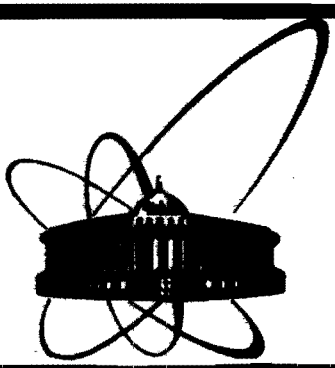

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THE CORE-SPLINES METHOD FOR SOLUTION OF QUANTUM-MECHANICAL SYSTEMS OF DIFFERENTIAL EQUATIONS FOR BOUND STATES

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The core-splines method (CSM) [1-3] is generalized in the present work towards the solution of the general problem for bound states of a system of M linear differential equations with coefficients depending on the spectral parameter (eigenvalue). The recursion scheme for construction of basic splines [1] is described in sect.3. The wave functions are expressed as linear combinations of basic splines, the latter being approximate partial solutions of the system. The spectral parameter is determined from the condition for existence of nontrivial solution of a $(M \times M)$ linear algebraic system at the last collocation point. The nontrivial solution of this system determines $(M - 1)$ coefficients of the linear spans, expressing the wave function. The last coefficient is determined from an additional boundary condition for the system which is, usually, a common normalization condition for all functions of the system. Computational aspects of the method are discussed in sect.4 and an up-to-date realization of a concrete algorithm is given on which computer program RODSOL is based. The last section presents, as an example, a numerical solution of the Dirac-system for the bound states of a hydrogen atom.

1. FORMULATION OF THE PROBLEM

Given the real intervals $X = [x_a, x_b]$, $Z = [z_a, z_b]$, $G = [y_a, y_b]$ and matrix $H(x, z) = \{H_{\lambda\lambda'}(x, z)\}_{\lambda\lambda' = 1, 2, \ldots, M}$, whose elements are

$$H_{\lambda\lambda'}(x, z) = \sum_{\nu=1}^{n_{\lambda\lambda'}} a_{\lambda\lambda'}^{(\nu)}(x, z) \frac{d^\nu}{dx^\nu} + a_{\lambda\lambda'}^{(0)}(x, z),$$

where $n_{\lambda\lambda'}$ are some natural numbers and

$a_{\lambda\lambda'}^{(\nu)}(x, z) \in C^{0,1}(P) \quad \forall \ \nu, \quad P = X \times Z.$

Consider the solution of the following differential system:

$$\begin{cases} H(x, z)\, y(x, z) = 0, & (1) \\ g(z, y(x, z)) = \bar{\gamma} \quad (\bar{\gamma} \in G, \ \bar{\gamma} \neq 0) & (2) \end{cases}$$

with respect to the unknown pair

$$(z, y) \in Z \times F_{p,n}, \qquad (3)$$

where

$y = (y_1(x, z), \ldots, y_M(x, z))^T$, $y_\lambda \in C^{n,1}(P_0)$, $n = \max_{\lambda,\lambda'} \{n_{\lambda\lambda'}\}$,

$F_{p,n} = \{\phi(x)p(x, z)/\phi(x) = \mathrm{diag}(\phi_1(x), \ldots, \phi_M(x)),\ \phi_\lambda(x) \in C^n(X_0)\}$,

$p = (p_1(x, z), \ldots, p_M(x, z))^T$, $p_\lambda(x, z) \in C^{n,1}(P_0)$, $P_0 = X_0 \times Z$, $X_0 = [0, \infty]$

($p(x, z)$ - is a given core of the solution /1/). Functional $g(z, y(x, z)): Z \times C^{n,1}(P_0) \to G$ is bounded and real. One assumes that upon substitution $y = \gamma y^*$, where $y^*(x, z) \in C^{n,1}(P_0)$, ($\gamma \in R^1$, $\gamma \neq 0$), equation (2) is uniquely solvable in G.

For every $z \in Z$ elements of matrix H obey the following quantum-mechanical conditions (see, e.g., /4,5/):

i) $a^{(n_{\lambda\lambda'})}_{\lambda\lambda'}(x, z) \not\equiv 0 \ \forall\ x \in X_0$ and $\lim_{x \to 0} a^{(n_{\lambda\lambda'})}_{\lambda\lambda'}(x, z) > 0$;

ii) when $x \to 0$ (or $x \to \infty$), $a^{(\nu)}_{\lambda\lambda'}(x, z)$ $(\nu = 1, 2, \ldots, n_{\lambda\lambda'} - 1)$ can increase not faster than $\dfrac{1}{x^{t^{(\nu)}_{\lambda\lambda'}}}$ $(x^{t^{(\nu)}_{\lambda\lambda'}})$, where $t^{(\nu)}_{\lambda\lambda'} \in (0, n_\lambda - \nu]$, $n_\lambda = \max_{\lambda'} \{n_{\lambda\lambda'}\}$;

iii) when $x \to 0$, "potentials" $a^{(0)}_{\lambda\lambda'}(x, z)$ can increase infinitely, if they are positive in the vicinity of 0^+; if they are negative in the vicinity of 0^+, they can increase not faster than $1/x^{t^{(0)}_{\lambda\lambda'}}$, where $t^{(0)}_{\lambda\lambda'} \in (0, n_\lambda)$. At the same time it is necessary that $\lim_{x \to \infty} a^{(0)}_{\lambda\lambda'}(x, z) \neq -\infty$.

