty(r), \Omega_+(r), \Omega_0(r), \Omega_-(r))$$

where dimensions of the submatrices $\Omega_{\infty,+,0,-}$ are equal to $2n \times n_-$, $2n \times n_+$, $2n \times n_-$, and $2n \times n_+$, respectively (here n_-, n_+ are the numbers of negative and positive eigenvalues of the matrix $w^{-1}q_M$, $n = n_- + n_+$). The columns $\Omega_\infty(r)$ correspond to solutions which diverge exponentially and columns $\Omega_0(r)$ to exponentially decaying solutions as $r \to \infty$. Columns $\Omega_\pm(r)$ correspond to oscillating solutions as $r \to \infty$. Suppose that we have calculated 'right-hand' solutions with desired accuracy at the point $\hat{r}$ choosing it at a 'sufficiently' large distance from the origin. If we are interested in the discrete spectrum we should compute the matrix $\hat{\Omega}_0 \equiv \Omega_0(\hat{r})$, on the other hand, to determine the complete spectrum we should compute matrices $\hat{\Omega}_{\pm 0} \equiv \Omega_{\pm 0}(\hat{r})$.

Remark 2. *In some cases it is impossible to match with desired accuracy the 'left-hand' and 'right-hand' solutions at a point $\hat{r}$, then it is necessary to use either the power series expansion for the fundamental matrix in the neighbourhood(s) of intermediate point(s) or a numerical integration of (5) over the interval (r_0, r_∞), where $0 < r_0 < r_\infty < \infty$.*

5.1. Discrete spectrum

At first we compose a matrix A of the dimension $2n \times (n_- + n_0)$ from the matrices $\hat{\Omega}_0$ and $\hat{\Phi}_0$ at some value of the energy E:

$$A = (\hat{\Omega}_0, -\hat{\Phi}_0) = A(E).$$

Let $(n_- + n_0)$-dimensional vectors $a^{(1)}, \ldots, a^{(\alpha)}$ form a basis of the null-space of the matrix A. It means that the following equality holds:

$$\begin{aligned} &Aa^{(i)} = 0 \qquad i = 1, \ldots, \alpha \\ &\alpha \equiv \dim \mathrm{Ker}(A) = (n_- + n_0) - \mathrm{rank}A. \end{aligned} \tag{24}$$

Note that if $\alpha = 0$ then such vectors do not exist, so this particular value of E does not belong to the discrete spectrum. We present vectors $a^{(i)}$ in the following form:

$$a^{(i)} = \begin{pmatrix} a_\infty^{(i)} \\ a_0^{(i)} \end{pmatrix} \qquad i = 1, \ldots, \alpha$$

where $a_0^{(i)}$ and $a_\infty^{(i)}$ are n_0-dimensional and n_--dimensional vectors, respectively. The procedure of the calculation of an eigenvalue $E = E_0$ from the discrete spectrum within some interval (E', E'') is reduced to solving the equation

$$\omega(E) = 0 \tag{25}$$

where

$$\omega(E) = \begin{cases} \det A(E) & \text{if matrix } A \text{ is quadratic} \\ \det[A^*(E)A(E)] & \text{if matrix } A \text{ is not quadratic.} \end{cases}$$

Then after determination of an eigenvalue E_0 from equation (25) and solving equation (24) we obtain a basis of α linearly independent solutions of the equation (5) and their derivatives for the value E_0 from the discrete spectrum:

$$\phi^{(i)}(r) = \begin{cases} \Omega_0(r)a_\infty^{(i)}, & r \geqslant \hat{r} \\ \Phi_0(r)a_0^{(i)}, & r \leqslant \hat{r} \end{cases} \qquad i = 1, \ldots, \alpha. \tag{26}$$

5.2. Continuous spectrum

In the case of the continuous spectrum we compose a matrix B of the dimension $2n \times (n+n_+ + n_0)$ from the matrices $\hat{\Omega}_{\pm 0}$, $\hat{\Phi}_0$ at a given value of the energy E from the C-set:

$$B = (\hat{\Omega}_+, \hat{\Omega}_0, \hat{\Omega}_-, -\hat{\Phi}_0) = B(E).$$

Let the vectors $b^{(j)}$, $j = 1, \ldots, \beta$ of the dimension $(n + n_+ + n_0)$ form a basis of the null-space of the matrix B:

$$\begin{aligned} &Bb^{(j)} = 0 \qquad j = 1, \ldots, \beta \\ &\beta \equiv \dim \mathrm{Ker}(B) = (n + n_+ + n_0) - \mathrm{rank}B. \end{aligned} \tag{27}$$

