

**Note**

**Continuous Analog of Newton's Method for the Calculation of Quasibound States of Hydrogen  $\mu$ -Molecules**

1

In the present paper the continuous analog of Newton's method (CAMEN scheme) [1, 2] is used for numerical solution of scattering problem in quantum mechanics taking account of closed channels.

Such problems can be formulated as follows. Given the system of ordinary differential equations

$$\left(\frac{d^2}{dx^2} - \frac{L(L+1)}{x^2} + 2ME\right)\chi_i(x) - \sum_{j=1}^m V_{ij}(x)\chi_j(x) = 0, \quad (1)$$

$$0 \leq x < \infty, \quad i = 1, 2, \dots, m$$

in which the coefficients (potentials)  $V_{ij}(x)$  obey the asymptotic conditions

$$x^2 V_{ij}(x) \rightarrow \text{const} \quad \text{when } x \rightarrow 0,$$

with

$$V_{mm}(\infty) \geq V_{m-1,m-1}(\infty) \geq \dots \geq V_{11}(\infty) = 0.$$

At  $x = 0$  the boundary conditions

$$\chi_i(0) = 0, \quad i = 1, 2, \dots, m \quad (2)$$

are considered.

By the conventional terminology the equations following from system (1) in the limit  $x \rightarrow \infty$  are called the reaction channels. In the case  $V_{SS}(\infty) > 2ME > V_{S-1,S-1}(\infty) > 0$  the wave functions  $\chi_i(x)$  in the closed channels ( $m \geq i \geq S$ ) when  $x \rightarrow \infty$  are exponentially decreasing:

$$\chi_i(x) \sim \exp(-\kappa_i x), \quad (3)$$

where

$$\kappa_i = (V_{ii}(\infty) - 2ME)^{1/2},$$

and for the open channels ( $i < S$ ) their asymptotic form is oscillating

$$\chi_i^{(\omega)}(x) \rightarrow A_i^{(\omega)} \sin(k_i x - (L\pi/2) + \delta_L^{(\omega)}(k_i)), \quad (4)$$

where

$$k_i = (2ME - V_{ii}(\infty))^{1/2}, \delta_L^{(i)} = \delta_L(k_i) \delta_{iv} + \pi/2 (1 - \delta_{iv}).$$

## 2

In the scattering problem the functional dependence of the scattering phases  $\delta_L^{(i)}$  on energy  $E$  is usually investigated. Such an approach to the problem determines the numerical methods of its solution which reduce to the integration of system (1) with some initial conditions and a given energy  $E$  (or consequences of this system, e.g., the equations for the phase and amplitude functions [3]) on a sufficiently large interval  $0 \leq x \leq x_m$ .

In the proposed approach the problem (1)–(4) given on the semiaxis  $0 \leq x < \infty$  reduces to the Sturm–Liouville problem on the finite interval  $[0, x_m]$  with the given values of phases  $\delta_L^{(i)}$  and boundary conditions which are the approximation of conditions (3), (4) at the point  $x_m$ . The collision energy  $E$  and the wavefunctions  $\chi_i^{(i)}(x)$  corresponding to a set of phases  $\delta_L^{(i)}$  are then found as the eigenvalue and eigenfunctions of the given problem. Such an approach to the scattering problem is especially effective in the resonance situations when the phase  $\delta_L^{(i)} = \delta_L^{(i)}(k_i)$  changes sharply with slightly changing  $E$ .

## 3

Here we consider the problem on the calculation of quasibound states of hydrogen  $\mu$ -molecules by which one can trace the possibilities of the proposed method and the peculiarities of its application.

In the adiabatic representation of the three-body problem [4] the energy levels and wavefunctions of mesomolecules are obtained from system (1) at  $m = 2$  with the effective mass of the three-body system

$$M = \left( \frac{1}{m_\mu} + \frac{1}{M_1 + M_2} \right) \left( \frac{1}{M_1} + \frac{1}{M_2} \right)^{-1}$$

where  $m_\mu$ ,  $M_1$  and  $M_2$  are the masses of the  $\mu$ -meson and nuclei, respectively. The effective potentials  $V_{ij}(x)$  are calculated when solving the two-center problem [5]. The method of their construction is given in the paper [6].

