Three-body scattering model: diatomic homonuclear molecule and atom in collinear configuration

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ABSTRACT

Three-body model comprising a diatomic homonuclear molecule and an atom, the solutions of which are necessary for modelling interactions of three-body systems with laser radiation and spectroscopy, is formulated in the collinear configuration of the adiabatic representation. The mapping of the relevant 2D boundary-value problems (BVPs) in the Jacobi coordinates and in polar (hyperspherical) coordinates is reduced to a 1D BVP for a system of coupled second-order ordinary differential equations (ODEs) by means of the Kantorovich expansion in basis functions of one of the two independent variables, depending on the other independent variable parametrically. The efficiency of the proposed approach and software is demonstrated by benchmark calculations of the discrete spectrum of Be_3 trimer in the collinear configuration.

Keywords: trimer of atoms, collinear configuration, interatomic potentials, diatomic molecules, bound states

1. INTRODUCTION

The recent studies of tunnelling of bound particles through repulsive barriers revealed the effect of resonance quantum transparency of the barrier: when the cluster size is comparable with the spatial width of the barrier, one can observe enhanced barrier transparency, the mechanism of which is analogous to blooming of optical systems.[1] At present this effect and its possible applications are a subject of extensive theoretical and experimental studies in different physical fields, e.g., the quantum diffusion of molecules,[2] the processes of resonance scattering of diatomic molecules by atoms via weakly-bound and metastable states[3] and the quantum control of molecular processes in laser fields.[4]

The model of quantum tunnelling of a diatomic molecule through Gaussian barriers in the collinear configuration was formulated as 2D boundary-value problems (BVPs) in the Jacobi and polar coordinates.[5,6] The considered situation corresponds to the scattering of a diatomic homonuclear molecule in the potential field of the third atom having the infinite mass, resembling the scattering of electron by helium ion.[7] Using the solutions of different auxiliary boundary-value problems as basis functions of transverse or angular variable, parametrically depending upon the *(hyper)radial* variable, the 2D BVPs were reduced to systems of coupled second-order ordinary differential equations (ODEs). In the Jacobi coordinates, the effective potentials decrease exponentially (below the dissociation threshold) and in the polar coordinates they decrease as inverse powers of the independent variable. In the latter case it is necessary to calculate the asymptotic expansions of matrix elements and fundamental solutions of the ODE system. For this aim the symbolic-numeric algorithms, implemented

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in the Maple computer algebra system were developed[6,8] that offer a way to new optimal calculation schemes and software required for further study of bound and metastable states and resonance scattering in three-body systems.[9]

In this paper we consider a model of a diatomic molecules interacting with an atom in collinear configuration. We briefly discuss the computational model using the Kantorovich expansion of the 2D solution in the parametric basis functions in Jacobi and polar coordinates and the software implementation of the technique. Comparative analysis of benchmark calculations using these coordinates is presented for the discrete spectrum and bound states of Be_3 trimer.

The paper is organized as following. Section II formulates the 2D boundary-value problem. Sections III and IV present the calculation schemes and benchmark calculations of the bound states spectrum of Be_3 trimer in collinear configuration using the Kantorovich method in the Jacobi and polar coordinates, respectively. In the Conclusion the results and perspectives are discussed.

2. SETTING OF THE PROBLEM

Consider a 2D model of three identical particles with the mass M and the coordinates $x_i \in \mathbf{R}^1$, $i = 1, 2, 3$, coupled via the pair potential $\tilde{V}(|x_i - x_j|)$ $i, j = 1, 2, 3$. Performing the change of variables at cyclic permutation $(\alpha, \beta, \gamma) = (1, 2, 3)$:

$$x \equiv x_{(\alpha\beta)} = x_\alpha - x_\beta, \quad y \equiv y_{(\alpha\beta)\gamma} = \frac{x_\alpha + x_\beta - 2x_\gamma}{\sqrt{3}}, \quad x_0 = \frac{\sqrt{2}}{\sqrt{3}}(x_1 + x_2 + x_3), \quad \begin{pmatrix} x_{(\alpha\beta)} \\ y_{(\alpha\beta)\gamma} \end{pmatrix} = - \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} x_{(\beta\gamma)} \\ y_{(\beta\gamma)\alpha} \end{pmatrix}$$

or in the case of a diatomic molecule with identical nuclei coupled via the pair potential $\tilde{V}(|x_1 - x_2|)$ in the potential field $\tilde{V}^b(|x_i - x_3|)$, $i = 2, 1$ of the third atom having the infinite mass

$$x = x_1 - x_2, \quad y = x_1 + x_2,$$

we arrive at the Schrödinger equation(SE) for the wave function $\Psi(y, x)$ in the center-of-mass system $\{x_i \in \mathbf{R}^1 | x_1 + x_2 + x_3 = 0\}$ or in the laboratory frame with the origin $x_3 = 0$ placed at the third atom having the infinite mass

$$\left(-\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2} + \frac{M}{\hbar^2}(\tilde{V}(x, y) - \tilde{E}) \right) \Psi(y, x) = 0, \tag{1}$$

where the potential function for a trimer with the pair potentials (see Fig. 6),

$$\tilde{V}(x, y) = \tilde{V}(|x_1 - x_2|) + \tilde{V}(|x_2 - x_3|) + \tilde{V}(|x_1 - x_3|) = \tilde{V}(|x|) + \tilde{V}(|\frac{x - \sqrt{3}y}{2}|) + \tilde{V}(|\frac{x + \sqrt{3}y}{2}|), \tag{2}$$

or the potential function for a dimer in the field of barrier potentials

$$\tilde{V}(x, y) = \tilde{V}(|x_1 - x_2|) + \tilde{V}^b(|x_2 - x_3|) + \tilde{V}^b(|x_1 - x_3|) = \tilde{V}(|x|) + \tilde{V}^b(|\frac{x - y}{2}|) + \tilde{V}^b(|\frac{x + y}{2}|),$$

is symmetric with respect to the straight line $x = 0$ (i.e., $x_1 = x_2$), which allows one to consider the solutions of the problem in the half-plane $x \geq 0$. Using the Dirichlet or Neumann boundary condition at $x = 0$ one can obtain the solutions, symmetric and antisymmetric with respect to the permutation of two particles. If the pair potential possesses a high maximum in the vicinity of the pair collision point, then the solution of the problem in the vicinity of $x = 0$ is exponentially small and can be considered in the half-plane $x \geq x_{\min}$. In this case setting the Neumann or Dirichlet boundary condition at $x_{\min}$ makes only a minor contribution to the solution. The equation, describing the molecular subsystem, has the form