Note, that if $\beta = 0$ then such vectors do not exist and this value of E does not belong to the spectrum of the problem. Similar to the problem of the discrete spectrum we present vectors $b^{(j)}$ in the form:

$$b^{(j)} = \begin{pmatrix} b_\infty^{(j)} \\ b_0^{(j)} \end{pmatrix} \qquad j = 1, \ldots, \beta$$

where $b_0^{(j)}$, $b_\infty^{(j)}$ are n_0-vectors and $(n + n_+)$-vectors, respectively. Then, solving equation (27) with respect to $b^{(j)}$, we obtain a basis of β linearly independent solutions of the equation (5) and their derivatives corresponding to a given value E from the continuous spectrum:

$$\phi^{(j)}(r) = \begin{cases} \Phi_0(r) b_0^{(j)} & r \leqslant \hat{r} \\ (\Omega_+(r), \Omega_0(r), \Omega_-(r)) b_\infty^{(j)} & r \geqslant \hat{r} \end{cases} \qquad j = 1, \ldots, \beta. \tag{28}$$

5.3. S-matrix, in(out)-solutions

In this section we construct an S-matrix and in(out)-solutions for a given value E from the continuous spectrum (we set $n_0 = n$). It is convenient to represent $2n \times (2n + n_+)$ matrix B and vectors $b^1, \ldots, b^{n_+}$ from (27) in the following form:

$$B = (\hat{\Omega}_-, \hat{\Omega}_+, \hat{\Omega}_0, -\hat{\Phi}_0) \equiv (\hat{\Omega}_-, \Xi)$$

where Ξ is a $(2n \times 2n)$ matrix and

$$(b^{(1)}, \ldots, b^{(n_+)}) = \begin{pmatrix} 1_{n_+} \\ X \end{pmatrix} \equiv \begin{pmatrix} 1 \\ X \end{pmatrix}$$

where X is a $2n \times n_+$ matrix to be determined. We have

$$B \begin{pmatrix} 1 \\ X \end{pmatrix} = 0.$$

Hence

$$X = -\Xi^{-1} \hat{\Omega}_-.$$

Let columns of the matrix T_∞ be normalized and

$$k_\alpha \equiv -\mathrm{i}(B_0^+)_{n_- + \alpha, n_- + \alpha} = k_\alpha(E) \qquad v_\alpha \equiv \left| \frac{\mathrm{d}k_\alpha}{\mathrm{d}E} \right|^{-1} = v_\alpha(E) \qquad \alpha = 1, \ldots, n_+.$$

Then, coefficients

$$\Sigma_{\alpha\beta} \equiv X_{\alpha\beta} \left| \frac{v_\alpha}{v_\beta} \right|^{1/2} \qquad \alpha, \beta = 1, \ldots, n_+$$

determine some unitary matrix $\Sigma = (\Sigma_{\alpha\beta}) = \Sigma(E)$ that describes the scattering. Since this matrix is determined with no relation to the initial three-dimensional Hamiltonian (2), it may

differ from the true partial S-matrix. This is evident in the case of radial equations describing a 'scalar' particle ($n = 1$) in a spherically symmetric potential. In this case $\Sigma = -\eta S$, where $\eta = (-1)^{l+1}$. A similar example ($n = 2$, $\Sigma = (-1)^{(l+1)}S$) is presented in section 6. Choosing vectors $b^{(1)}, \ldots, b^{(n_+)}$ in the form of $\binom{1}{X}$, we obtain partial in-solutions in (28). Out-solutions are constructed analogously. All these scattering states $F_\alpha^{\mathrm{in(out)}}(r; E)$ are normalized to $2\pi v_\alpha \delta(E - E')\delta_{\alpha\beta}$ ($\hat{r} \to \infty$). In the case of a real Hamiltonian these solutions are the complex conjugate of each other and matrices Σ and S are symmetric.

