JOURNAL OF COMPUTATIONAL PHYSICS 54, 221–236 (1984)

Numerical Solution of a System of Integrodifferential Equations Arising from the Quantum Mechanical Three-Body Problem with Coulomb Interaction

V. S. MELEZHIK, I. V. PUZYNIN, T. P. PUZYNINA, AND L. N. SOMOV

Joint Institute for Nuclear Research, Dubna, Moscow, U.S.S.R

Received August 28, 1980; revised September 23, 1983

Two iterative schemes are proposed for numerically solving an eigenvalue problem for a large system of integrodifferential equations arising from the three-body problem with Coulomb interaction in quantum mechanics. The iterative corrections are determined by solving a set of well-conditioned boundary problems for a system of differential equations.

1. INTRODUCTION

The quantum mechanical three-body problem with Coulomb interaction has a number of important physical applications. For instance, this system is used as a model for the description of μ-atomic and μ-mesic molecular processes in hydrogen isotope mixtures [1, 2].

The values of the total energy $\varepsilon_{n\tau}$ and the wave functions $\Psi(\mathbf{r}, \mathbf{R})$ of different states $|n\tau\rangle$ of μ-mesic molecules are found from the Schrödinger equation in six-dimensional space $(\mathbf{r}, \mathbf{R})$ [3–5],

$$(H - \varepsilon_{n\tau})\, \Psi_{n\tau}(\mathbf{r}, \mathbf{R}) = 0. \tag{1.1}$$

Here $\mathbf{R}$ is the vector connecting the nuclei of mesic molecules a and b with the masses M_a and M_b $(M_a \geqslant M_b)$ and $\mathbf{r}$ is the vector connecting the midpoint of R and μ^--meson with the mass m_μ. The quantities r_a and r_b are the distances from nuclei a and b to the μ^--meson. Quantum numbers n and τ specify the motion of the μ^--meson (n) in a mesic molecule and the relative motion of nuclei (τ). We shall consider the energy levels of mesic molecules that correspond to the ground state $n = 0$. For such states with $n = 0$ and a given parity, the wave function depends only on quantum numbers $\tau = (J, \theta)$, where J and θ are the rotation and vibration quantum numbers, respectively. In the units $e = \hbar = 1$ the operator $\hat{H}$ has the form $\hat{H} = \hat{T}_a + \hat{h}_a + 1/R$,

$$\hat{T}_a = -\frac{1}{2M}\left[\left(\nabla_{\mathbf{R}} + \frac{\kappa}{2}\nabla_{\mathbf{r}}\right)^2 + \left(\frac{1+\kappa}{2}\right)^2 \Delta_{\mathbf{r}}\right],$$

$$\hat{h}_a = -\frac{1}{2m_a}\Delta_{\mathbf{r}} - \frac{1}{r_a} - \frac{1}{r_b}, \qquad M^{-1} = M_a^{-1} + M_b^{-1}, \tag{1.2}$$

$$m_a^{-1} = m_\mu^{-1} + M_a^{-1}, \qquad \kappa = \frac{M_b - M_a}{M_b + M_a}.$$

0021-9991/84 $3.00

At present there are two well-known methods for the numerical solution of Eq. (1.1), namely, variational [4, 5] and adiabatic [3].

Variational calculations have been used to obtain values of the binding energy of the ground state and of some excited states of μ-mesic molecules. These calculations are cumbersome and are not always effective in determining the energy levels of weakly bound excited states, unless a proper choice of basic functions is made.

New experimental measurements of formation rates of mesic molecules stimulate new interest in high accuracy calculations of energy levels and wave functions of weakly bound excited states of μ-mesic molecules. Based on an assumption about the existence of energy levels of weakly bound excited states of mesic molecules, a theoretical prediction of resonance dependence of formation rates of mesic molecules $dd\mu$ and $dt\mu$ [6] on temperature can be made, which is in agreement with experiments [7, 8]. Although variational calculations were not of much help in computational schemes the adiabatic approach allows one to calculate energy levels of all bound states of μ-mesic molecules and to determine the weakly bound excited states of mesic molecules $dd\mu$ and $dt\mu$. The results obtained are in good agreement with the variational calculations when the latter are carried out carefully [9]. Progress in the creation of numerical schemes for the solution of Eq. (1.1) utilizing the adiabatic method is closely related to the development of effective algorithms for the numerical solution of the quantum-mechanical problem of two Coulomb centers [10, 11].

The adiabatic representation of the three-body problem with Coulomb interaction is based on the expansion of the wave function $\Psi(\mathbf{r}, \mathbf{R})$ of Eq. (1.1) over the set of wave functions of the two-center problem [3, 9],

$$\Psi(\mathbf{r}, \mathbf{R}) = \sum_j \phi_j(\mathbf{r}; R)\, \chi_j(\mathbf{R}) + \sum_s \int \phi_s(\mathbf{r}, k; R)\, \chi_s(k, \mathbf{R})\, dk. \tag{1.3}$$

Substitution of this expression in Eq. (1.1) and subsequent integrations over the coordinates of vector $\mathbf{r}$ and angular variables of vector $\mathbf{R}$ leads to an infinite system of integrodifferential equations ($m_a = 1$) [9],

$$\begin{aligned}
&\left[\frac{d^2}{dR^2} - \frac{J(J+1) - 2m^2}{R^2} - \frac{2M}{R} + 2M\varepsilon_{J\theta}\right] \hat{I}\chi_i(R) \\
&\quad - \sum_{j=1}^{\infty} \hat{u}_{ij}(R)\, \chi_j(R) - \sum_{s=1}^{\infty} \int_0^{\infty} \hat{u}_{is}(k, R)\, \chi_s(k, R)\, dk = 0, \\
&\left[\frac{d^2}{dR^2} - \frac{J(J+1) - 2m^2}{R^2} - \frac{2M}{R} + 2M\varepsilon_{J\theta}\right] \hat{I}\chi_s(k, R) \\
&\quad - \sum_{j=1}^{\infty} \hat{u}_{sj}(k, R)\, \chi_j(R) - \sum_{s'=1}^{\infty} \int_0^{\infty} \hat{u}_{ss'}(k, k', R)\, \chi_{s'}(k', R)\, dk' = 0,
\end{aligned} \tag{1.4}$$

with the boundary conditions,

$$\chi_i(0) = \lim_{R \to \infty} \chi_i(R) = 0, \qquad \chi_s(k, 0) = \lim_{R \to \infty} \chi_s(k, R) = 0, \tag{1.5}$$

for the radial wave functions from which the values of binding energy levels can be determined. Here m is the magnetic quantum number.