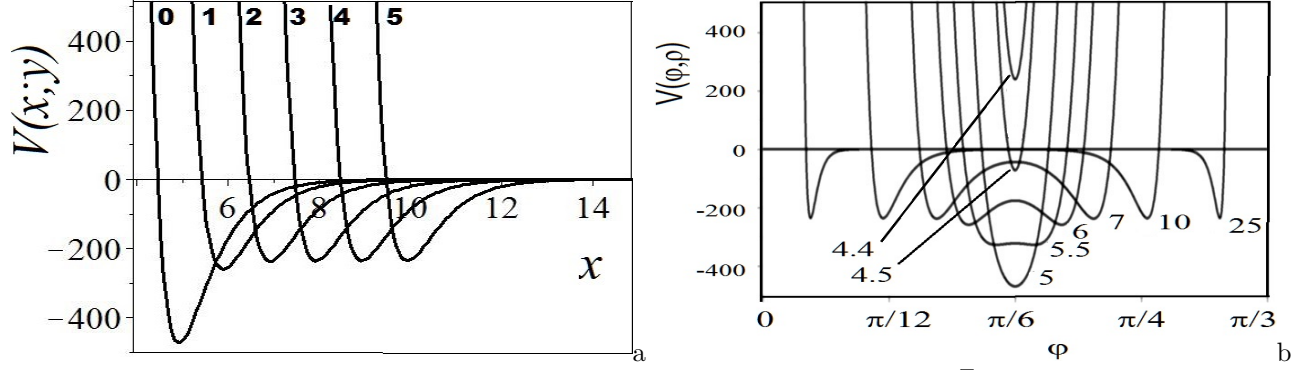$$\left(-\frac{d^2}{dx^2} + \frac{M}{\hbar^2}(\tilde{V}(x) - \tilde{\varepsilon}) \right) \phi(x) = 0. \tag{3}$$

Figure 1. The potential V that enters Eq. (3) in sector 2: a) $V(x;y)$ versus x at $y = \pm n/\sqrt{3}$, for $n = 0, ..., 5$ and b) $V(\phi; \rho)$ versus ϕ in the finite interval $\phi \in (0, \pi/3)$ for $\rho = 4.4, 4.5, 5, 5.5, 6, 7, 10, 25$.

We assume that the molecular subsystem has a discrete spectrum, consisting of a finite number n of bound states with the eigenfunctions $\phi_j(x)$, $j = 1, n$ and the eigenvalues $\tilde{\varepsilon}_j = -|\tilde{\varepsilon}_j|$, and the continuous spectrum of eigenvalues $\tilde{\varepsilon} > 0$ with the corresponding eigenfunctions $\phi_{\tilde{\varepsilon}}(x)$. As a rule, the solutions of the BVP for Eq. (3) can be found numerically, using a reduction on the appropriate finite interval in Jacobi or polar coordinates, such that the continuum spectrum is overlapped by the discrete one $\tilde{\varepsilon}_j > 0$, $j = n + 1, ...$, corresponding to pseudostates or parametric surface functions.[6,8] The proposed approach, algorithms and software are illustrated below by the example of the molecular interaction approximated by the Morse potential for Be_2 with the reduced mass of the nuclei M/2=4.506 Da[2,5]

$$V(x) = \frac{M}{\hbar^2}\tilde{V}(x), \quad \tilde{V}(x) = D\{\exp[-2(x - \hat{x}_{eq})\alpha] - 2\exp[-(x - \hat{x}_{eq})\alpha]\}, \tag{4}$$

where $\alpha = 2.96812$ Å^{-1} is the potential well width, $\hat{x}_{eq} = 2.47$ Å is the average distance between the nuclei, and $D = 1280$ K is the potential well depth or $\bar{D} = 236.510$ Å$^{-2} = (M/\hbar^2)D$ (1 K=0.184766 Å^{-2},1 Å^{-2}=5.412262 K). This potential supports five bound states[10] with the energies $\varepsilon_i = (M/\hbar^2)\tilde{\varepsilon}_i$, $i = 1, ..., n = 5$: $-\tilde{\varepsilon}_1$=1044.879 649 K, $-\tilde{\varepsilon}_2$=646.157 093 K, $-\tilde{\varepsilon}_3$=342.791 979 K, $-\tilde{\varepsilon}_4$=134.784305 K, $-\tilde{\varepsilon}_5$=22.134 with $(D = 1280 \text{ K})/(\hat{D} = 236.510$ Å$^{-2}) = 5.412262$ $(\hat{D} = 236.510$ Å$^{-2})/$(D=1280 K)=0.184766; The values of the parameters are determined from the condition $(\tilde{\varepsilon}_2 - \tilde{\varepsilon}_1)/(2\pi\hbar c) = 277.124$ cm^{-1}, 1K/($2\pi\hbar$ c)=0.69503476 cm^{-1}.