There are several definitions of quasibound states in quantum mechanics [7] with different ranges of applicability. Without going into details, we accept the following definition

$$\delta_L^{(1)}(k_1) = \pi(n + \frac{1}{2}) \quad (5)$$

which holds with good accuracy for the states with  $k_1 \ll 1$  and  $L \neq 0$  [7, 11]. The collision energy  $E$  is defined as a real part of the complex energy of the quasibound state

$$E_{\text{qst}} = E - i(\Gamma/2),$$

where  $n$  is the number of zeros of the wavefunction  $\chi_1(x)$  in the range of potentials  $V_{ij}(x)$ . All quasibound states of  $\mu$ -molecules with unequal nuclei ( $M_1 \neq M_2$ ) are in the range of values

$$V_{22}(\infty) > 2ME > V_{11}(\infty) = 0.$$

For determining the width of the levels  $\Gamma$  we use the relation [7]

$$\Gamma = (k_1/M) \int_0^{x_0} \chi_1^2(x) dx.$$

The function  $\chi_1(x)$  is normalized by the condition (4) at  $A_1 = 1$  and the  $x_0$  value is chosen as the position of the first zero  $\chi_1(x)$  beyond the range of potentials  $V_{ij}$ .

A similar approach to the scattering problems for the radial Schrodinger equation was considered in [8, 9].

#### 4

To solve the problem (1)–(1) for finding the quasistationary levels and wavefunctions of  $\mu$ -molecules, one uses the CAMEN scheme thoroughly discussed in [2]. It is a generalization of the algorithm for solving the Sturm–Liouville problem given in [1]. Note some details of the application of the calculation scheme characteristic of the considered case.

To make the approximation of boundary conditions for system (1) on the interval  $0 \leq x \leq x_m$  more accurate, the asymptotic form (3), (4) of the wavefunctions is defined in more detail and, taking account of (5), has the form:

$$\tilde{\chi}_1(x) = (-1)^{n+1} \left[ \left( -1 + \sum_{j=1}^{s_1} d_j \xi^{-2j} \right) \cos(\xi - (L\pi/2)) + \sum_{j=1}^{s_2} b_j \xi^{-2j+1} \sin(\xi - (L\pi/2)) \right] \quad (6)$$

where  $\xi = k_1 x$  and

$$\tilde{\chi}_2(x) = \exp\{-\kappa_2 x\} \sum_{j=0}^{s_3} a_j x^{-j}. \quad (7)$$

Using the known asymptotic form of the potentials  $V_{ij}(x)$  [1, 6] one can easily obtain the expressions for the coefficients  $a_j$ ,  $b_j$  and  $d_j$  in expansions (6), (7). The upper limits of the summation  $s_1$ ,  $s_2$ ,  $s_3$  in them depend on the values  $k_1$ ,  $x_m$ ,

and on necessary calculation accuracy. For the wavefunctions  $\chi_i(x)$  at the point  $x_m$ , we consider the boundary conditions of the type:

$$((d/dx) + f_i(E, x)) \chi_i(x)|_{x=x_m} = 0, \quad i = 1, 2 \quad (8)$$

where  $f_i(E, x)$  are the logarithmic derivatives constructed taking account of expansions (6), (7).

The Eqs. (1), (2), (8) which are the approximation of the considered problem on the finite interval  $0 \leq x \leq x_m$  are supported by the normalization condition of the wavefunction  $\chi_2(x)$  in the closed channel

$$\int_0^{x_m} \chi_2^2(x) dx + c \int_{x_m}^{\infty} \tilde{\chi}_2^2(E, x) dx = 1 \quad (9)$$

where  $c = \chi_2(x_m)/\tilde{\chi}_2(E, x_m)$ . Then the CAMEN scheme can be completely applied for this problem.

For the approximation of differential operators of system (1), boundary conditions (8), and the normalization condition (9) in the proposed algorithm we have used the three-point finite-difference approximation and quadrature formulas of second-order of accuracy with respect to step  $h$  of the uniform difference net. The calculation errors in dependence on the values of the parameters  $s_i$  ( $i = 1, 2, 3$ ) in formulas (6), (7),  $x_m$  and the step  $h$  of the difference net have been investigated.

In accordance with general estimates [10], the absolute accuracy of the calculation of energy  $E$  and wavefunctions  $\chi_i(x)$  is of the order  $O(h^2)$  and is  $\sim 10^{-4}$  when choosing  $s_1 = 3$ ,  $s_2 = 4$ ,  $s_3 = 6$ ,  $x_m = 30$ , and  $h = 0.01$  taking account of the terms  $\sim x^{-6}$  in the asymptotic form of the potentials  $V_{ij}(x)$ .