Often it is possible to obtain the asymptotic solutions $y_0 = (y_{01}, \ldots, y_{0M})^T$ and $y_\infty = (y_{\infty 1}, \ldots, y_{\infty M})^T$ for system (1) having properties i)-iii). Functions y_0 and y_∞ are solutions of systems:

$$H_0(z)y_0(x, z) = 0 \quad \text{and} \quad H_\infty(z)y_\infty(x, z) = 0, \tag{4}$$

where $H_0(z) = \lim_{x \to 0} H(x, z)$ and $H_\infty(z) = \lim_{x \to \infty} H(x, z)$.

In particular, when coefficients $a^{(\nu)}_{\lambda\lambda'}$ are holomorphic in $x = 0$, solutions $y_{0\lambda}(x, z)$ $(\lambda = 1, 2, \ldots, M)$ can be found in the form of a formal series (Frobenius series):

$$y_{0\lambda} = x^{s_\lambda}(b_{\lambda 1} + b_{\lambda 2}\, x + \ldots), \tag{5}$$

where s_λ are roots of the corresponding characteristic system (e.g., see /5/ p.12). In the general case we assume that functions $y_0(x, z)$ and $y_\infty(x, z)$ give only a rough behaviour of solutions of system (1) at boundaries of the interval X_0; e.g., the leading asymptotic term $y_{0\lambda} = x^{s_\lambda}$ in the case of expansion (5). In what follows y_0 and y_∞ are used to specify the core-function $p(x, z)$ whose components have the form

$$p_\lambda(x, z) = y_{0\lambda}(x, z)\, y_{\infty\lambda}(x, z) \quad (\lambda = 1, 2, \ldots, M). \tag{6}$$

Components of the core-function should obey the following conditions:

$$p_\lambda(x, z) \neq 0 \quad \forall \quad (x, z) \in P_0, \tag{7}$$

$$\lim_{x \to \infty} p_\lambda(x, z) = 0 \quad \forall \quad z \in Z. \tag{8}$$

2. THE APPROXIMATE SOLUTIONS

For a given integer $N \geq m + 3$ divide the interval X by two meshes:

$$\bar{\Delta}_N = \{\bar{x}_j / \bar{x}_1 = x_a, \bar{x}_{N+1} = x_b, \bar{x}_j = \bar{x}_{j-1} + h,\ h = \frac{x_b - x_a}{N},\ j = 2, 3, \ldots, N\},$$

$$\Delta_N = \{x_{j_\sigma} / x_1 = x_a, x_N = x_b,\ x_{j_\sigma} = \bar{x}_j + \delta_\sigma;\ \sigma = 1 \text{ when } j = 1, 2, \ldots, m, N$$

($j_1 \equiv j$, $\delta_1 \equiv \delta$) and $\sigma = 1, 2, \ldots, \sigma^*$ when $j = m + 1, m + 2, \ldots, N - 1$;

where σ^* is integer ($1 \leq \sigma^* \leq m$); $0 < \delta_{\sigma^*} < \delta_{\sigma^*-1} < \ldots < \delta \leq h\}$.

Polynomial splines $s_{m\lambda}(x)$ $(\lambda = 1, 2, \ldots, M)$ of degree m and defect σ^*, interpolating functions $\phi_\lambda(x)$ $(\lambda = 1, 2, \ldots M)$ on the mesh Δ_N, are defined on the mesh $\bar{\Delta}_N$ by the following conditions (see. ref. /6/ pp.34, 83):

$$s_{m\lambda}(x) = \{\sum_{i=0}^{m} a^{(i)}_{j,\lambda}\, x^i / a^{(i)}_{j,\lambda} \in R^1,\ \bar{x}_j < x < \bar{x}_{j+1}\},\ j = 1, 2, \ldots, N, \tag{9}$$

$$s_{m\lambda}(x_{j_\sigma}) = \phi_\lambda(x_{j_\sigma}) \quad \begin{pmatrix} j = 1, 2, \ldots, m, N;\ \sigma = 1 \\ j = m + 1, m + 2, \ldots, N - 1;\ \sigma = 1, 2, \ldots, \sigma^* \end{pmatrix}, \tag{10}$$

$$s_{m\lambda}(x) \in C^{m-\sigma^*}(X), \tag{11}$$

$$a^{(i)}_{1,\lambda} = a^{(i)}_{2,\lambda} = \ldots = a^{(i)}_{m,\lambda};\ a^{(i)}_{N-1,\lambda} = a^{(i)}_{N,\lambda} \quad (i = 0, 1, \ldots, m). \tag{12}$$

All splines $s_{m\lambda}(x)$, interpolating functions $\phi_\lambda(x) \in C^n(X)$, on the mesh Δ_N, form a manifold $S_{N\lambda}(X)$. The basic idea of the core-splines method /1-3/ consists in replacing the original problem (1), (2) under assumption (3) by an approximate problem solved with respect to approximate unknowns $(\tilde{z}, \tilde{y}(x, \tilde{z}))$. The approximate problem includes eqs. (1), (2), but the manifold $F_{p,n}$ in (3) is replaced by the manifold

$$\tilde{F}_{p,n} = \{s_m(x)p(x, z)/s_m(x) = \mathrm{diag}(s_{m1}(x), \ldots, s_{mM}(x)),\ s_{m\lambda}(x) \in S_{N\lambda}(X)\}.$$

Now the interpolation conditions (10) are converted into collocation conditions for the system (1) (see, e.g., /7/):

$$f(x_{j\sigma}, \bar{z}) \equiv H(x, \bar{z})(s_m(x)p(x, \bar{z}))\Big/_{x = x_{j\sigma}} = 0 \qquad (13)$$

$$\left(\begin{array}{l} j = 1,2,\ldots, m, N;\ \sigma = 1 \\ j = m+1, m+2, \ldots, N-1;\ \sigma = 1, 2, \ldots, \sigma^* \end{array} \right)$$