Using a procedure which is analogous to the one of section 5.1, it is possible to calculate the poles of an S-matrix at complex energies $\zeta = E + \mathrm{i}G$, ($G < 0$) and the corresponding eigenfunctions, i.e. resonance states; besides, if required, one can calculate antibound states [3, 15] at real energies.

6. Example of applications: discrete and continuum hole Coulomb states

In this section the method is applied to solving the Schrödinger equation in the case of a matrix Hamiltonian with a nontrivial 'spin–orbit-coupling' term and Coulomb potential energy term, namely the Luttinger Hamiltonian [1]. This Hamiltonian describes hole Coulomb states, like shallow acceptor or exciton states in semiconductors with degenerate valence bands.

In the framework of the so-called spherical approximation [16], the Luttinger Hamiltonian can be written as [16, 17]

$$H = \boldsymbol{p}^2 - \mu(P^{(2)} \cdot J^{(2)}) + \frac{2Z}{r}. \tag{29}$$

Here $\bar{h}\boldsymbol{p}$ is the momentum operator; $P^{(2)}$ and $J^{(2)}$ are irreducible spherical tensor operators of the second rank [7], derived from the components of $\boldsymbol{p}$, and the vector $\boldsymbol{J}$ representing the pseudospin angular momentum with $j = \frac{3}{2}$; $\mu = (4\gamma_2 + 6\gamma_3)/5\gamma_1$, where γ_i are empirical constants—so-called Luttinger parameters of the valence band [1]; the energy and the distances are measured in units of $R_a = m_0 e^4/2\bar{h}\kappa^2\gamma_1$ and of $a = \bar{h}\kappa\gamma_1/m_0 e^2$ respectively, m_0 is the mass of a free electron, κ is the static permittivity of the crystal, Z is the magnitude of the impurity ion charge.

The Hamiltonian (29) 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 [17]

$$\Psi = r^{-1}\{(\beta F_H + F_L)|ljfm_f\rangle + (F_H - \beta F_L)|l+2, jfm_f\rangle\} \tag{30}$$

where the functions $|ljfm_f\rangle$ are eigenfunctions of the total angular momentum in the l–j coupled scheme, $F_H(r)$ and $F_L(r)$ are the 'heavy-' and 'light-hole' radial functions, respectively, and the constant $\beta = 3^{l-f+1}[(f+\frac{3}{2})/(f-\frac{1}{2})]^{1/2}$. Then the Schrödinger equation is reduced to coupled sets of radial equations (5) ($M = 2$, $n = 2$), where $F = \binom{F_H}{F_L}$, with a diagonal matrix w: $w = \mathrm{diag}(1-\mu, 1+\mu)$. Each set is characterized by a given value of f and the parity $(-1)^l$.

It is interesting to note that in the present case equation (5) is similar to a system of two coupled 'hydrogen-like" radial equations with two different masses of the particle, namely $1/(1-\mu)$ (heavy hole) and $1/(1+\mu)$ (light hole) and with a coupling which arises due both to the potential energy term and to terms containing differential operators.

The results of sections 3–5 give a complete solution to the problem of finding discrete and continuum eigenstates of the Hamiltonian (29). Below we present results of calculations for states with $f = \frac{3}{2}$ and $l = 0$. In this case matrices of coefficients in (5) are as follows:

$$p_0 = \begin{pmatrix} 0 & 3\mu \\ -3\mu & 0 \end{pmatrix} \qquad q_0 = \begin{pmatrix} -\mu - 2 & 2 - \mu \\ \mu + 2 & \mu - 2 \end{pmatrix} \qquad q_1 = 2Z \qquad q_2 = E.$$

Table 1. Energies (in the units of R_a) of discrete states ($f = \frac{3}{2}$, $l = 0$). 'Material' parameters: $Z = 1$, $\mu = 0.766$.

Level number	1	2	3	4	5
Present method	−2.2637	−0.6728	−0.3453	−0.2107	−0.1424
[18, 19]	−2.264	−0.673	−0.347	—	—
Level number	6	7	8	9	10
Present method	−0.1026	−0.0881	−0.0764	−0.0599	−0.0481

In table 1 we present results of the calculation of energies of the ten lowest discrete states which are characterized by the values $f = \frac{3}{2}, l = 0$ and material parameters $Z = 1, \mu = 0.766$ in the Hamiltonian (29). Note that these values are in fact the energies of even states of shallow acceptor impurities in Ge, the lowermost of which is the ground state energy. For a comparison we also present available data of the previous calculations based on the numerical integration of coupled radial Schrödinger equations [18,19]. All digits in the results of the present calculation are significant and there is a natural way to control errors in our calculations: the results must be stable when changing the matching point. Note that simultaneously with the energies of discrete levels we have determined analytically defined (sections 3–5) wavefunctions.