3. REDUCTION OF THE BVP IN JACOBI COORDINATES USING KANTOROVICH METHOD

The SE for the wave function $\Psi(x, y) \in \mathcal{W}_2^2(\Omega_{x,y})$ in the Jacobi coordinates $x = x_{(12)}$, $y = y_{(12)3}$ has the form

$$\left(-\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2} + (V(x, y) - E)\right)\Psi(y, x) = 0, \tag{5}$$

where the potential function for a trimer of atoms with the pair potentials is

$$V(x, y) = \frac{M}{\hbar^2}\tilde{V}(x, y), \quad \tilde{V}(x, y) = \tilde{V}(|x|) + \tilde{V}(|\frac{x - \sqrt{3}y}{2}|) + \tilde{V}(|\frac{x + \sqrt{3}y}{2}|). \tag{6}$$

To calculate the trimer bound states, we solve the BVP in the sector 2 $\Omega_2 = \{(x, y)|x > \sqrt{3}|y|\} = \{(r, \varphi)|\varphi \in (\pi/3, 2\pi/3)\}$, see Fig. 6. The solution of Eq. (5) is sought in the form of the Kantorovich expansion

$$\Psi_{i_o}(y, x) = \sum_{j=1}^{j_{max}} \phi_j(x; y)\chi_{ji_o}(y). \tag{7}$$
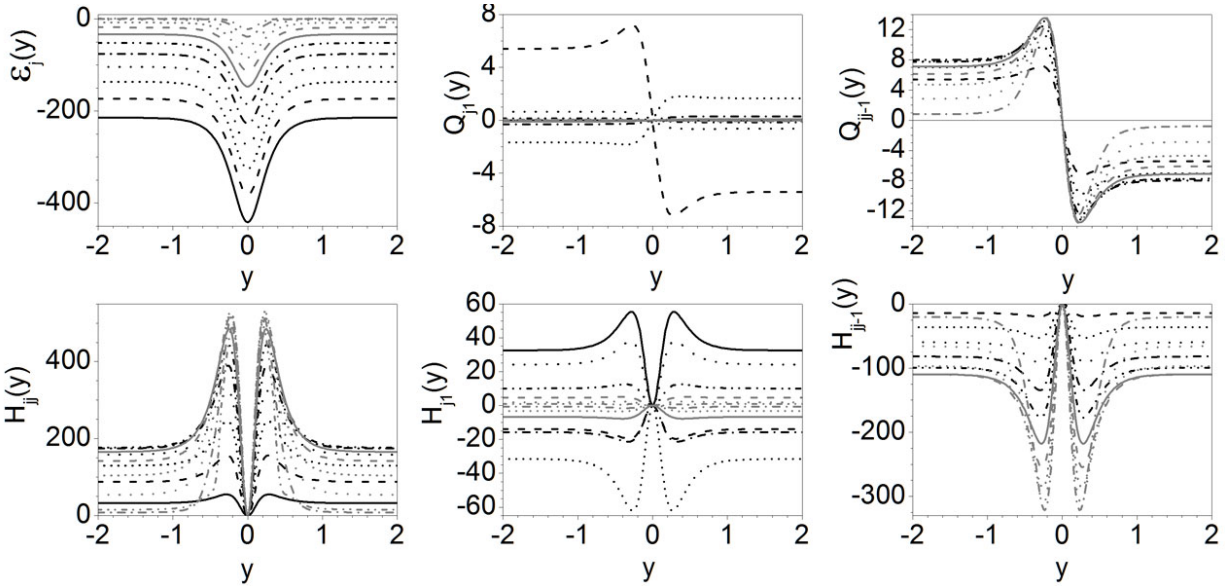
Figure 2. The potential curves $\varepsilon_j(y)$ of the BVP (8) in sector 2 and the effective potentials $H_{ji}(y)$ and $Q_{ji}(y)$ (11) in Å^{-2}.
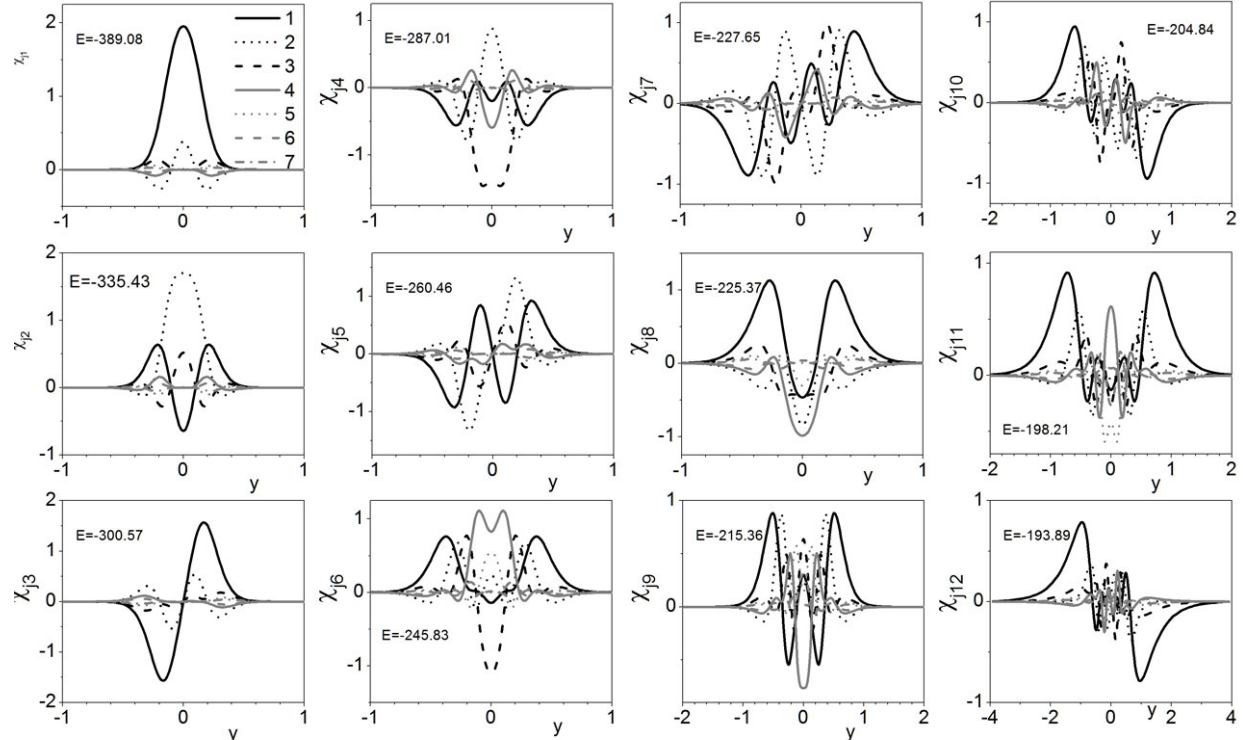