Smoothness conditions (11) and collocation conditions (13) lead to the following equations valid for every $\lambda = 1,2,\ldots, M$:

$$\sum_{i=\mu}^{m} \frac{i!}{(i-\mu)!}\left(a^{(i)}_{j,\lambda} - a^{(i)}_{j-1,\lambda}\right) = 0 \qquad \left(\begin{array}{l} j = m+1, m+2, \ldots, N-1 \\ \mu = 0,1,\ldots, m-\sigma^* \end{array} \right) \qquad (14)$$

$$\sum_{\lambda'=1}^{M} \sum_{i=0}^{m} h^{(i)}_{j_\sigma, \lambda\lambda'} a^{(i)}_{j,\lambda'} = 0 \qquad \left(\begin{array}{l} j = 1,2,\ldots, m, N;\ \sigma = 1 \\ j = m+1, m+2, \ldots, N-1; \\ \alpha = 1,2,\ldots, \sigma^* \end{array} \right) \qquad (15)$$

where

$$h^{(i)}_{j_\sigma, \lambda\lambda'} \equiv \sum_{\mu=0}^{i} \rho(\mu) \frac{i!}{(i-\mu)!} g_{j_\sigma, \mu; n_{\lambda\lambda'}} x_{j_\sigma}^{i-\mu},$$

$$g_{j_\sigma, \mu, n_{\lambda\lambda'}} \equiv \sum_{\nu=\mu}^{n_{\lambda\lambda'}} \frac{\nu!}{\mu!(\nu-\mu)!} a^{(\nu)}_{\lambda\lambda'}(x_{j_\sigma}, z) p^{(\nu-\mu)}_{j_\sigma, \lambda'},$$

$$p^{(\nu-\mu)}_{j_\sigma, \lambda'} \equiv \left(\frac{d^{\nu-\mu}}{dx^{\nu-\mu}} p_{\lambda'}(x, z) \right)\Big|_{x = x_{j_\sigma}},$$

$$\rho(\mu) = \begin{cases} 1, & \text{if } \mu \le m^*, \\ 0, & \text{if } \mu > m^*, \end{cases} \qquad m^* = \begin{cases} m, & \text{if } m \le n_{\lambda\lambda'} \\ n_{\lambda\lambda'}, & \text{if } m > n_{\lambda\lambda'}. \end{cases}$$

For a fixed value of z equalities (12), (14) and (15) form a linear system of $\mathfrak{M} = M(m+1)N$ equations with respect to $\mathfrak{M}$ unknown coefficients $\mathfrak{L} = \{a^{(i)}_{j,\lambda}\}_{\substack{i = 0,1,\ldots, m \\ j = 1,2,\ldots, N \\ \lambda = 1,2,\ldots, M}}$ of the splines $s_{m\lambda}(x)$. Thus, the problem for finding approximate solutions $(\bar{z}, \bar{y}(x, \bar{z}))$ reduces to the construction of a nontrivial solution of system (12), (14), (15). The condition for existence of such a solution (generally, nonunique) becomes a condition determining the spectral parameter $\bar{z}$. In what follows one of the possible numerical ways to solve this problem is given.

3. COMPUTATIONAL SCHEME FOR THE CONSTRUCTION OF THE BASIC SPLINES

In refs. /1-3/ the simplest case of system (12), (14), (15) is considered: construction of the basic spline in the case $M = 1$, $m = 2$, $\sigma^* = 1$ and $n \le 2$, (i.e. when system (1) is reduced only to one equation and quadratic splines are used). In the present work the CSM /1-3/ is extended to the solution of problem (1), (2) in the general case. Linear system (12), (14), (15) is solved by a successive expression of the unknowns $\mathfrak{L}_1 = \{a^{(i)}_{j,\lambda}\}_{\substack{i = 1,2,\ldots, m \\ j = 1,2,\ldots, N \\ \lambda = 1,2,\ldots, M}}$, starting from the mesh-point x_a, through unknowns $a^{(o)}_{1,1}, a^{(o)}_{1,2}, \ldots, a^{(o)}_{1,M}$. The latter are defined by solving a linear homogeneous system at the last collocation point x_b and from condition (2).

Let $\bar{z} \in Z$ be a fixed value of the spectral parameter. The first part of equations (12) with equations (15) together for $\lambda = 1,2,\ldots, M$ and $j = 1,2,\ldots, m$ $(\sigma = 1)$ lead to the following relation between unknowns $\{a^{(i)}_{1,\lambda}\}_{\substack{i = 1,2,\ldots, m \\ \lambda = 1,2,\ldots, M}}$ and $\{a^{(o)}_{1,\lambda}\}_{\lambda = 1,2,\ldots, M}$

$$AX = -\sum_{\lambda'=1}^{M} a^{(o)}_{1,\lambda'} Y_{\lambda'}, \qquad (16)$$

where

$$A = \{A_{\ell\ell'}\}_{\ell, \ell' = 1,2,\ldots, \mathfrak{M}_1},$$

$$X = (X_1, X_2, \ldots, X_{\mathfrak{M}_1})^T, \qquad Y_{\lambda'} = (Y_{\lambda' 1}, Y_{\lambda' 2}, \ldots, Y_{\lambda' \mathfrak{M}_1})^T,$$

are matrices with components $A_{\ell\ell'} = h^{(i)}_{j,\lambda\lambda'}$, $X_{\ell'} = a^{(i)}_{1,\lambda'}$, $Y_{\lambda'\ell} = h^{(o)}_{j,\lambda\lambda'}$; indices ℓ, ℓ' are given by the formulae $\ell = (\lambda - 1)m + j$, $(j = 1,2,\ldots, m)$, $\ell' = (\lambda' - 1)m + i$ $(i = 1,2,\ldots, m)$ and $\mathfrak{M}_1 = mM$.