The system of Eqs. (1.4) is given in the "two-component form,"

$$\hat{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \chi_i(R) = \begin{pmatrix} \chi_{ia}(R) \\ \chi_{ib}(R) \end{pmatrix}, \qquad \chi_s(k, R) = \begin{pmatrix} \chi_{sa}(k, R) \\ \chi_{sb}(k, R) \end{pmatrix}.$$

The coefficients of Eqs. (1.4) represent 2×2 dimensional matrices, for instance,

$$\hat{u}_{ij}(R) = \begin{pmatrix} u_{iaja}(R) & u_{iajb}(R) \\ u_{ibja}(R) & u_{ibjb}(R) \end{pmatrix},$$

where the components are matrix elements [12] for the two Coulomb centers problem. Asymptotic properties as $R \to 0$ and $R \to \infty$ have been investigated [13], for example, as $R \to \infty$, $u_{1a1a}(R) \to 0$. Here we consider the general case of $M_a \neq M_b$. For identical nuclei, one can use the one-component notation, since [3],

$$u_{iaja}(R) = u_{ibjb}(R), u_{iajb}(R) = u_{ibja}(R) = 0.$$

Formulae (1.4), (1.5) can be written symbolically as

$$[D^{\infty} + S^{\infty}]\chi = \lambda\chi, \tag{1.6}$$

where D^{∞} is the differential operator determined on the semiaxis $0 \leqslant R < \infty$, and S^{∞} is the integral operator on the semiaxis $0 \leqslant k < \infty$, $\lambda = -2M\varepsilon_{J\theta}$.

In developing algorithms and programs for the numerical solution of the system (1.4), one should take into account the specific properties of the adiabatic representation. These characteristics are:

(i) The effective potentials of the system of Eqs. (1.4) have long-range characters, i.e., slowly reach the asymptotes as $R \to \infty$ [13].

(ii) Numerical analysis of the convergence of the expansion (1.3) leads to a solution of sequences of finite systems of Eqs. (1.4), a number which can be large.

(iii) The effective potentials of the system of a finite number of Eqs. (1.4) are given as tables for a large number of nodes.

(iv) The energy levels of weakly bound excited states of mesic molecules are of an order of 10^{-3} of the depth of the effective potentials.

This paper describes two computational Schemes A and B for the solution of the local spectral problem for the system (1.4) containing a finite number of equations, and analysis of the convergence of expansion (1.3). The schemes depend on the neglect of different elements in the potential matrix (1.4). The peculiarities of these schemes are demonstrated by the calculation of the energy levels of mesic molecules $pd\mu$ and $dd\mu$, both of the ground states and excited states. The spectrum of the mesic molecule $dd\mu$ includes a weakly bound level ($J = \theta = 1$) with binding energy of about 2 eV (the depth of the effective potential well is about 600 eV).

2. Approximation of the Singular Spectral Problem (1.4), (1.5)

Numerical analysis of the convergence of expansion (1.3) is reduced to the solution of system (1.4) with boundary conditions (1.5), in which indices i and s take the values $1, 2, \ldots, N_i$ and $1, 2, \ldots, N_s$, respectively, for different values of $\{N_i, N_s\}$. Therefore, for each given pair the singular Sturm–Liouville problem should be solved for the system of integrodifferential equations in the range $0 \leqslant R < \infty$ and $0 \leqslant k < \infty$. An approximate solution can, however, only be obtained in the rectangle $0 \leqslant R \leqslant R_m$, $0 \leqslant k \leqslant k_m$. A semidiscrete representation of the problem (1.4), (1.5) on a chosen net of nodes with respect to k; $\{k_\alpha\}$ is obtained by approximating the integrals over k in the system of Eqs. (1.4) by the quadrature formula, $\int_{k_0}^{k_m} f(k)\,dk \to \sum_{\alpha}^{N_k} f(k_\alpha) P(k_\alpha) \Delta k_\alpha$. As a result, we get the following system of differential equations:

$$\begin{aligned}
&\left[\frac{d^2}{dR^2} - \frac{J(J+1)-2m^2}{R^2} - \frac{2M}{R} + 2M\varepsilon_{J\theta}\right] \hat{I}\chi_i(R) \\
&\quad - \sum_{j=1}^{N_i} \hat{u}_{ij}(R)\chi_j(R) - \sum_{s=1}^{N_s}\sum_{\alpha=1}^{N_k} \hat{u}_{is}(k_\alpha, R) P(k_\alpha) \Delta k_\alpha \chi_s(k_\alpha, R) = 0, \\
&\left[\frac{d^2}{dR^2} - \frac{J(J+1)-2m^2}{R^2} - \frac{2M}{R} + 2M\varepsilon_{J\theta}\right] \hat{I}\chi_s(k_\alpha, R) \\
&\quad - \sum_{j=1}^{N_i} \hat{u}_{sj}(k_\alpha, R)\chi_j(R) \\
&\quad - \sum_{s'=1}^{N_s}\sum_{\alpha'=1}^{N_k} \hat{u}_{ss'}(k_\alpha, k'_\alpha, R) P(k_\alpha) P(k'_\alpha) \Delta k_\alpha \Delta k'_\alpha \chi'_s(k'_\alpha, R) = 0.
\end{aligned} \tag{2.1}$$

Here Δk_α is the node step with respect to k, and $P(k_\alpha)$ is the weight of the quadrature formula. Simpson's rule of accuracy $O(\Delta k_\alpha^4)$ has been used in the calculations. In matrix notation for brevity the indices (J, θ) will be omitted,

$$\left[\left(\frac{d^2}{dR^2} + 2M\varepsilon\right)\hat{I} - \hat{U}(R)\right]\chi(R) = 0, \tag{2.2}$$

where

$$\hat{U}(R) = \begin{pmatrix} \hat{U}^{dd}(R) & \hat{U}^{dc}(R) \\ \hat{U}^{cd}(R) & \hat{U}^{cc}(R) \end{pmatrix}.$$