Figure 3. The even $\boldsymbol{\chi}_1$, $\boldsymbol{\chi}_2$, $\boldsymbol{\chi}_4$, $\boldsymbol{\chi}_6$, $\boldsymbol{\chi}_8$, $\boldsymbol{\chi}_9$, $\boldsymbol{\chi}_{11}$, and odd $\boldsymbol{\chi}_3$, $\boldsymbol{\chi}_5$, $\boldsymbol{\chi}_7$, $\boldsymbol{\chi}_{10}$, $\boldsymbol{\chi}_{12}$ eigenfunctions of the BVP (9)–(11).
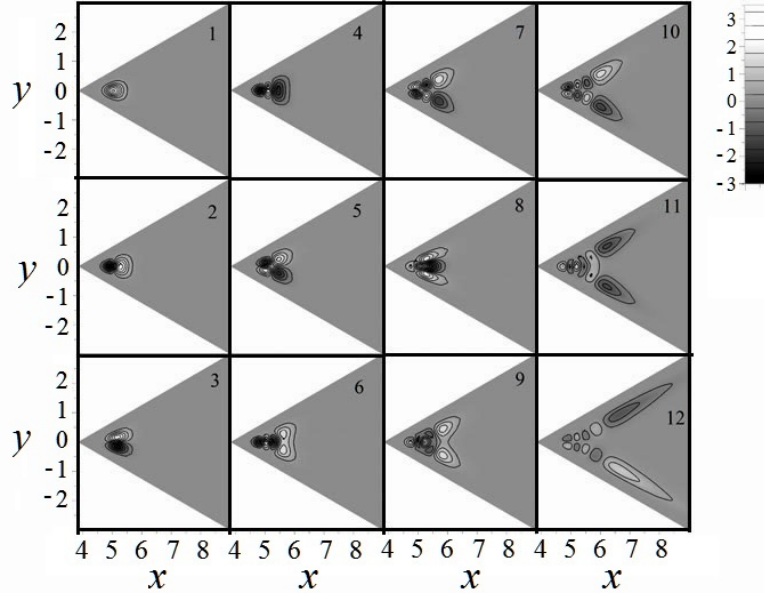
Figure 4. The isolines of even Ψ_1, Ψ_2, Ψ_4, Ψ_6, Ψ_8, Ψ_9, Ψ_{11}, and odd Ψ_3, Ψ_5, Ψ_7, Ψ_{10}, Ψ_{12} eigenfunctions of the BVP (9)–(11) in plane (y, x) of sector 2.
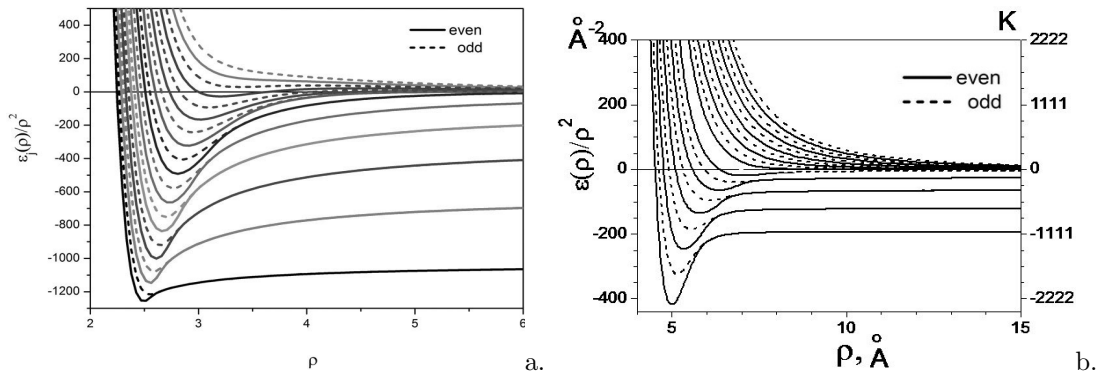

Figure 5. The potential curves $\tilde{\varepsilon}_j = \varepsilon_j(\rho)/\rho^2$ (in K, 1 K=0.18 Å^{-2}):a) Be$_2$ and b) Be$_3$.

Here the eigenfunctions $\phi_j(y; x) \in \mathcal{W}_2^2(\Omega_{y;x})$ corresponding to the eigenvalues $\varepsilon_j(y), j = \overline{1, j_{max}}$ are solutions of the BVP in $\Omega_2(x; y) = \{x \in (x_{\min}(y) = 3.8 + \sqrt{3}y, x_{\max}(y) = 9.8 + \sqrt{3}y)\}$ depending on y as a parameter $y \in \Omega_y = [-y_{\min}, y_{\max}]$:

$$\left(-\frac{\partial^2}{\partial x^2} + V(x,y) - \varepsilon_i(y)\right)\phi_i(x;y) = 0, \quad \phi_i(x_{\min}(y);y) = \phi_i(x_{\max}(y);y) = 0, \quad \int_{x_{\min}(y)}^{x_{\max}(y)} \phi_i(x;y)\phi_j(x;y) = \delta_{ij}. \quad (8)$$