The initial approximation for the function  $\chi_2(x)$  in the closed channel is chosen following [1], and for the function  $\chi_1(x)$  in the open channel as a sinusoid with the deformation to fulfill conditions (2), (6), and the given number of zeroes  $n$  in the range of potentials  $V_{ij}(x)$ . The calculation time of characteristics of the quasibound state at the computer CDC-6200 is about 2 min.

## 5

The calculation results for the hydrogen  $\mu$ -molecules are given in Table I. Figure 1 represents the wavefunctions  $\chi_1(x)$  and  $\chi_2(x)$  of the quasibound state of the mesomolecule  $d\mu$  with quantum numbers  $L = 3$ ,  $n = 0$ . The energy and width of this level are equal to  $E = 4.6 \cdot 10^{-3}$  and  $\Gamma = 5.4 \cdot 10^{-4}$ , respectively.

In the proposed computational scheme the eigenvalues and eigenfunctions are defined in the unique computation process and with the same absolute accuracy. The scheme is stable, and this is especially important for the problems with long-range potentials as well as when finding small eigenvalues.

TABLE I  
Energies and Widths of Quasibound States of Hydrogen Molecules<sup>a</sup>

	$L$	$n$	$E$	$E(\text{eV})$	$\Gamma$	$\Gamma(\text{eV})$							
$dd\mu$	3	0	$6.80 \cdot 10^{-3}$	37.2	$1.45 \cdot 10^{-3}$	7.9							
$tt\mu$	2	1	$8.2 \cdot 10^{-4}$	4.5	$1.9 \cdot 10^{-4}$	1.1							
$pd\mu$	2	0	$1.03 \cdot 10^{-2}$	55.6	$6.31 \cdot 10^{-3}$	35.0							
$pt\mu$	2	0	$8.29 \cdot 10^{-3}$	44.9	$4.48 \cdot 10^{-3}$	24.0 </tr <tr> <td><math>dt\mu</math></td> <td>3</td> <td>0</td> <td><math>4.57 \cdot 10^{-3}</math></td> <td>25.1</td> <td><math>5.3 \cdot 10^{-4}</math></td> <td>2.9</td> </tr>	$dt\mu$	3	0	$4.57 \cdot 10^{-3}$	25.1	$5.3 \cdot 10^{-4}$	2.9
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<sup>a</sup>In the calculations the following masses of hydrogen isotopes are used:  $m_\mu = 206.769$ ,  $M_p = 1836,109$ ,  $M_d = 3670,398$ ,  $M_t = 5496,753$ .

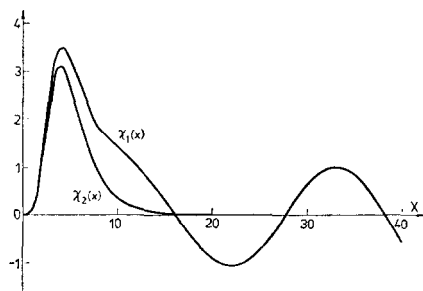


FIG. 1. The wavefunctions of the quasistationary state of mesomolecule  $dt\mu$  ( $M = 10.89$ ,  $L = 3$ ,  $n = 0$ ):  $\chi_1(x)$ —the solution in the open channel, and  $\chi_2(x)$  in the closed one.

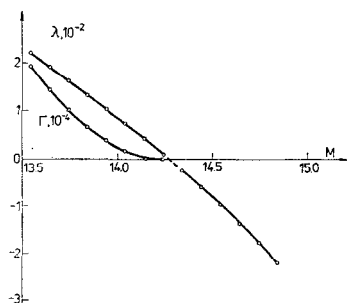


FIG. 2. The dependence of the energy  $E$  and width  $\Gamma$  of the quasistationary state  $L = 2$ ,  $n = 1$  on the effective mass  $M$  of the problem near the continuum ( $\lambda = 2ME$ ).

From Fig. 2 we can see the evolution of the quasistationary level ( $L = 1$ ,  $n = 1$ ,  $E = 8, 2 \cdot 10^{-4}$ ,  $\Gamma = 2 \cdot 10^{-4}$ ) of the mesomolecule  $tt\mu$  with increasing effective mass of the system  $M$  which is equal to 13.54. It is seen that when  $M > 14.27$  the quasistationary level becomes discrete and the dependence  $E = E(M)$  is approximately linear. This example shows the efficiency of the algorithm when calculating both the discrete and quasistationary levels in the vicinity of the continuum  $E = 0$ .

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