Here $\hat{U}^{dd}(R)$ is the matrix of the potentials,

$$\hat{U}^{dd}(R) = \left[\frac{J(J+1)-2m^2}{R^2} + \frac{2M}{R}\right]\delta_{ij}\hat{I} + \hat{u}_{ij}(R)$$

connecting the discrete spectrum states of the two-center problem, and $\hat{U}^{dc}(R)$ and $\hat{U}^{cd}(R)$ are the matrices of the potentials connecting the states of the discrete and continuous spectra of the two-center problem,

$$\hat{U}^{dc}(R) = \hat{u}_{is}(k_\alpha, R)\, P(k_\alpha)\, \Delta k_\alpha; \qquad \hat{U}^{cd}(R) = \hat{u}_{sj}(k_\alpha, R).$$

The matrix $\hat{U}^{cc}(R)$ connects the states of the continuous spectrum of the two-center problem,

$$\hat{U}^{cc}(R) = \left[\frac{J(J+1) - 2m^2}{R^2} + \frac{2M}{R}\right] \delta_{ss'}\, \delta_{\alpha\alpha'} \hat{I} + \hat{u}_{ss'}(k_\alpha, k'_\alpha, R)\, P(k_\alpha)\, P(k'_\alpha)\, \Delta k_\alpha\, \Delta k'_\alpha.$$

The boundary conditions (1.5) are replaced by

$$\chi(0) = 0, \qquad \left[\frac{d}{dR}\hat{I} + \hat{F}(\varepsilon, R_m)\right] \chi(R_m) = 0, \tag{2.3}$$

which makes the vector function $\chi(R)$ bounded for $0 \leqslant R < \infty$ and allow one to take into account the asymptotics of the wave functions as $R \to \infty$. Such a substitution also brings in an error in the solution, which can be estimated by comparing the solutions for different values of R_m.

3. Statement of the Problem

After these approximations it is necessary to find the solution of the regular Sturm–Liouville problem for the system $2N = 2(N_i + N_k \times N_s)$ of second-order differential equations (2.2) with boundary conditions (2.3) on the interval $[0, R_m]$. Note that an error in the solution $\{\varepsilon^*, \chi^*\}$ of the approximate problem (2.2), (2.3) depends on the number of equations $2N$, the upper limit of integration k_m, net step with respect to $k - \Delta k$, and the boundary point of the interval $[0, R_m] - R_m$ under consideration.

Consider two computational schemes for the matrices of the coefficients, a special form of system (2.2) (see Fig. 1). In the first case the matrix of the potentials $\hat{U}^{dd}(R)$ are completely filled, $\hat{U}^{dc}(R)$ and $\hat{U}^{cd}(R)$ contain just one row, and $\hat{U}^{cc}(R)$ just the diagonal. In the second case the matrix $\hat{U}(R)$ contains the first row, the first column, and the diagonal, and all other elements are zero. Each element of $\hat{U}(R)$ is a 2×2 matrix with dimension $2N \times 2N$.

4. The Iteration Method of Solution

Problem (2.2), (2.3) is treated as a nonlinear functional equation,

$$\varphi(Z) = 0, \qquad \varphi = (\varphi^{(1)}, \varphi^{(2)}, \varphi^{(3)}, \varphi^{(4)}), \tag{4.1}$$

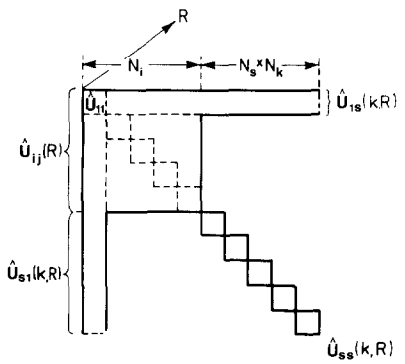

FIGURE 1

with respect to the pair $Z = (\lambda, \chi) \in R \times C^2[0, R_m]$, $(\lambda = -2M\varepsilon)$, where the components $\varphi^{(j)}$ are determined as follows:

$$\varphi^{(1)}(\lambda, \chi) \equiv \left[\frac{d^2}{dR^2}\hat{I} - (\lambda\hat{I} + \hat{U}(R))\right]\chi(R) = 0, \tag{4.1a}$$

$$\varphi^{(2)}(\lambda, \chi) \equiv \chi(0) = 0, \tag{4.1b}$$

$$\varphi^{(3)}(\lambda, \chi) \equiv \left[\frac{d}{dR}\hat{I} + \hat{F}(\lambda, R_m)\right]\chi(R_m) = 0. \tag{4.1c}$$

The fourth component is the normalization condition of the wave functions $\chi(R)$,

$$\varphi^{(4)}(\lambda, \chi) \equiv (\chi, \chi) - 1 = 0. \tag{4.1d}$$

Here

$$(\chi, \chi) = \sum_{i=1}^{N} \int_0^{R_m} [\chi_{ia}^2(R) + \chi_{ib}^2(R)]\, dR.$$

Suppose that a simple localized solution of Eq. (4.1) $Z = (\lambda^*, \chi^*)$ exists and the initial approximation $Z_0 = (\lambda_0, \chi_0)$ to this solution is known.

To solve the functional equation $\varphi(Z) = 0$, apply the continuous analog of Newton's method [14–16]. For the continuous parameter $0 \leqslant t < \infty$ the following relations are valid:

$$\varphi'(Z(t))\, Z'(t) = -\varphi(Z(t)), \qquad Z(0) = Z_0. \tag{4.2}$$

Here φ' is a Frechet derivative of the operator φ, and $Z'(t) = (\lambda'(t), \chi'(t)) = (\mu(t), \mathbf{V}(t))$. This approach is referred to as the invariant imbedding method [16]. In [15] it is shown that the smoothness of the operator φ in the vicinity of an unknown isolated solution Z^* leads to the asymptotic relation

$$\lim_{t \to \infty} \|Z^* - Z(t)\| = 0. \tag{4.3}$$

The evolution equation (4.2) is solved by the Euler method. The semiaxis $0 \leqslant t < \infty$ is divided by nodes t_k $(k = 0, 1,...)$ with step τ_k

$$t_{k+1} = t_k + \tau_k.$$

The process of solving Eq. (4.2) may be considered as the iteration process of solving Eq. (4.1).