Step 1. Let

$$\det A \neq 0, \qquad (17)$$

then solve the linear system

$$AX_{\lambda^*} = -Y_{\lambda^*} \qquad (18)$$

with respect to the unknown vector

$$X_{\lambda^*} = (X_{\lambda^* 1}, X_{\lambda^* 2}, \ldots, X_{\lambda^* \mathfrak{M}_1})^T, \quad X_{\lambda^* \ell'} = a^{(i)}_{1,\lambda'\lambda^*}.$$

Solution of different in λ^* systems (18) corresponds to construction of M different approximate partial solutions of system (1)

$$\bar{y}_{\lambda\lambda^*}(x, \bar{z}) = s_{m\lambda\lambda^*}(x) p_\lambda(x, \bar{z}).$$

At the following step the coefficients $\mathfrak{L}^* = \{a^{(i)}_{j,\lambda\lambda^*}\}_{\substack{i=0,1,\dots,m \\ j=m+1,m+2,\dots,N-1 \\ \lambda,\lambda^*=1,2,\dots,M}}$

of the splines $s_{m\lambda\lambda^*}(x)$ on X are detrmined.

Step 2. From eqs.(14) we express unknowns

$\mathfrak{L}^*_1 = \{a^{(\mu)}_{j,\lambda\lambda^*}\}_{\substack{\mu=0,1,\dots,m-\sigma^* \\ j=m+1,m+2,\dots,N-1 \\ \lambda,\lambda^*=1,2,\dots,M}}$ through unknowns

$\{a^{(\mu)}_{j-1,\lambda\lambda^*}\}$, using the following recursion relations:

$$\begin{cases} a^{(0)}_{1,\lambda\lambda^*} = \begin{cases} 1, & \text{if } \lambda = \lambda^*, \\ 0, & \text{if } \lambda \neq \lambda^*, \end{cases} \\ a^{(\mu)}_{j,\lambda\lambda^*} = a^{(\mu)}_{j-1,\lambda\lambda^*} + (-1)^{m-\mu} \dfrac{m!}{\mu!(m-\mu)!} \bar{x}_j^{m-\mu} (a^{(m)}_{j,\lambda\lambda^*} - a^{(m)}_{j-1,\lambda\lambda^*}). \end{cases} \tag{19}$$

To determine unknowns $\mathfrak{L}^*_2 = \{a^{(\mu)}_{j,\lambda\lambda^*}\}_{\substack{\mu=m-\sigma^*+1,m-\sigma^*+2,\dots,m \\ j=m+1,m+2,\dots,N-1 \\ \lambda,\lambda^*=1,2,\dots,M}}$

one should substitute relations (19) into eqs. (15) thus obtaining a set of linear systems (every one of dimension $\mathfrak{M}_2 = \sigma^* M$):

$$\{B_j X_{j\lambda^*} = -Y_{j\lambda^*}\}_{\substack{j=m+1,m+2,\dots,N-1, \\ \lambda^*=1,2,\dots,M}} \tag{20}$$

where

$B_j = \{B_{j,\ell\ell'}\}_{\ell,\ell'=1,2,\dots,\mathfrak{M}_2}$,

$X_{j\lambda^*} = (X_{j\lambda^*,1}, X_{j\lambda^*,2}, \dots, X_{j\lambda^*,\mathfrak{M}_2})^T$,

$Y_{j\lambda^*} = (Y_{j\lambda^*,1}, Y_{j\lambda^*,2}, \dots, Y_{j\lambda^*,\mathfrak{M}_2})^T$,

are matrices with elements

$$B_{j,\ell\ell'} = h^{(i)}_{j_\sigma,\lambda\lambda'} + \delta_{im}\, t^{(m-\sigma^*)}_{j_\sigma,\lambda\lambda'}, \quad \delta_{im} = \begin{cases} 1, & \text{if } i = m, \\ 0, & \text{if } i \neq m, \end{cases}$$

$$t^{(m-\sigma^*)}_{j_\sigma,\lambda\lambda'} = \sum_{i=0}^{m-\sigma^*} (-1)^{m-i} \frac{m!}{i!(m-i)!} x_j^{m-i}\, h^{(i)}_{j_\sigma,\lambda\lambda'},$$

$$X_{j\lambda^*,\ell'} = a^{(i)}_{j,\lambda'\lambda^*} - a^{(i)}_{j-1,\lambda'\lambda^*},$$

$$Y_{j\lambda^*,\ell} = \sum_{\lambda'=1}^{M} \sum_{i=0}^{m} h^{(i)}_{j_\sigma,\lambda\lambda'}\, a^{(i)}_{j-1,\lambda'\lambda^*}.$$

Indices ℓ, ℓ' are given by the formulae

$\ell = (\lambda - 1)\sigma^* + j_\sigma$ $(j = m+1, m+2, \dots, N-1;\ \sigma = 1,2,\dots,\sigma^*)$,

$\ell' = (\lambda' - 1)\sigma^* + m - i + 1$ $(i = m - \sigma^* + 1,\ m - \sigma^* + 2, \dots, m)$.