The system of coupled self-adjoint ODEs for the unknown functions $\boldsymbol{\chi}_{i_o}(y) = \{\chi_{j i_o}(y)\}_{j=1}^{j_{max}} \in \mathcal{W}_2^2(\Omega_y)$ has the form

$$\left[-\frac{d^2}{dy^2} + \varepsilon_i(y) - E\right]\chi_{i i_o}(y) + \sum_{j=1}^{j_{max}} W_{ij}(y)\chi_{j i_o}(y) = 0, \quad W_{ij}(y) = H_{ji}(y) + \frac{d}{dy}Q_{ji}(y) + Q_{ji}(y)\frac{d}{dy}, \quad (9)$$

$$\chi_{j i_o}(y_{\min}) = \chi_{j i_o}(y_{\max}) = 0, \quad \int_{y_{\min}}^{y_{\max}} dy \sum_{j=1}^{j_{max}} \chi_{j i_o}(y)\chi_{j i'_o}(y) = \delta_{i_o i'_o}. \quad (10)$$
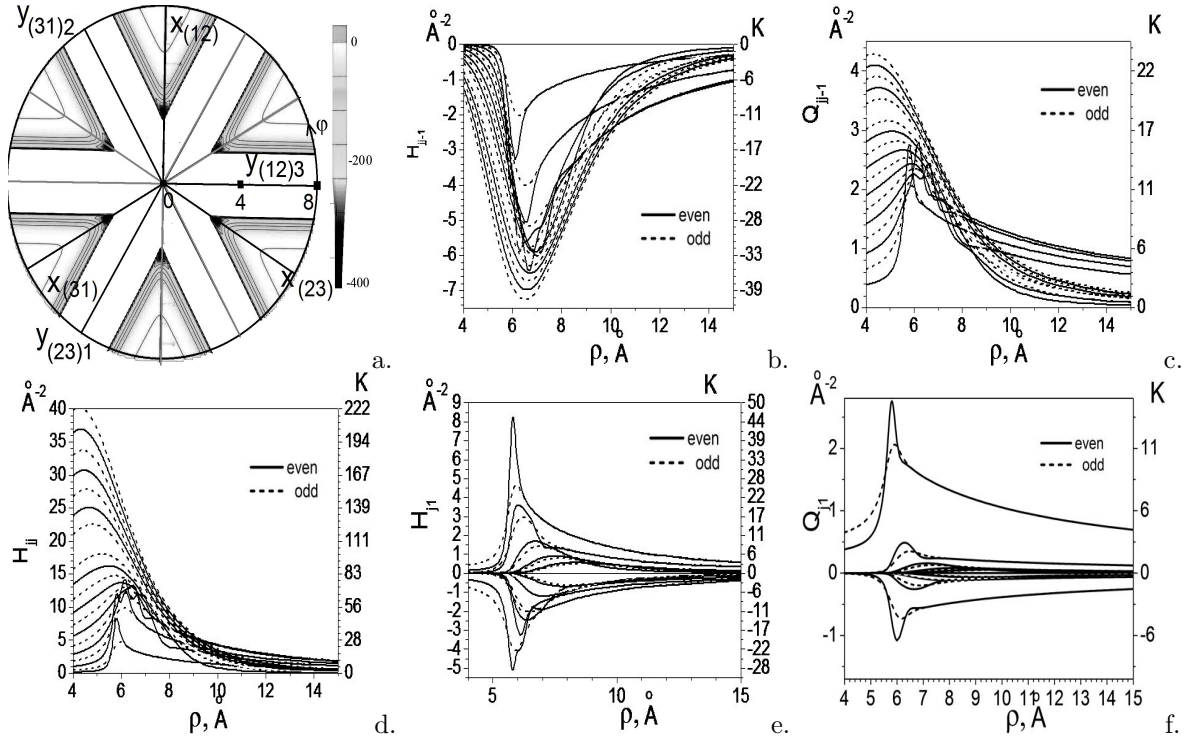
Figure 6. a)The isolines of 2D potentials (6), (16) and b)-f)the effective potentials (22)of Be$_3$ trimer.

The eigenvalues of the BVP (8) and the corresponding effective potentials (see fig. 2) are defined by the integrals

$$Q_{ij}(y) = -\int_{x_{\min}(y)}^{x_{\max}(y)} dx\,\phi_i(x;y)\frac{d\phi_j(x;y)}{dy},\ H_{ij}(y) = \int_{x_{\min}(y)}^{x_{\max}(y)} dx\,\frac{d\phi_i(x;y)}{dy}\frac{d\phi_j(x;y)}{dy},\tag{11}$$

In the system of ODEs the effective potentials tend to nonzero constants $\boldsymbol{\varepsilon}$, $\mathbf{H}$ $\mathbf{Q}$ at $|y| \geq |y_{min}, y_{max}| \geq 1$.

$$\left(-\mathbf{I}\frac{d^2}{dy^2} + \mathbf{V} + 2\mathbf{Q}\frac{d}{dy} - E\,\mathbf{I}\right)\boldsymbol{\Phi}(y) = 0, \mathbf{V} = \boldsymbol{\varepsilon} + \mathbf{H}.\tag{12}$$

If $\mathbf{Q} = \mathbf{0}$, then this system has the general solution, explicitly depending upon the spectral parameter E

$$\boldsymbol{\Phi}(y) = \sum_{i=1}^{j_{\max}} \left(C_i F_i(E, -y)\boldsymbol{\Psi}_i + C_{j_{\max}+i}F_i(E, y)\boldsymbol{\Psi}_i\right),\tag{13}$$

where $F_i(E, y) = \exp(p_i y) = \exp(\sqrt{E-\lambda_i}y)$, C_i are unknown coefficients (for bound states the solutions decrease exponentially as $F_i(E, y) = \exp(-p_i|y|)$), λ_i and $\boldsymbol{\Psi}_i = \{\Psi_{1i}, ..., \Psi_{j_{\max}i}\}^T$ are solutions of the algebraic eigenvalue problem that is solved numerically

$$\mathbf{V}\boldsymbol{\Psi}_i = \lambda_i \boldsymbol{\Psi}_i.\tag{14}$$

In the case $\mathbf{Q} \neq \mathbf{0}$ we have no explicit expression for the general solution, but the approximated threshold energies $\lambda_i \equiv E^{\mathrm{trsh}}(j_{\max})$ are the same as in the case $\mathbf{Q} = \mathbf{0}$, while the value of p_i is to be modified.[11]