At each step number k, $(t = t_k)$ the linear problem,

$$\varphi'(Z_k)\,\Delta Z_k = -\varphi(Z_k), \tag{4.4}$$

is solved with respect to the iteration correction $\Delta Z_k = (\lambda'(t_k), \chi'(t_k)) = (\mu_k, \mathbf{V}_k)$ under the known approximation Z_k to the desired solution. Then a new approximation $Z_{k+1} = (\lambda_{k+1}, \chi_{k+1})$ is found,

$$Z_{k+1} = Z_k + \tau_k \Delta Z_k = (\lambda_k + \tau_k \mu_k, \chi_k + \tau_k \mathbf{V}_k), \tag{4.5}$$

if step τ_k is defined. For $\tau_k = 1$ we have the Newton method. In the vicinity of the desired solution, the method provides a minimum for [17],

$$\delta_k = \|\varphi(Z_k)\|.$$

Choose τ_k so that this property is fulfilled at each step.

The operator φ for Eq. (4.1) can be separated into two main components

$$\varphi(\lambda, \chi) = \begin{pmatrix} (D - \lambda\hat{I})\chi \\ (\chi, \chi) - 1 \end{pmatrix}, \tag{4.6}$$

where D is the differential operator (4.1a) including the boundary conditions (4.1b) and (4.1c). Equation (4.4) with respect to the iteration corrections $(\mu_k, \mathbf{V}_k)$ is the system of equations,

$$\begin{aligned} (D - \lambda_k \hat{I})\mathbf{V}_k - \mu_k \chi_k &= -(D - \lambda_k \hat{I})\,\chi_k, \\ 2(\chi_k, \mathbf{V}_k) &= 1 - (\chi_k, \chi_k). \end{aligned} \tag{4.7}$$

The inverse operator $[\varphi'(Z_k)]^{-1}$ for this system exists [18] and is bounded in the vicinity of the solution Z^*. To simplify the solution of the system (4.7) let

$$\mathbf{V}_k = -\chi_k + \mu_k \mathbf{v}_k, \tag{4.8}$$

where $\mathbf{v}_k$ is the solution of the boundary problem

$$(D - \lambda_k \hat{I})\mathbf{v}_k = -\chi_k. \tag{4.9a}$$

Solving this problem and substituting an expression for $\mathbf{V}_k$ (4.8) with an unknown μ_k into the second equation of the system (4.7), produces

$$\mu_k = \frac{1 + (\chi_k, \chi_k)}{2(\chi_k, \mathbf{v}_k)}. \tag{4.9b}$$

Formulae (4.9) and (4.5) correspond at $\tau_k = 1$ to an inverse iteration method [19]. As $\lambda_k \to \lambda^*$, where λ^* is a point of the spectrum of operator D, we are faced with the ill-conditioned problem (4.9a). To avoid the construction of special algorithms for its solution, consider the well-known modification of the Newton process,

$$\varphi'(Z_0)\,\Delta Z_k = -\varphi(Z_k), \tag{4.10}$$

$k = 0, 1, \ldots$, Z_0 is the given element. Now instead of formulae (4.8), (4.9), we have

$$(D - \lambda_0 \hat{I})\,\mathbf{v}_0 = -\chi_0, \tag{4.11a}$$

$$(D - \lambda_0 \hat{I})\,\mathbf{w}_k = -(D - \lambda_k \hat{I})\,\chi_k, \tag{4.11b}$$

$$\mu_k = \frac{1 - (\chi_k, \chi_k) - 2(\chi_0, \mathbf{w}_k)}{2(\chi_0, \theta_0)}, \tag{4.11c}$$

$$\mathbf{V}_k = \mathbf{w}_k + \mu_k \mathbf{v}_0. \tag{4.11d}$$

The ill-conditioned problem (4.9a) is replaced by two boundary problems (4.11a) and (4.11b) with a nondegenerate operator $(D - \lambda_0 \hat{I})^{-1}$. Equation (4.11a) is solved only once on the first step of the iteration process (4.11) at $\lambda_0 \neq \lambda^*$. Computation time is drastically reduced particularly. Deceleration of convergence in contrast with the classical Newton process (4.8), (4.9) can be compensated by choosing a good initial approximation.

5. Solution of the Boundary Problem for the Iteration Correction

The most complicated part in the numerical solution of the iteration process (4.11) is due to the boundary problem (4.11a), (4.11b). Consider problem (4.11a) in a form analogous to (2.2). The index $k = 0$ is omitted,

$$(D - \lambda \hat{I})\mathbf{v} = -\chi, \tag{5.1}$$

where

$$D = \begin{pmatrix} D^{dd}(R) & D^{dc}(R) \\ D^{cd}(R) & D^{cc}(R) \end{pmatrix} = \begin{pmatrix} (d^2/dR^2)\,\hat{I} - \hat{U}^{dd}(R) & -\hat{U}^{dc}(R) \\ -\hat{U}^{cd}(R) & (d^2/dR^2)\,\hat{I} - \hat{U}^{cc}(R) \end{pmatrix}, \tag{5.2}$$

and $0 < R < R_m$. For $R = 0$ and $R = R_m$ the operator is represented by formulae (2.3).

In solving the given large system of differential equations*, it is advantageous to use specific properties of the problem, the vacuity of the matrix of the coefficients of the system (5.1) (see Fig. 1); a low-accuracy iteration correction to the sought solution $\mathbf{v}$ is acceptable. Convergence of the Newton process (4.10) in this case requires a relative accuracy of about 10^{-1} [20] when calculating $\mathbf{v}$.

Consider two computational schemes for solving the equations for the iteration corrections.