In addition, the following inequalities are assumed to hold:

$$\det B_j \neq 0, \quad j = m+1, m+2, \dots, N-1. \tag{21}$$

Finally, from the second part of the spline-boundary conditions (12) the remaining part of unknowns $\mathfrak{L}^*_3 = \{a^{(i)}_{N,\lambda\lambda^*}\}_{\substack{i=0,1,\dots,m \\ \lambda,\lambda^*=1,2,\dots,M}}$ is expressed through unknowns $\{a^{(i)}_{N-1,\lambda\lambda^*}\}$. Thus, all the coefficients $\mathfrak{L}^* = \mathfrak{L}^*_1 \cup \mathfrak{L}^*_2 \cup \mathfrak{L}^*_3$ of the splines $\{s_{m\lambda\lambda^*}(x)\}_{\lambda,\lambda^*=1,\dots,M}$ are determined.

Approximate solutions $\tilde{y}_\lambda(x, \tilde{z})$ are expressed in terms of just constructed partial approximate solutions $\tilde{y}_{\lambda\lambda^*}(x, \tilde{z})$ by the relation

$$\tilde{y}_\lambda(x, \tilde{z}) = p_\lambda(x, \tilde{z}) \sum_{\lambda^*=1}^{M} a^{(o)}_{1,\lambda^*}\, s_{m\lambda\lambda^*}(x). \tag{22}$$

Splines $s_{m\lambda\lambda^*}(x)$ are analogues of the basic spline (see ref.[1] p.927) in the case of the system of differential equations (1), (2).

Step 3. The approximate solutions $\tilde{y}_\lambda(x, \tilde{z})$ $(\lambda = 1,2,\dots,M)$ satisfy the collocation condition (15) for $j = N$ $(x = x_N = x_b)$. This leads to an (MxM) - linear homogeneous system

$$\Phi(\tilde{z})\theta = 0 \tag{23}$$

for the unknown vector $\theta = (a^{(o)}_{1,1}, a^{(o)}_{1,2}, \dots, a^{(o)}_{1,M})^T$. The components of the functional matrix $\Phi(\tilde{z})$ read

$$\Phi_{\lambda\lambda^*} = \sum_{\lambda'=1}^{M} \sum_{i=0}^{m} h^{(i)}_{N,\lambda\lambda'}(x_b, \tilde{z})\, a^{(i)}_{N,\lambda\lambda^*}(\tilde{z}).$$

A necessary and sufficient condition for existence of non-trivial approximate solutions $\tilde{y}_\lambda(x, \tilde{z})$ $(\lambda = 1,2,\dots,M)$ is

$$\operatorname{rank} \Phi(\tilde{z}) = M - 1. \tag{24}$$

The values of the spectral parameter $\tilde{z}$ are determined from condition (24).

Let condition (24) be fulfilled for a certain $\tilde{z}^* \in Z$. Substitute $a^{(o)}_{1,M} = 1$. Then system (23) has a unique solution $\theta' = (a^{(o)}_{1,1}, a^{(o)}_{1,2}, \dots, a^{(o)}_{1,M-1}, 1)^T$ which determines functions $\tilde{y}_{\lambda\lambda^*}$ uniquely. The vector θ determining the approximate solutions $\tilde{y}_\lambda$ (22) is connected with θ' by the equality $\theta = a^{(o)}_{1,M}\,\theta'$.

The unknown $a^{(o)}_{1,M}$ is determined by condition (2), namely:

$$a^{(o)}_{1,M} = g^{-1}[\tilde{z}^*, \tilde{y}(x, \tilde{z}^*)]\bar{\gamma}. \tag{25}$$

From the assumption that the inverse function g^{-1} exists and from inequality $\bar{y} \neq 0$ it follows that the inequality $a^{(o)}_{1,M} \neq 0$ holds too.

The calculational scheme just described leads to the following statement for existence of approximate solutions of problem (1), (2) (a generalization of Theorem 1 in ref. /1/):

When inequalities (17) and (21) are fulfilled the approximate solution $(\bar{z}, \bar{y}(x, \bar{z}))$ exists if and only if there is a certain $\bar{z} \in Z$ for which equality (24) is valid. Approximate wave functions $\bar{y}_\lambda(x, \bar{z})(\lambda = 1,2,\ldots,M)$ are expressed with the help of the basic splines $s_{m\lambda\lambda^*}(x)$ according to eq.(22).

There is no generalization of Theorem 2 (of ref /1/) about proximity between approximate and exact solutions of problem (1), (2). The rates of convergence of CSM established in a numerical way are given at the end of the next section.

4. COMPUTATIONAL ASPECTS OF THE METHOD

The computational scheme of CSM in its basic spline variant can be realized algorithmically in a relatively simple way. A FORTRAN-program RODSOL is worked out on the basis of this algorithm whose main features are listed bellow:

4.1. The basic spline coefficients are determined by solving streams of linear systems (18), (20) for a fixed value of the spectral parameter $\bar{z}$. These systems are solved by the Gauss elimination with a partial choice of the leading element /8/ . Beforehand every matrix and the r.h.s.-vector of systems (18), (20) are divided by a scale factor equal to the maximal, in absolute value, element of the matrix. The triangle decomposition of the matrices is realized by the program DECOMP /8/ and then the program SOLVE /8/ is used to solve systems (18), (20).

4.2. In the basic variant spline coefficients $\{a^{(i)}_{1,\lambda}\}_{\substack{i=1,2,\ldots,m \\ \lambda=1,2,\ldots,M}}$ are determined by solving systems (18). In this case one uses the boundary information for system (1), entering only into the main part of the asymptotic solutions for $x \to 0$ (i.e. the cores of the solutions). There is another possibility of determining $a^{(i)}_{1,\lambda}$ in the cases when the solution of system (1) for $x \to 0$ can be found as series (5). Then the values of coefficients $a^{(i)}_{1,\lambda}$ can be calculated directly from the coefficients $b_{\lambda i}$ of series (5).