We calculated the parametric basis functions of BVP (8) and the effective potentials (11) for the Be$_3$ trimer in collinear configuration using the program ODPEVP .[12] The calculations have been performed in the fast-variable grid $\Omega_x = \{\sqrt{3}|y| + 3.8(60)\sqrt{3}|y| + 9.8\}$ depending on the parameter y, taking its values on the slow-variable grid $\Omega_y = \{-4(6) - 1(20)1(6)4\}$ of sector 2 with the sixth-order Lagrange elements.

Table 1. The total energy E and the binding energies E^b (in Å^{-2}, 1 Å^{-2}=5.412033094 K) of the even (e) and odd (o) states of the trimer Be$_3$ depending upon the number $j_{\max}$ of basis functions in Jacobi coordinates (sector 2): $E^b(j_{\max}=12)=E(j_{\max}=12)-E^{\text{trsh}}(j_{\max}=12)$ and $E^b(j_{\max}=40)=E(j_{\max}=40)-E^{\text{trsh}}(j_{\max}=40)$, relative to the approximate thresholds $E^{\text{trsh}}(j_{\max}=12)=192.42$ and $E^{\text{trsh}}(j_{\max}=40)=193.05$. The total energy and the and binding energies of the trimer Be_3 at $j_{\max}=12$ basis functions in polar coordinates: $\hat{E}^b(j_{\max}=12)=\hat{E}(j_{\max}=12)-\hat{E}^{\text{trsh}}$ relative to the exact threshold $\hat{E}^{\text{trsh}}=193.06$.

v	$E(j_{\max}=12)$	$E^b(j_{\max}=12)$	$E(j_{\max}=40)$	$E^b(j_{\max}=40)$	$\hat{E}(j_{\max}=12)$	$\hat{E}^b(j_{\max}=12)$
1e	-388.82	196.39	-389.08	196.03	-389.08	196.02
2e	-334.76	142.33	-335.43	142.38	-335.43	142.37
3o	-299.79	107.36	-300.57	107.52	-300.58	107.52
4e	-285.50	93.07	-287.01	93.96	-287.02	93.96
5o	-258.98	66.55	-260.46	67.41	-260.47	67.41
6e	-243.21	50.79	-245.83	52.78	-245.84	52.78
7o	-225.25	32.83	-227.65	34.60	-227.66	34.60
8e	-223.56	31.13	-225.37	32.32	-225.39	32.33
9e	-212.70	20.27	-215.36	22.31	-215.37	22.31
10o	-202.33	9.90	-204.84	11.79	-204.85	11.79
11e	-196.11	3.69	-198.21	5.16	-198.21	5.15
12o	-192.71	0.29	-193.89	0.84	-193.86	0.80

For this model the eigenvalues and the components of 2D eigenfunctions of the BVP for the set of ODEs (9) were calculated using the program KANTBP.[13] The discrete energy spectrum of the trimer Be$_3$ is shown in second, third, forth and fifth columns of Table 1 that demonstrate the convergence of the total energy $E(j_{\max})$ and the binding energies $E^b(j_{\max}) = E(j_{\max}) - E^{\text{trsh}}(j_{\max})$ relative to the approximate threshold $E^{\text{trsh}}(j_{\max}) = \lambda_1$ to the exact ones. The isolines of even and odd trimer eigenfunctions $\Psi_j(x,y)$ and their components $\chi_j(y)$ are shown in Figs. 4 and 3.

4. REDUCTION OF THE BVP IN POLAR COORDINATES USING KANTOROVICH METHOD

We rewrite Eq. (1) in the polar coordinates $(\rho, \varphi) : \{x = \rho \sin\varphi, \quad y = \rho \cos\varphi\}$ for $\Psi(\rho, \varphi) \in \mathcal{W}_2^2(\Omega_{\rho,\varphi})$

$$\left(-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + V(\rho,\varphi) - E\right)\Psi(\rho,\varphi) = 0, \tag{15}$$

in the domain $\Omega_{\rho,\varphi} = (\rho \in (0,\infty), \varphi \in [0,2\pi])$ (see Fig. 6) for the trimer with the pair potentials

$$V(\rho,\varphi) = V(\rho\sin\varphi) + V(\rho\sin(\varphi - 2\pi/3)) + V(\rho\sin(\varphi - 4\pi/3)), \tag{16}$$

or for a dimer of atoms, coupled by pair potential and interacting with the external barrier potentials

$$V(\rho,\varphi) = V(\rho\sin\varphi) + V^b(\rho\sin(\varphi - \pi/4)) + V^b(\rho\sin(\varphi + \pi/4)). \tag{17}$$

The solution of Eq. (15) is sought in the form of the Kantorovich expansion

$$\Psi_{i_o}(\rho,\varphi) = \sum_{j=1}^{j_{\max}} \phi_j(\varphi;\rho)\chi_{ji_o}(\rho). \tag{18}$$