Scheme A. The matrix D^{dd} is completely filled. Use the representation (5.2) for the operator D and rewrite Eq. (5.1) in the form

$$\begin{aligned}(D^{dd} - \lambda\hat{I})\,\mathbf{v}^d &= -\boldsymbol{\chi}^d - D^{dc}\mathbf{v}^c,\\ (D^{cc} - \lambda\hat{I})\,\mathbf{v}^c &= -\boldsymbol{\chi}^c - D^{cd}\mathbf{v}^d,\end{aligned} \tag{5.3}$$

where

$$\mathbf{v} = \begin{pmatrix}\mathbf{v}^d\\ \mathbf{v}^c\end{pmatrix}, \qquad \boldsymbol{\chi} = \begin{pmatrix}\boldsymbol{\chi}^d\\ \boldsymbol{\chi}^c\end{pmatrix}.$$

To solve Eq. (5.3) use the method of successive approximations. For the first step ($l = 1$) assume $\mathbf{v}^c = 0$ and solve the boundary problem

$$(D^{dd} - \lambda\hat{I})\,\mathbf{v}^d = -\boldsymbol{\chi}^d. \tag{5.4}$$

Substitute the solution $\mathbf{v}^d$ in the right-hand side of the second matrix equation of (5.3) and solve the boundary problem

$$(D^{cc} - \lambda\hat{I})\,\mathbf{v}^c = -\boldsymbol{\chi}^c - D^{cd}\mathbf{v}^d. \tag{5.5}$$

Having found $\mathbf{v}^c$ repeat the solution of Eqs. (5.4), (5.5) with the right-hand side of the first matrix equation (5.3) containing $\mathbf{v}^c_{l-1}$.

The iteration process (with respect to l) for solving the problem (5.1) is described by the equations,

$$\begin{aligned}(D^{dd} - \lambda\hat{I})\,\mathbf{v}^d_l &= -\boldsymbol{\chi}^d - D^{dc}\mathbf{v}^c_{l-1},\\ (D^{cc} - \lambda\hat{I})\,\mathbf{v}^c_l &= -\boldsymbol{\chi}^c - D^{cd}\mathbf{v}^d_l.\end{aligned} \tag{5.7a}$$

Convergence of the iteration process (5.7a) is investigated numerically. Equation (4.11a) is solved only once at $k = 0$. An analogous "inner" iteration process is constructed at each step of the "outer" Newton process (4.10) and for the solution of the boundary problem (4.11b).

Problem (5.4) is solved numerically by the method of finite differences. Approximation of the operator D with accuracy of order $O(h^2)$ (h is the step of the difference

* It is shown below that to achieve the required accuracy, one should solve a system of about 300 equations.

net) and an alternating implicit matrix algorithm are used [21]. The numerical algorithm is easily obtained, since system (5.5) consists of $N_k \times N_s$ independent matrix equations (see Fig. 1) ($i = N_i + 1, \ldots, N$),

$$\left[\frac{d^2}{dR^2}\hat{I} - (\lambda\hat{I} + \hat{U}_{ii}^{cc}(R))\right]\mathbf{v}_i^c(R) = -\chi_i^c(R) + \sum_j^{N_i} \hat{U}_{ij}^{cd}(R)\,\mathbf{v}_j^d(R). \tag{5.6}$$

Scheme B. In matrix D the diagonal, the first row, and first column are assumed to be nonzero.

Numerical investigations show that replacing the matrix of effective potentials (2.2) by a matrix of a special type (see Fig. 1),

$$\hat{U}(R) = \begin{pmatrix} \hat{U}_{11}(R) & \hat{U}_{12}(R) & \hat{U}_{13}(R) & \cdots & \hat{U}_{1N}(R) \\ \hat{U}_{21}(R) & \hat{U}_{22}(R) & 0 & \cdots & 0 \\ \hat{U}_{31}(R) & 0 & \hat{U}_{33}(R) & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ \hat{U}_{N1}(R) & 0 & 0 & \cdots & \hat{U}_{NN}(R) \end{pmatrix}, \tag{5.8}$$

determines eigenvalues which differ slightly from the true eigenvalues of the original problem (2.2) [9]. This allows one to modify the described computational scheme for special matrices (5.8) by treating the problem as a possible adiabatic representation of the original problem (1.1). This modification leads to the construction of an iteration procedure for solving the boundary problems,

$$\begin{aligned} &(D_{11} - \lambda\hat{I})\,\mathbf{v}_{1l} = -\boldsymbol{\chi}_1 - \sum_{i=1}^{N} D_{1i}\mathbf{v}_{il-1}; \qquad \mathbf{v}_{i0} = 0;\ i = 2, 3, \ldots, N, \\ &(D_{ii} - \lambda\hat{I})\,\mathbf{v}_{il} = -\boldsymbol{\chi}_i - D_{i1}\mathbf{v}_{1l}, \end{aligned} \tag{5.7b}$$

that corresponds to the matrix structure (5.8). The numerical procedure of the iteration process (5.7b) is analogous to that of (5.7a). The correction μ_k is determined numerically by approximating the integrals in formula (4.11c) with Simpson's rule using the modes of the difference net.

6. Some Details of the Computational Procedure

The computational schemes under consideration are programmed in FORTRAN for a CDC-6500 computer. The programs will calculate energy levels of mesic molecules and their wave functions [9] using boundary conditions $\chi(0) = \chi(R_m) = 0$. Numerical investigations have shown fast convergence of "inner" iteration processes (5.7). A relative accuracy of the calculation of the iteration corrections $\mathbf{v}_0$, $\mathbf{w}_k \sim 10^{-2}$ is achieved per two to three iterations with respect to computational Scheme A. The convergence of iterations (5.7b) is somewhat slower ($l_{\max} \sim 3$–4). Computational

Scheme B is simpler and reduces computational time by a factor of five in contrast with Schema A. Convergence of the Newton process (4.11) is checked by the decrease in the quantity,

$$\delta_k = \max_i |(D_h - \lambda_{hk}\hat{I})\chi_{hk}(R_i)|, \tag{6.1}$$

where D_h is the finite-difference approximation of the differential operator D (5.2) and i is the number of the node of the difference net.

In solving the boundary value problems (5.7) by the matrix implicit alternating direction method, only three neighboring mesh points $R_i - h$, R_i, $R_i + h$ [21] are required. This minimizes computer storage containing potentials $\hat{U}(R_i)$ with only three neighbouring nodes of the difference network in R being required while other values are stored on tape. This structure makes it possible to increase the number of mesh points without increasing the computer storage size occupied by the routine.