4.3. The approximate eigenvalues $\bar{z}$ are solutions of the equation

$$F(\bar{z}) \equiv \det \Phi(\bar{z}) = 0. \qquad (26)$$

This is a sufficient condition for equality (24) to hold. The determinant $F(z)$ is calculated, after the triangle decomposition of matrix $\Phi(z)$ by the program DECOMP, as a product of the principal diagonal elements. To avoid computer overflows, this product is calculated as a sum of logarithms of the diagonal elements.

The calculation of eigenvalues as roots of eq.(26) goes through the following procedures:

4.3.1. For big enough values of x_b and N one checks the sign of $F(z)$ on a given "fine" mesh in the interval Z:

$$z_o = z_a,\ z_i = z_o + i h_z (i = 1,2,\ldots,i^*;\ i^* \geq 1),\ h_z = \text{const.} \geq 0$$

is a mesh step. After finishing this procedure a subinterval $Z_{i^*} = [z_{i^*-1},\ z_{i^*}]$ containing a root of eq.(26) is found;

4.3.2. A more precise value of the root is obtained by the dichotomy:

$$z_{i^*,o} = z_{i^*},$$

$$z_{i^*,j} = z_{i^*,j-1} - \frac{h_z}{2^j} \operatorname{sign}[F(z_{i^*,j-1}) F(z_{i^*,j})] \quad (j = 1,2,\ldots,\bar{j}).$$

This procedure ends when the counter j reaches a given number $\bar{j} \geq 1$ or when inequality $|F(z_{i^*,j^*})| \leq T_{z1}$ is satisfied ($j^* \in \{1,2,\ldots,\bar{j}\}$, $T_{z1} = \text{const.} \geq 0$ is a given small number);

4.3.3. This approximation of the root $z_{i^*,\bar{j}}$ (or z_{i^*,j^*}) is further precised by the autoregularized Newton iteration process /9/ :

$$z_o = z_{i^*,\bar{j}} \quad (\text{or } z_o = z_{i^*,j^*}),$$

$$z_{k+1} = z_k - \frac{F'(z_k) F(z_k)}{F'^2(z_k) + \epsilon_k} \qquad (k = 0,1,\ldots,\bar{k};\ \bar{k} \geq 0),$$

$$\epsilon_k = \frac{1}{2}\left[\sqrt{F'^4(z_k) + 4\mathfrak{N}_o |F'(z_k) F(z_k)|} - F'^2(z_k)\right] + \epsilon_L,$$

$$\mathfrak{N}_o = \epsilon_o(\epsilon_o + F'^2(z_o))/|F'(z_o) F(z_o)|,\quad \epsilon_o, \epsilon_L = \text{const.} \geq 0.$$

This process ends by achieving a given number of iterations $\bar{k}$ or by satisfying inequalities $|F(z_{k^*})| \leq T_{zg}$ or $100\,|z_{k^*+1} - z_{k^*}|/|z_{k^*}| \leq T_{z3}$. ($T_{z2}, T_{z3}$ are given small positive numbers).

4.4. For a qualitative estimate of thus found solution $\bar{z}^* = z_{k^*}$ the criteria $MD(\bar{z}^*)$ and $\bar{\chi}^2(\bar{z}^*)$ are used. On the mesh $\{x_{j_k} = \bar{x}_j + (k-1)\frac{h}{\bar{k}}\}_{\substack{j=1,2,\ldots,N \\ k=1,2,\ldots,\bar{k};\ \bar{k} \geq 2}}$ the defects of the collo-

cation conditions $f(x_{j_k}, \tilde{z}^*)$ (13) are calculated, and one forms quantities:

$$MD(\tilde{z}^*) = \max_{j,k} |f(x_{j_k}, \tilde{z}^*)| , \tag{27}$$

$$\bar{\chi}^2(\tilde{z}^*) = [\sum_{j=1}^{N} \sum_{k=1}^{\tilde{k}} f^2(x_{j_k}, \tilde{z}^*)] / (\tilde{k}N) . \tag{28}$$

These criteria are used to compare solutions of problem (1), (2) obtained at different values of x_b and N.

In table 1 convergence rates of the method established by numerical experience on the basis of the program RODSOL are given.

Table 1.

The rates of convergence of the method as a function of the spline mesh-step in the case M = 1.

n	m	σ*	δ	convergence rate
1,2	2	1	1/2	$O(h^2)$
	3	1	3/4	$O(h^3)$
	4	1	1	$O(h^4)$
4	4	1	1/2	$O(h^2)$
	6	2	$\delta_2 = 1/2$, $\delta_1 = 1$	$O(h^3)$
	6	3	$\delta_3 = 1/3$, $\delta_1 = 1$, $\delta_2 = 2/3$	$O(h^2)$

5. APPLICATION OF CSM WITH QUADRATIC SPLINES FOR SOLVING THE SYSTEM OF TWO EQUATIONS

By the core-splines method the problem for calculation of spin-dependent bound states of quarkonium system was solved /10/. Here we consider, as an example, a solution of the Dirac system for the bound states of a hydrogen atom /4/ :

$$\left.\begin{aligned} (-\frac{d}{dx} + \frac{r}{x}) y_1(x, z) + (+\mu - z - \frac{\eta}{x}) y_2(x, z) = 0 , \\ -(\mu + z + \frac{\eta}{x}) y_1(x, z) + (\frac{d}{dx} + \frac{r}{x}) y_2(x, z) = 0 , \end{aligned}\right\} \tag{29}$$

$$\int_0^\infty [y_1^2(x, z) + y_2^2(x, z)] dx = 1 , \tag{30}$$

where η = const. > 0 is the strength of the Coulomb force, $r = \omega(J + \frac{1}{2})$,

$$\omega = \begin{cases} +1 \text{ for states with parity } (-1)^{J+1/2} \\ -1 \text{ for states with parity } (-1)^{J-1/2} \end{cases}$$