Here the eigenfunctions $\phi_j(\varphi;\rho) \in \mathcal{W}_2^2(\Omega_{\rho;\varphi})$ corresponding to the eigenvalues $\varepsilon_j(\rho), j = \overline{1,j_{max}}$ are solutions of the BVP in the interval $\Omega_{\phi;\rho} = \{\varphi \in (0,2\pi)\}$ depending on ρ as a parameter $y \in \Omega_\rho = [\rho_{\min}, \rho_{\max}]$:

$$\left(-\frac{d^2}{d\varphi^2} + \rho^2 V(\rho,\varphi) - \varepsilon_j(\rho)\right)\phi_j(\varphi;\rho) = 0, \quad \int_0^{2\pi} d\varphi\phi_i(\varphi;\rho)\phi_j(\varphi;\rho) = \delta_{ij}. \tag{19}$$
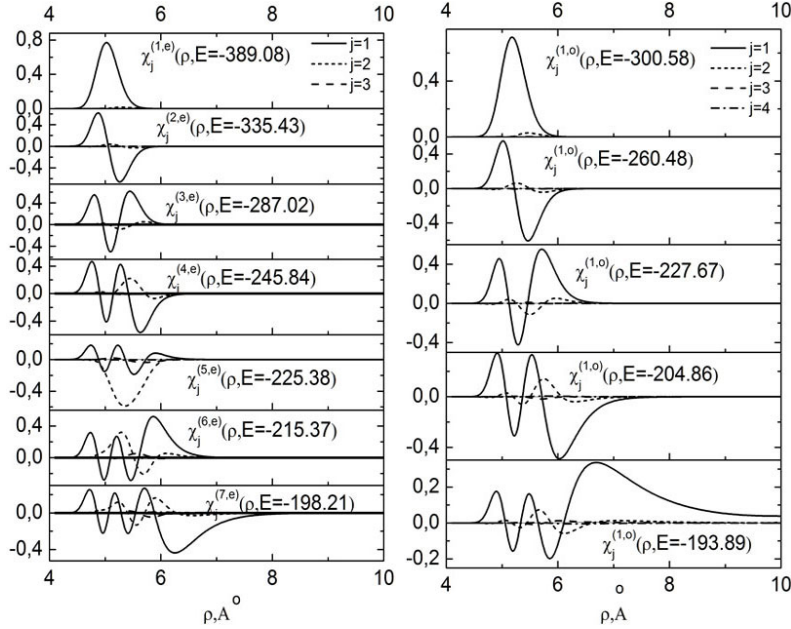
Figure 7. Components $\chi_j^{i,\sigma=e,o}(\rho, E) \equiv \chi_j^{(i)}(\rho)$ of even (e) and odd (o) bound states with the total energy E in Å^{-2}.

For the problems under consideration the potential function $V(\rho, \varphi)$ depending on the parameter ρ can be determined as follows:

Task 1. The case of one pair potential in the intervals $\varphi \in (0, \varphi_\alpha = \pi/3)$, $\varphi \in (0, \varphi_\alpha = \pi/4)$ or $\varphi \in (0, \varphi_\alpha = \pi/2)$

$$V(\rho, \varphi) = V(\rho \sin \varphi),$$

Task 2. The case of three pair potentials in the interval $\varphi \in (0, 2\varphi_\alpha = \pi/3)$

$$V(\rho, \varphi) = V(\rho \sin \varphi) + V(\rho \sin(\varphi - 2\pi/3)) + V(\rho \sin(\varphi - 4\pi/3)),$$

Task 3. The case of one pair potential and two barrier potentials in the interval $\varphi \in (0, \varphi_\alpha = \pi/4)$

$$V(\rho, \varphi) = V(\rho \sin \varphi) + V(\rho \sin(\varphi - \pi/4)) + V(\rho \sin(\varphi + \pi/4)).$$

The solutions symmetric with respect to the permutation of two particles satisfy the Neumann boundary condition at $\varphi = 0$ and $\varphi = 2\varphi_\alpha$, $\left.\frac{\phi_j(\varphi;\rho)}{d\varphi}\right|_{\varphi=0} = \left.\frac{\phi_j(\varphi;\rho)}{d\varphi}\right|_{\varphi=2\varphi_\alpha} = 0$, while the antisymmetric ones satisfy the Dirichlet boundary condition $\phi_j(0; \rho) = \phi_j(2\varphi_\alpha; \rho) = 0$.

If the pair potential possesses a high peak in the vicinity of the pair collision point, then the solution of the problem (15) will be considered in the half-plane $\Omega_{\rho,\varphi} = (\rho \in (\rho_{\min}, \infty), \varphi \in [\varphi_{\min}(\rho), 2\varphi_\alpha - \varphi_{\min}(\rho)])$ with the Neumann or Dirichlet boundary condition. Since the potential of the boundary-value problem (19) is symmetric with respect to $\varphi = \varphi_\alpha$, the even (e) $\phi_j(\varphi; \rho) = \phi_j(2\varphi_\alpha - \varphi; \rho)$ and odd (o) $\phi_j(\varphi; \rho) = -\phi_j(2\varphi_\alpha - \varphi; \rho)$ solutions, satisfying the Neumann boundary condition $\left.\frac{\phi_j(\varphi;\rho)}{d\varphi}\right|_{\varphi=\varphi_\alpha} = 0$, and the Dirichlet boundary condition $\phi_j(\varphi_\alpha; \rho) = 0$, respectively, will be considered separately in the interval $\varphi \in [\varphi_{\min}(\rho), \varphi_\alpha]$.

The set of coupled self-adjoint ODEs for the unknown functions $\boldsymbol{\chi}_{i_o}(\rho) = \{\chi_{ji_o}(\rho)\}_{j=1}^{j_{\max}} \in \mathcal{W}_2^2(\Omega_\rho)$ has the
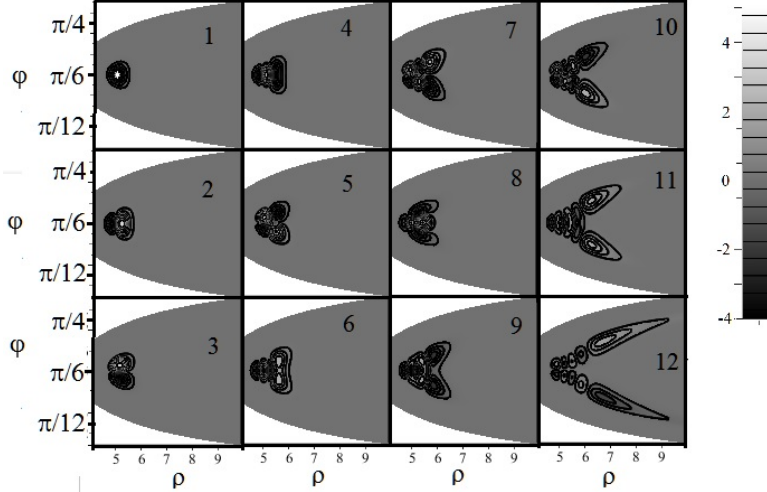
Figure 8. The isolines of even Ψ_1, Ψ_2, Ψ_4, Ψ_6, Ψ_8, Ψ_9, Ψ_{11}, and odd Ψ_3, Ψ_5, Ψ_7, Ψ_{10}, Ψ_{12} eigenfunctions of the BVP (9)–(11) in plane (ρ, φ).