In Table I some quantities characterising the convergence of the computational scheme (4.11) are presented. The Newton process converges in three to five iterations. The time of one iteration by Scheme B ~2 min, the number of equations to be solved ~300, and the number of mesh points ~300. An initial condition for the iterations uses the "two-level approximation" of the adiabatic representation (two equations in the system (2.2)) [22]. Step τ_k in the initial approximation is determined from the condition of minimum of the quantity (6.1) allowing extended range of convergence of the method. With increasing N put τ equal to 1 (Newton method).

Briefly, consider errors in the numerical solution of (1.6), where the matrix structure of coefficients of the system (1.4) is given. Errors, both of the approximation (see Introduction) and of the numerical solution of Eqs. (2.2), (2.3), are included.

If the difference nodes for Eqs. (4.11a)–(4.11c) are fixed, the iteration process

TABLE I

Convergence of the Computer Scheme

Mesic Molecule	k	δ_k	$-\varepsilon^k_{J\theta}$(eV)	λ_k
$dd\mu$	0	0.48	2.50	0.880×10^{-2}
$J = \theta = 1$	5	0.14×10^{-6}	1.91	0.671×10^{-2}
$pd\mu$	0	0.18	225.00	0.52826
$J = \theta = 0$	3	0.4×10^{-7}	221.52	0.52010

Note. Here k is the iteration number of the computational process, δ_k is determined by formula (6.1), $\varepsilon^k_{J\theta}$ is the level of energy of the mesic molecule on the kth step, $\lambda_k = -2M\varepsilon^k_{J\theta}$ is the eigenvalue in the units of the problem ($m_a = \hbar = e = 1$). The calculations are performed by the Scheme B at $\chi(0) = \chi(R_m) = 0$, $R_m = 60$, $N = 84$ for $pd\mu$, and $N = 131$ for $dd\mu$. As the wave functions of the initial approximation ($k = 0$) we have used the wave functions which have been obtained while solving the first two equations (one equation for $dd\mu$) in the system (2.2).

(4.11), (4.5) in the vicinity of a sought solution at $\tau_k = 1$ can be considered as a modified Newton method for solving the nonlinear system of algebraic equations,

$$\varphi_h(Z_h) = \begin{pmatrix} D_h \chi_h - \lambda_h \chi_h \\ (\chi_h, \chi_h) - 1 \end{pmatrix} = 0, \qquad Z_h = \{\lambda_h, \chi_h\}, \tag{6.2}$$

approximating Eqs. (2.2), (2.3) with accuracy of order $O(h^2)$. That system (6.2) has a solution for the Hermitian operator with boundary condition (4.1c) which is λ-independent, follows from [23]. How accurately the problem (6.2) is solved by the modified Newton method can be seen from the estimate achieved in the course of iterations of the quantity δ_K (6.1), where K is the number of iterations and $(\chi_{hK}, \chi_{nK}) = 1$. For the convergence of iterations the estimate [18],

$$\|Z_h^* - Z_{hK}\| \leqslant c_1 \delta_K, \tag{6.3}$$

is valid, where Z_h^* is a solution of Eq. (6.2). According to [14] the eigenvalue λ_h^* satisfies

$$|\lambda_h^* - \lambda_{hK}| < c_2 \delta_K, \tag{6.4}$$

where c_1, $c_2 = \text{const.} > 0$.

For the chosen difference scheme with approximation order $O(h^2)$ convergence of the difference solution $\{\lambda_h^*, \chi_h^*\}$ to solution $\{\lambda^*, \chi^*\}$ of Eqs. (2.2), (2.3) is quadratic in h [24], i.e.,

$$\|Z^* - Z_h^*\| < c_3 h^2, \qquad c_3 = \text{const.} > 0. \tag{6.5}$$

Therefore,

$$|\lambda^* - \lambda_{hK}| + \|\chi^* - \chi_{hK}\| = \|Z^* - Z_{hK}\| < c_4(\delta_K + h^2), \qquad c_4 > 0. \tag{6.6}$$

For $\delta_K \ll h^2$, the main error is generated by the difference approximation.

A contribution to the error of the approximation of Eq. (1.6) comes from the error $\sigma(K_m)$ caused by replacing the infinite integration interval $k \in [0, \infty)$ by the finite one, the operator $[D^\infty + S^\infty]$ by $[D^\infty + S^{km}]$, and also from the error of order $O(\Delta k^4)$ originating from the approximation of operator S^{km} by Simpson's rule. In [9] a numerical analysis of the error $\sigma(K_m)$ and the choice of the step Δk of quadrature formulae is described. It is also necessary to take into account the error $\sigma(R_m)$ due to the change of the boundary conditions (1.5) to (2.3). It is known [25] that for the change of D^∞ to D^{R_m}, as $R_m \to \infty$ we have the convergence of solutions of regular problems (4.1), however, the rate of convergence is determined by operator properties D^∞. This analysis is a difficult problem. Therefore, the dependence of the error on R_m is analysed numerically. The boundary point R_m is chosen from the dependence $\varepsilon = \varepsilon(R_m)$ obtained numerically. As follows from Table II, to calculate energy levels of mesic molecules with an accuracy of 0.1 eV, it is sufficient to put $R_m = 20$. Note

TABLE II

Dependence of the Energy Level—$\varepsilon_{J\theta}$ on R_m

R_m	$pd\mu$ $J=\theta=0$	$dd\mu$ $J=\theta=1$
20	221.516	1.393
40	221.520	1.908
60	221.520	1.906

Note. The $\varepsilon_{J\theta}$ are given in eV and R_m in the units of the problem. The energy levels are calculated for $N=84$ for the $pd\mu$ mesic molecule and $N=131$ for $dd\mu$. The calculation has been performed by Scheme B for $\chi(0)=\chi(R_m)=0$.

strong dependence of ε on R_m for the weakly bound state $J=\theta=1$ of a mesic molecule $dd\mu$.