$J = \frac{1}{2}, \frac{3}{2}, \ldots$; μ is the reduced mass, z is the energy of the system in c.m.s. $(-\mu < z < \mu)$. System (29) corresponds to a particular case of system (1) with M = 2, $n_{11} = n_{22} = 1$, $n_{12} = n_{21} = 0$. The core functions of the problem (29) have the form

$$y_{01}(x) = y_{02}(x) = x^s , \quad s = \sqrt{r^2 - \eta^2} \quad (\eta < J + \tfrac{1}{2}) , \tag{31}$$

$$y_{\infty 1}(x, z) = y_{\infty 2}(x, z) = e^{-\kappa x} , \quad \kappa = \sqrt{\mu^2 - z^2} . \tag{32}$$

Solutions of the Dirac system are known in the analytic form:

$$\bar{z}_{n^* J} = \frac{\mu(n^* + s)}{\sqrt{(n^* + s)^2 + \eta^2}} \quad (n^* = 0, 1, 2, \ldots) , \tag{33}$$

$$\bar{y}_{(n^*)\lambda}(x, z) = x^s \mathcal{P}_{n^*\lambda}(x) e^{-\kappa x} \quad (\lambda = 1, 2) , \tag{34}$$

where $\mathcal{P}_{n^*\lambda}(x)$ are polynomials of degree n^*.

Having in mind that

$$\mu + z + \frac{\eta}{x} \neq 0 \qquad x \in X_0 \quad (\mu, z, \eta > 0) ,$$

one can make the substitution

$$y_1(x, z) = \frac{1}{\mu + z + \eta/x} (\frac{d}{dx} + \frac{r}{x}) y_2(x, z)$$

which reduces system (29) to a single second order equation:

$$\{\frac{d^2}{dx^2} + \frac{\eta}{[\eta + (\mu + z) x] x} \frac{d}{dx} - \\ - [\kappa^2 - \frac{2\eta z}{x} + (s^2 + r - \frac{r\eta}{\eta + (\mu + z) x}) \frac{1}{x^2}] y_2(x, z) = 0 . \tag{35}$$

The core functions of y_2 are identical to those given by eqs. (31), (32).

The Dirac problem with $\mu = 1$, $\eta = 1/2$, $J = 1/2$, $\omega = -1$, $r = -1$, $s = \sqrt{3}/2$ in both variants (29) and (35) was solved by the core-splines method with $m = 2$, $\sigma^* = 1$ and $\delta = 1/2$. The approximate eigenvalues $\tilde{z}_{n^*}$ found at different values of the basic parameters x_b and N as well as the values of criteria MD and $\bar{\chi}^2$ are presented in table 2. Exact functions y_1 and y_2 and relative errors of the corresponding approximate functions are plotted in the Figure.

Table 2.

Exact and approximate values of some first eigenvalues of Dirac system.

n^*	x_b	N	$\tilde{z}_{n^*}$	MD	$\bar{\chi}^2$	equation
	-	-	$\bar{z}_0 = 0.866\ 025\ 403\ 8$	-	-	-
		100	0.866 025 403 0	$3.8\ 10^{-6}$	$1.9\ 10^{-14}$	(29)
0	20.	200	0.866 025 400 3	$8.6\ 10^{-6}$	$9.8\ 10^{-12}$	(29)
		300	0.866 025 419 9	$6.5\ 10^{-6}$	$5.7\ 10^{-12}$	(29)
		100	0.866 025 403 8	$3.4\ 10^{-10}$	$1.2\ 10^{-23}$	(35)
	-	-	$\bar{z}_1 = 0.965\ 925\ 826\ 3$	-	-	-
		100	0.965 925 817 3	$2.2\ 10^{-5}$	$4.4\ 10^{-11}$	(29)
1	40.	200	0.965 925 827 3	$5.3\ 10^{-7}$	$2.6\ 10^{-14}$	(29)
		300	0.965 925 802 6	$2.7\ 10^{-5}$	$6.5\ 10^{-11}$	(29)
		100	0.965 925 826 3	$3.1\ 20^{-11}$	$1.6\ 10^{-23}$	(35)
	-	-	$\bar{z}_2 = 0.985\ 121\ 054\ 8$	-	-	-
		100	0.985 122 808 9	$1.1\ 10^{-2}$	$1.2\ 10^{-4}$	(29)
2	60	200	0.985 121 294 2	$2.9\ 10^{-3}$	$7.7\ 10^{-7}$	(29)
		300	0.985 122 787 3	$5.8\ 10^{-3}$	$3.0\ 10^{-6}$	(29)
		100	0.985 121 054 8	$1.9\ 10^{-11}$	$2.9\ 10^{-24}$	(35)
	-	-	$\bar{z}_3 = 0.991\ 740\ 120\ 7$	-	-	-
		100	0.991 735 855 9	$3.8\ 10^{-2}$	$6.6\ 10^{-5}$	(29)
		100	0.991 736 218 6	$4.4\ 10^{-3}$	$2.0\ 10^{-6}$	(35)
		200	0.991 739 822 9	$9.6\ 10^{-3}$	$4.2\ 10^{-6}$	(29)
3	85.	200	0.991 740 204 5	$2.4\ 10^{-3}$	$4.8\ 10^{-7}$	(35)
		300	0.991 739 982 6	$2.6\ 10^{-3}$	$3.0\ 10^{-7}$	(29)
		300	0.991 740 516 6	$1.2\ 10^{-3}$	$1.2\ 10^{-7}$	(35)