As follows from the results of section 5, to calculate the wavefunctions of the continuous spectrum of the Hamiltonian (29) one should match two 'left-hand' solutions of (5) and linear combinations of four linearly independent 'right-hand' solutions. We choose linear combinations of 'right-hand' solutions that yield radial in-solutions, whose asymptotic behaviour ($r \to \infty$) is as follows:

$$F_H^{\text{in}}(r) \sim \frac{\mathrm{i}^{-l}}{2ik_H} \begin{pmatrix} (-1)^{l+1}\exp(-\mathrm{i}k_H r) + S_{HH}\exp(\mathrm{i}k_H r) \\ \left(\frac{1-\mu}{1+\mu}\right)^{1/4} \cdot S_{LH}\exp(\mathrm{i}k_L r) \end{pmatrix}$$
$$F_L^{\text{in}}(r) \sim \frac{\mathrm{i}^{-l}}{2\mathrm{i}k_L} \begin{pmatrix} \left(\frac{1+\mu}{1-\mu}\right)^{1/4} \cdot S_{HL}\exp(\mathrm{i}k_H r) \\ (-1)^{l+1}\exp(-\mathrm{i}k_L r) + S_{LL}\exp(\mathrm{i}k_L r) \end{pmatrix} \tag{31}$$

where $k_{H,L} = (E/(1 \mp \mu)^{1/2}$, coefficients $S_{\alpha\beta}$, $\alpha, \beta = H, L$ are the elements of the partial S-matrix which corresponds to a given value of f and the parity.

Since the radial Hamiltonian is real, the S-matrix is symmetric:

$$S_{\alpha\beta} = S_{\beta\alpha} \qquad \alpha, \beta = H, L. \tag{32}$$

For the S-matrix is unitary and symmetric, we have

$$S_{LL} = -\bar{S}_{HH}\frac{S_{HH}}{\bar{S}_{LH}}. \tag{33}$$

In table 2 the results of calculations are presented of the partial S-matrix as a function of the energy E for the states of continuous spectrum which are characterized by the same values of quantum numbers as in table 1: $f = \frac{3}{2}$, $l = 0$ and the same material parameters: $Z = 1$, $\mu = 0.766$. It corresponds to scattering of holes by attractive Coulomb potential of an impurity ion in Ge.

Only values of elements S_{HH} and S_{HL} are presented in the table because the rest of them is determined unambiguously by relations (32) and (33). All digits in results presented in table 2 are significant. In the present case of states of continuous spectrum both unitarity + symmetry of $S_{\alpha\beta}$ and stability of results when changing the matching point can be used to control errors in computations.

Table 2. Partial S-matrix as a function of the energy (E in the units of R_a) for the state with $f = \frac{3}{2}$, $l = 0$. 'Material' parameters: $Z = 1$, $\mu = 0.766$.

E	S_{HH}	S_{HL}
0.5	−0.847 91 − i0.517 51	−0.083 32 − i0.079 27
1.0	−0.670 08 − i0.726 29	−0.142 72 + i0.055 87
2.0	−0.488 17 + i0.852 49	−0.142 07 + i0.121 52
5.0	−0.835 75 + i0.512 46	−0.166 63 + i0.105 57
10.0	−0.983 66 − i0.026 32	−0.170 95 + i0.049 92
20.0	−0.815 13 − i0.560 22	−0.147 32 − i0.003 87
50.0	−0.300 82 − i0.947 83	−0.096 94 − i0.041 60
100.0	+0.098 96 − i0.991 96	−0.062 90 − i0.047 58
500.0	+0.691 79 − i0.721 11	−0.018 56 − i0.032 81

7. Conclusions

A numerical-analytical method has been developed for solving a Schrödinger equation, when a matrix Hamiltonian is a quadratic form of the momentum and contains the potential energy term of a rather general form, in particular, Coulomb and polynomial potentials. Reduction to a system of coupled radial equations is described and the behaviour of radial functions as $r \to 0$ and $r \to \infty$ is explicitly derived. A method of solving coupled radial Schrödinger equations, based on the matching of exact solutions, constructed as algebraic combinations of convergent power series and logarithmic function, and of asymptotic expansions of solutions in the neighbourhood of an irregular singularity at $r = \infty$ has been developed. Using the matching method one can calculate the following for radial matrix Hamiltonians: (1) in/out-solutions, (2) S-matrix, (3) poles of resolvent with corresponding eigenfunctions, in particular, poles of S-matrix—bound, antibound and resonance states included.