The approximation parameters for the initial problem h, Δk, R_m, k_m are determined so that the absolute error in the value of an energy level does not exceed 0.1 eV [9]. From the same considerations the quantity (6.1) was estimated ($\delta_K < \varepsilon = 10^{-6}$).

7. Numerical Analysis of the Convergence of the Adiabatic Expansion

Convergence of expansion (1.3) is analysed by the numerical solution of the sequence of problems (2.2), (2.3) for different N at h, Δk, R_m, k_m chosen by Scheme B. In Table III the dependence of the mesomolecule binding energies on the number of solved equations of the system (2.2) is given, i.e., on the number of states of the two-center problem considered in the expansion (1.3). The contribution of discrete and continuous spectra of the two-center problem into the binding energy is taken into account for given N with an accuracy of 0.1 eV. The calculation was carried out by Scheme B, since the problem (2.2), (2.3) with the potential matrix (5.8) approximated the initial problem with a high absolute accuracy $\sim 10^{-2}$ eV, as follows from Table IV. Note that the results obtained agree with results of [9], where the convergence of expansion (1.3) was investigated by perturbative formulae [26]. The authors present values of energy levels of all mesic molecules and compare adiabatic and variational [4, 5] calculations.

The above method allows for the contribution in the energy level $\varepsilon_{J\theta}$ from omitted states of the discrete (N, ∞) spectrum and from low-lying states of the continuous $[0, k_0]$, one of the two-center problems [27]. Values do not exceed $\sim$0.1 eV for deep and $\sim$0.05 eV for weakly bound states.

TABLE III

Dependence of the Energy Level $\varepsilon_{J\theta}$ on the Number of Equations Solved N

	Number of Pairs of Equations N	$pd\mu$ $(J=\theta=0)$		Number of Equations	$dd\mu$ $(J=\theta=1)$	
		$-\varepsilon_N$	$\Delta\varepsilon_N=\varepsilon_N-\varepsilon_{N-1}$		$-\varepsilon_N$	$\Delta\varepsilon_N=\varepsilon_N-\varepsilon_{N-1}$
States of the	1	215.680		1	0.640	
discrete spectrum	3	218.598	2.918	4	1.392	0.752
of the two-	6	219.114	0.516	8	1.522	0.130
center problem	9	219.302	0.188	12	1.562	0.040
States of	27	220.140	0.838	30	1.678	0.117
continuous	49	221.227	1.087	52	1.769	0.090
spectrum	71	221.447	0.260	74	1.812	0.043
of the	84	221.520	0.033	87	1.824	0.012
two-center				109	1.881	0.057
problem				131	1.906	0.025

Note. The values of ε_N are given in eV for a different number of equations in the system (2.2). N corresponds to a successive filling of states three shells $n=n_1+n_2+m+1$, and partially in the fourth shell $n=4$ (the states $n=[n_1n_2m]=[300]$, $[210]$, $[120]$) of the discrete spectrum, and in six shells of the continuous spectrum $[n_2m]=[00]$, $[10]$, $[20]$, $[30]$, $[61]$, $[11]$ of the two-center problem. N differs for $J=0$ and $\theta=1$, since at $J=1$ the eigenvalue is contributed by the matrix elements $\hat{U}_{ij}(R)$ $(i,j=\left\{\begin{smallmatrix}[n_1n_2m]\\[k[n_2m]]\end{smallmatrix}\right\})$ with $m=1$. The calculation has been performed for the zero boundary conditions $\chi(0)=\chi(R_m)=0$ at $R_m=60$ by Scheme B.

TABLE IV

Energy Levels $\varepsilon_{J\theta}$ of Mesic Molecules $pd\mu$ and $dd\mu$

Mesic Molecules	Quantum Numbers		Binding Energy $-\varepsilon_{J\theta}$ (eV)	
	J	θ	Scheme A	Scheme B
$dd\mu$	0	0	325.046	325.043
	0	1	35.808	35.813
	1	0	226.605	226.607
	1	1	1.392	1.393[a]
	2	0	86.314	86.324
$pd\mu$	0	0	221.515	221.516
	1	0	97.357	97.399

Note. For the calculations we have used the following values of particle masses (in the units of electron mass) and the value of Ry [29]: $m_\mu=206.769$, $M_p=1836.152$, $M_d=3670.481$, $Ry=13.6058$ eV. The $\varepsilon_{J\theta}$ are presented with three numbers after the decimal in order to compare Schemes A and B though the absolute accuracy of calculations is about 0.1 eV and for a weakly coupled level $dd\mu$ $(J=\theta=1)$ is about 0.05 eV. The calculation has been performed for $\chi(0)=\chi(R_m)=0$, $R_m=20$, $N=84$ for $pd\mu$, and $N=131$ for $dd\mu$.

[a] At $R_m=60$, $\varepsilon_{11}=-1.906$ eV.

Conclusion

Numerical methods for solving a local Sturm–Liouville problem for a system of integrodifferential equations are presented. These methods calculate energy levels and wave functions of μ-mesic molecules of hydrogen isotopes in the adiabatic representation.

The absolute accuracy of the calculation of energy levels is about 0.1 eV and can be increased when the system of equations is extended by choosing R_m and k_m and by increasing the accuracy of the finite-difference scheme. Possible ways to increase accuracy are also suggested [28].

Acknowledgments

The authors are grateful to Professor L. I. Ponomarev for the formulation of the problem and his support during the course of the work, and to Dr. S. I. Vinitsky for numerous discussions and help in this work.