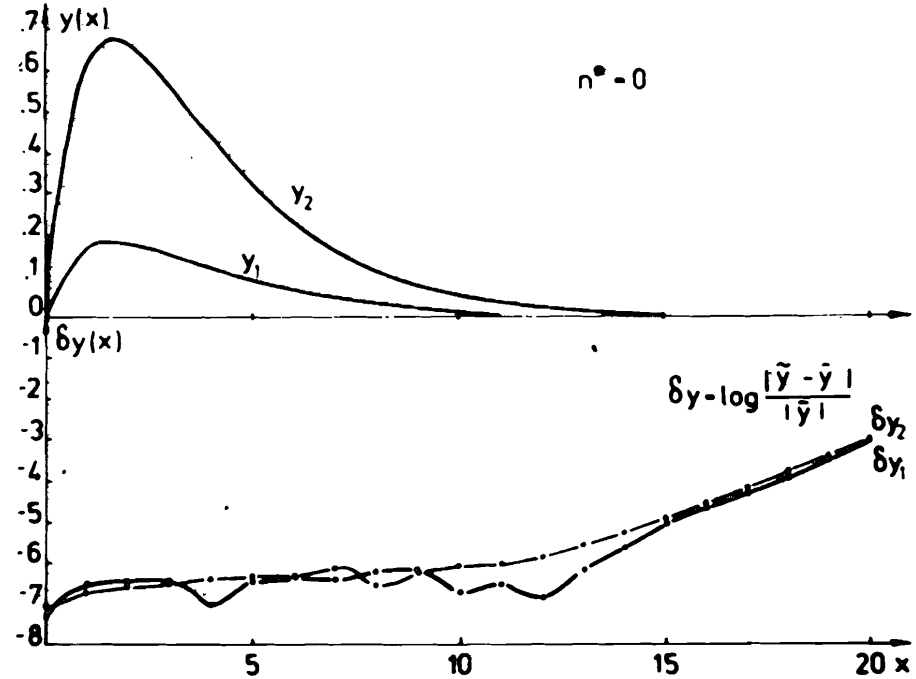

Fig.1. Exact wave functions of the ground state of the Dirac system and the logarithms of relative errors of the corresponding approximate functions.

REFERENCES

1. Aleksandrov L., Karadjov D. J.Comput.Math. and Math.Phys., 1980, 20, p.923 (sov.ed.).
2. Aleksandrov L., Drenska M., Karadjov D. J.Comput.Math. and Math.Phys., 1982, 22, p.375 (sov.ed.).
3. Aleksandrov L. et al. JINR, P11-80-752, Dubna, 1980.
4. Sommerfeld A. Wave Mechanics, GTTI, Leningrad-Moscow, 1933, (sov.ed.).
5. Fedorjuk M.V. Asymptotic Methods for Linear Ordinary Differential Equations, Nauka, Moscow, 1983.
6. Stechkin S.B.,Subbotin Ju.N.Splines in Computational Mathematics, Nauka, Moscow, 1976.
7. De Boor C. A Practical Guide to Splines, In: Applied Math. Sci. vol.27, Springer-Verlag, New York-Heidelberg-Berlin, 1978.
8. Forsythe G.E., Malcolm M.A., Moler C.B. Computer Methods for Mathematical Computations, Prentice-Hall,inc., Englewood Cliffs N.J., 1977.

9. Aleksandrov L. J.Comput.Math. and Math.Phys., 1971, 11, p.36, (sov.ed.); JINR, P5-5515, Dubna, 1970.
10. Aleksandrov L., Karadjov D., Morozov P. JINR, P2-86-349, Dubna, 1986.

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Александров Л., Дренска М., Караджов Д. E5-86-713

Метод стержневых сплайнов для решения квантовомеханических систем дифференциальных уравнений для связанных состояний

Приводится обобщение метода стержневых сплайнов для решения полной задачи на связанные состояния для систем из M линейных дифференциальных уравнений с коэффициентами, зависящими от спектрального параметра. Описана рекурсивная вычислительная схема построения базисных сплайнов. Волновые функции выражаются как линейные комбинации от базисных сплайнов, являющихся приближенными частными решениями системы. Спектральный параметр определяется из условия существования нетривиального решения линейной алгебраической системы размерностью /MxM/ в последнем коллокационном узле. Нетривиальное решение этой системы определяет /M - 1/ коэффициентов линейных оболочек, выражающих волновые функции. Последний коэффициент определяется из дополнительного краевого /нормировочного/ условия для системы. Обсуждаются вычислительные аспекты метода и его конкретная алгоритмическая реализация, использованная в компьютерной программе RODSOL. В качестве примера приводится численное решение системы Дирака для связанных состояний атома водорода.

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Aleksandrov L., Drenska M., Karadjov D. E5-86-713

The Core-Splines Method for Solution of Quantum-Mechanical Systems of Differential Equations for Bound States

A generalization of the core-splines method is given in the case of solution of the general bound-states problem for a system of M linear differential equations with coefficients depending on the spectral parameter. The recursion scheme for construction of basic splines is described. The wave functions are expressed as linear combinations of basic splines, which are approximate partial solutions of the system. The spectral parameter (the eigenvalue) is determined from the condition for existence of a nontrivial solution of a (MxM) linear aigebraic system at the last collocation point. The nontrivial solutions of this system determine (M - 1) coefficients of the linear spans, expressing the wave functions. The last unknown coefficient is determined from a boundary (or normalization) condition for the system. The computational aspects of the method are discussed, in particular, its concrete algorithmic realization used in the program RODSOL. The numerical solution of the Dirac-system for the bound states of a hydrogen atom is given as an example.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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