The wavefunctions calculated are represented in analytical form.

The method is applied to solving Schrödinger equation in a case of matrix Hamiltonian [1] describing discrete and continuum Coulomb states of charge carriers in semiconductors with degenerate valence bands. Analytical expressions for the wavefunctions have been derived, the energies of ten lowest discrete states of definite symmetry have been calculated and partial S-matrix, describing the scattering of holes by Coulomb potential of an impurity ion, has been calculated for the first time.

We note in conclusion that the method of matching can be extended to the following important cases:

(1) Matrix potentials of the form

$$V(\boldsymbol{r}) \sim \sum_{k=-1}^{\infty} V_k(\theta, \phi, \boldsymbol{L}) r^k \qquad r \to 0$$

$$V(\boldsymbol{r}) \sim r^v \sum_{k=0}^{\infty} \tilde{V}_k(\theta, \phi, \boldsymbol{L}) r^{-k} \qquad r \to \infty \qquad 0 \leqslant v = \text{integer}.$$

(2) Problems on intervals (a, b), where $-\infty \leqslant a < b \leqslant +\infty$.

(3) First-order Dirac-type equations.

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Appendix A. The structure of the leading matrix α_0

In this appendix we show that in case of Hamiltonians under consideration matrix α_0 is a simple one and all its eigenvalues are certain integers.

Let us first consider indices (l, τ) of the vector-function $F(\cdot)$ in equation (5). Let quantum numbers $l_1, l_2, \ldots, l_{n_0}$ be presented in the indices (l, τ) respectively $\nu(1)$, $\nu(2), \ldots, \nu(n_0)$ times, i.e. n_0 is the number of different values of l in the indices of $F(\cdot)$. Let $l_1 < l_2 < \cdots < l_{n_0}$. Obviously, $\sum_{k=1}^{n_0} \nu(k) = n$, i.e. $\nu(k)$ is a multiplicity of τ for a given l_k. According to the Wigner–Echart theorem [7] and using the form of the matrix α_0 along with the following relations for the reduced matrix elements:

$$\langle l \| \boldsymbol{p}^2 \| l' \rangle r^\zeta \propto r^{\zeta-2}(\zeta - l)(\zeta + l + 1)\delta_{ll'}$$

$$\langle l \| P^{(2)} \| l' \rangle r^\zeta \propto r^{\zeta-2} \begin{cases} (\zeta - l)(\zeta + l + 1), & l' = l \\ (\zeta + l + 1)(\zeta + l + 3), & l' = l + 2 \\ (\zeta - l)(\zeta - l - 2), & l' = l - 2 \end{cases}$$

we obtain that if the indices of $F(\cdot)$ are ordered in a definite way, namely, when the index $i = (l, \tau)$ increases the value of l does not decrease, the following properties hold:

(1) $l_k = l_1 + 2(k-1)$, $k = 1, \ldots, n_0$.

(2) The eigenvalues of the matrix α_0 are the following numbers (corresponding multiplicities are written down in parenthesis):

$$l_1 + 1(\nu(1)), \ldots, l_{n_0} + 1(\nu(n_0)), -l_1(\nu(1)), \ldots, -l_{n_0}(\nu(n_0)).$$