References

1. S. S. Gerstein and L. I. Ponomarev, *Phys. Lett. B* **72** (1977), 80; L. I. Ponomarev, "Tenth European Conference on Controlled Fusion and Plasma Physics," September 1981, Moscow, U.S.S.R.
2. S. S. Gerstein and L. I. Ponomarev, Mesomolecular process induced by π^- and μ^- mesons, *in* "Muon Physics," (V. Hughes and C. S. Wu, Eds.), Vol. III, Academic Press, New York/London, 1975.
3. M. Born, *Akad. Wiss. Goattingen Nachr.* **1** (1951); H. F. Mott and H. S. Massey, "Theory of Atomic Collisions," 3rd ed., Oxford Univ. Press, London/New York, 1965; L. I. Ponomarev and S. I. Vinitsky, *J. Phys. B* **12**(1979), 567; L. I. Ponomarev, S. I. Vinitsky, and F. R. Vucajlovic, *J. Phys. B* **13** (1980), 847; L. I. Ponomarev, L. N. Somov, and F. R. Vucajlovic, *J. Phys. B* **14** (1981), 591.
4. B. P. Carter, *J. Comput. Phys.* **4** (1969), 54; *J. Comput. Phys.* **4** (1969), 325; Y. Accad, C. L. Pekeris, and B. Schiff, *Phys. Rev. A* **4** (1971), 516.
5. B. P. Carter, *Phys. Rev.* **141** (1966), 863; A. Halpern, *Phys. Rev. Lett.* **13** (1964), 660.
6. S. I. Vinitsky, L. I. Ponomarev, I. V. Puzynin, T. P. Puzynina, L. N. Somov, and M. P. Faifman. *Zh. Exsp. Teor. Fiz.* **74** (1978), 849. [Russian]; *Sov. Phys. JETP* **47** (1979), 444.
7. V. M. Bystritsky, V. P. Dzhelepov, V. I. Petrukhin, A. I. Rudenko, L. N. Somov, V. M. Suvorov, V. V. Filchenkov, G. Hemnits, N. N. Khovansky, B. A. Khomenko, and D. Horvat, *Zh. Exsp. Teor. Fiz*, **76** (1979), 460. [Russian]; *Sov. Phys. JETP* **49** (1979), 232.
8. V. M. Bystritsky, V. P. Dzhelepov, Z. V. Ershova, V. V. Filchenkov, V. K. Kapyshev, S. M. Mukhamet-Galeeva, V. S. Nadezhdin, L. A. Rivkis, A. I. Rudenko, V. I. Satarov, N. V. Sergeeva, L. N. Somov, V. A. Stolupin, and V. G. Zinov, *Phys. Lett. B* **94** (1980), 476.
9. S. I. Vinitsky, V. S. Melezhik, L. I. Ponomarev, I. V. Puzynin, T. P. Puzynina, L. N. Somov, and N. F. Truskova, *Zh. Exsp. Teor. Fiz.* **79** (1980), 698. [Russian]; *Sov. Phys. JETP* **52** (1980), 353.
10. D. R. Bates, K. Ledsham, and A. L. Stewart, *Phil. Trans. Roy. Soc. London A* **246** (1953), 215; J. D. Power, *Phil. Trans. Roy. Soc. London A* **274** (1973), 663.
11. I. V. Komarov, L. I. Ponomarev, and S. Yu. Slavjanov, "Spheroidal and Coulomb Spheroidal Function," [Russian] Nauka, Moscow, 1976.

12. L. I. PONOMAREV, T. P. PUZYNINA, AND N. F. TRUSKOVA, *J. Phys. B* **11** (1978), 3861; L. I. PONOMAREV, T. P. PUZYNINA, AND L. N. SOMOV, *J. Phys. B* **10** (1977), 1335; L. I. PONOMAREV, S. YU. SLAVJANOV, AND L. N. SOMOV, *J. Phys. B* **13** (1980), 3737.
13. M. P. FAIFMAN, L. I. PONOMAREV, AND S. I. VINITSKY, *J. Phys. B* **9** (1976), 2255; D. I. ABRAMOV, S. YU. SLAVJANOV, AND L. N. SOMOV, *J. Phys. B* **13** (1980), 4717.
14. M. K. GAVURIN, *Izv. Vyssh. Uchebn. Zaved. Mat.* **5** (1958), 18; MR 25, 1380; Usp. Mat. Nauk 12 (1957), 173.
15. E. P. ZHIDKOV, G. I. MAKARENKO, AND I. V. PUZYNIN, *Part. Nucl.* **4** (1) (1973), 127.
16. R. E. BELLMAN AND R. E. KALABA, "Quasilinearization and Nonlinear Boundary-Value Problems," Amer. Elsevier, New York, 1965; R. E. BELLMAN, R. E. KALABA, AND G. M. WING. *J. Math. Phys.* **1** (1960), 280; R. HUSS, R. KALABA, AND R. VASUDEVAN, *J. Math. Phys.* **15** (1974), 1285.
17. L. A. KIVISTIK, *Dokl. Akad. Nauk USSR* **136** (1961), 22.
18. L. A. LYUSTERNIK AND V. I. SOBOLEV, "Elements of Functional Analysis," Nauka, Moscow, 1965. [Russian]
19. E. K. BLUM AND A. F. CHANG, *J. Inst. Maths. Its Appl.* **22** (1978), 29.
20. V. S. MELEZHIK, I. V. PUZYNIN, T. P. PUZYNINA, AND L. N. SOMOV, JINR Communication, No. P5-12789, Dubna, 1979.
21. A. A. SAMARSKY, "Introduction to Theory of Difference Schemes," Nauka, Moscow, 1971.
22. L. I. PONOMAREV, I. V. PUZYNIN, AND T. P. PUZYNINA, *J. Comput. Phys.* **13** (1973), 1.
23. N. N. KALITKIN, *Z. Vychisl. Mat. i Mat. Fiz* **5** (1965), 1107.
24. A. A. SAMARSKY, "Theory of Difference Schemes," Nauka, Moscow, 1977. [Russian]
25. I. M. GLASMAN, "Direct Methods for Exchange Analysis of Singular Difference Operators," Fizmatgis, Moscow, 1963.
26. S. I. VINITSKY AND L. I. PONOMAREV, *Zh. Eksp. Teor. Fiz.* **72** (1977), 1670; *Sov. Phys. JETP* **45** (1977), 876.
27. S. I. VINITSKY, V. S. MELEZHIK, AND L. I. PONOMAREV, *Zh. Eksp. Teor. Fiz.* **82** (1982), 670.
28. V. S. MELEZHIK AND L. N. SOMOV, JINR Communication, No. P11-81-856, Dubna, 1981; S. I. VINITSKY, I. V. PUZYNIN, AND T. P. PUZYNINA, JINR Communication, No. P11-82-421, Dubna, 1982.
29. E. R. COHEN AND V. N. TAYLOR, *J. Phys. Chem. Ref. Data* **2** (1973), 663.