(3) Corresponding linear-independent eigenvectors of the matrix α_0 compose a $2n \times 2n$ matrix of the form

$$\begin{pmatrix} X & Y \\ XD & Y\tilde{D} \end{pmatrix}$$

where

$$X = \begin{pmatrix} 1_{\nu(1)} & & & \\ & 1_{\nu(2)} & & * \\ & & \ddots & \\ 0 & & & 1_{\nu(n_0)} \end{pmatrix} \qquad Y = \begin{pmatrix} 1_{\nu(1)} & & & \\ & 1_{\nu(2)} & & 0 \\ & & \ddots & \\ * & & & 1_{\nu(n_0)} \end{pmatrix}$$

$$D = \operatorname{diag}(\underbrace{l_1 + 1}_{\nu(1)\text{times}}, \ldots, \underbrace{l_{n_0} + 1}_{\nu(n_0)\text{times}}) \qquad \tilde{D} = \operatorname{diag}(\underbrace{-l_1}_{\nu(1)\text{times}}, \ldots, \underbrace{-l_{n_0}}_{\nu(n_0)\text{times}})$$

are $n \times n$ matrices and 1_k is the unit $k \times k$ matrix.

(4) As follows from item (3) matrix α_0 is a simple one—it is similar to a diagonal matrix.

Appendix B. Calculation of matrices U_k^p and C_s^p

We put $U_k^p \equiv 0$, if $k < \lambda_p - \lambda_g$. Note that matrices $U^p_{\lambda_p-\lambda_g}$ are defined ambiguously. For definiteness we set them in the following form:

$$U^p_{\lambda_p-\lambda_g} = \begin{pmatrix} 0 \\ 1 \\ 0' \end{pmatrix} \tag{B1}$$

where 0, $0'$ are zero matrices of the dimensions equal to $[(\sum_{k=0}^{p-1} d_k) \times d_p]$ and $[(\sum_{k=p+1}^{d_g} d_k) \times d_p]$, respectively, 1 is the unit $(d_p \times d_p)$-matrix.

Let us consider equation (14) successively for each $p = 0, 1, \ldots, g$. If $p = 0$ then all matrices U_k^0, $k = \lambda_0 - \lambda_g + 1, \ldots, N$ are easily calculated.

The case $p > 0$. If $k \neq \lambda_t - \lambda_g$ for any t, $0 \leqslant t < p$ in equation (14) then the calculation of matrices $U^r_{\lambda_t-\lambda_g}$ is straightforward.

If $k = \lambda_t - \lambda_g$ for some t, $0 \leqslant t < m$, then the determination of $U^m_{\lambda_t-\lambda_g}$ becomes more complicated. Using the fact that matrices $U_k^m, C_l^m (k < \lambda_t - \lambda_g, l > t)$ were already determined we obtain

$$(\lambda_t - A_0)U^m_{\lambda_t-\lambda_g} = -(t+1)U^t_{\lambda_t-\lambda_g}C_t^m + H_t^m \tag{B2}$$

where

$$H_t^m = \sum_{l=1}^{\min(k,M)} A_l U^m_{k-l} - \sum_{p=1}^{m}(m+1-p)U_k^{m-p}C^m_{m-p}.$$

It is convenient for further consideration to rewrite equation (B2) using index notations:

$$(\lambda_t - A_0)_{ii}(U^m_{\lambda_t-\lambda_g})_{ii'} = -(t+1)\sum_{j=1}^{d_t}(U^t_{\lambda_t-\lambda_g})_{ij}(C_t^m)_{ji'} + (H_t^m)_{ii'}. \tag{B3}$$

As is easily seen, the left-hand side of equation (B3) equals zero for a given index i' when $i = d_0 + \cdots + d_{t-1} + 1, \ldots, d_0 + \cdots + d_{t-1} + d_t$. Therefore, in this case we put

$$(U^m_{\lambda_t-\lambda_g})_{ii'} = 0 \tag{B4}$$

and using our definition (B1) we can calculate d_t values of $(C_t^m)_{ji'}$ corresponding just to these values of the index i:

$$(C_t^m)_{ji'} = \frac{(H_t^m)_{d_0+\cdots+d_{t-1}+j,i'}}{t+1}.$$

Then using equation (B4) in the case when index $i \neq d_0 + \cdots + d_{t-1} + 1, \ldots, d_0 + \cdots + d_{t-1} + d_t$ we have

$$(U^m_{\lambda_t-\lambda_g})_{ii'} = \frac{(H_t^m)_{ii'}}{(\lambda_t - A_0)_{ii}}.$$

Finally, changing the value of index i' step by step from 1 to d, k from $\lambda_m - \lambda_g$ to N, m from 0 to g we compute all the matrices we need.

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