form

$$\left[-\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} + \frac{\varepsilon_i(\rho)}{\rho^2} - E \right] \chi_{ii_o}(\rho) + \sum_{j=1}^{j_{\max}} W_{ij}(\rho)\chi_{ji_o}(\rho) = 0, \quad W_{ij}(\rho) = H_{ji}(\rho) + \frac{1}{\rho}\frac{d}{d\rho}\rho Q_{ji}(\rho) + Q_{ji}(\rho)\frac{d}{d\rho}, \quad (20)$$

$$\chi_{ji_o}(\rho_{\min}) = \chi_{ji_o}(\rho_{\max}) = 0, \quad \sum_{j=1}^{j_{\max}}\int_{y_{\min}}^{y_{\max}} \rho d\rho \chi_{ji_o}(\rho)\chi_{ji'_o}(\rho) = \delta_{i_o i'_o}. \tag{21}$$

The potential curves (molecular terms) $\varepsilon_j(\rho)$ and the effective potentials $Q_{ij}(\rho) = -Q_{ji}(\rho)$, $H_{ij}(\rho) = H_{ji}(\rho)$ (see Fig. 6) are given by the integrals

$$Q_{ij}(\rho) = -\int_0^{2\varphi_\alpha} d\varphi \phi_i(\varphi; \rho)\frac{d\phi_j(\varphi; \rho)}{d\rho}, H_{ij}(\rho) = \int_0^{2\varphi_\alpha} d\varphi \frac{d\phi_i(\varphi; \rho)}{d\rho}\frac{d\phi_j(\varphi; \rho)}{d\rho}, \tag{22}$$

and for Task 1 the barrier potentials $V_{ij}^b(\rho)$ can be expressed as

$$V_{ij}^b(\rho) = \int_0^{2\varphi_\alpha} d\varphi \phi_i(\varphi; \rho)(V^b(\rho\sin(\varphi - \pi/4)) + V^b(\rho\sin(\varphi + \pi/4)))\phi_j(\varphi; \rho).$$

The discrete energy spectrum of the dimer Be$_2$ calculated of the grid $\Omega_1(1.8, 10) = \{1.8(24)3(10)4(5)5(10)10\}$ and the set of binding energies of the trimer Be$_3$ calculated on the radial-variable grid $\Omega_\rho(4.1, 10) = \{4.1(20)7(10)10\}$ with the twelfth-order Lagrange elements and the angular-variable grid $\Omega_\phi = \{1.5/\rho(25)\pi/6\}$ at $\rho \leq 48/\pi$ and $\Omega_\phi = \{1.5/\rho(15)4/\rho(10)\pi/6\}$ at $\rho > 48/\pi$ with the eleventh-order Lagrange elements are shown in Table 1.

As an example, we calculated the parametric basis functions of BVP (8) and (19), the effective potentials (22) for the models of Be$_2$ dimer and Be$_3$ trimer in collinear configuration using the programme ODPEVP.[12] The results are shown in Figs.5, and 6. For this model the eigenvalues and the hyperradial components of 2D eigenfunctions of the BVP for the set of ODEs (20) were calculated using the program KANTBP.[13] The discrete energy spectrum and a set of the binding energies of the trimer Be$_3$ is shown in the sixth and the seventh column of Table 1. The isolines of even and odd trimer eigenfunctions $\Psi_j(\rho, \varphi)$ and their components $\chi_j(\rho)$ are shown in Figs. 8 and 7 as functions of the radial variable $\rho = \sqrt{x^2 + y^2}$. They are seen to be more delocalized in comparison with eigenfunctions in the Jacobi variables (x, y) in Figs. 4 and 3. Note, that the solution calculated in one of the six sectors of the circle can be extended over all other five sectors (see Fig. 6) similar to Ref.[14]

5. CONCLUSIONS

The model of a three-body system comprising a diatomic homonuclear molecule and an atom in the collinear configuration is formulated as a 2D boundary-value problem for the Schrödinger equation. Using the Kantorovich expansions of the 2D solution in parametric basis functions, we reduce the problem in Jacobi and polar coordinates to the boundary-value problem for a set of self-adjoint second-order ordinary differential equations. In these equations the parameter of the Kantorovich basis is an independent variable.

In polar coordinate, the calculation scheme using the Kantorovich expansion has exact threshold energies and relative momenta that can be applied both below and above the three-body threshold. In the case of polar coordinates the asymptotic behavior of the effective potential and the ODEs fundamental solutions is presented by the long-range expansion in inverse powers of the radial variable, while in the case of Jacobi coordinates the effective potentials exponentially tend to nondiagonal constant matrices. An important result, demonstrtated in our benchmark calculations of the discrete-energy spectrum of the trimer Be_3 is the convergence of the total energy $E(j_{max})$ and the binding energies $E^b(j_{max}) = E(j_{max}) - E^{trsh}(j_{max})$ relative to the threshold $E^{trsh}(j_{max}) = \lambda_1$ in Jacobi coordinates to the exact ones, calculated in polar coordinates (Table 1). This fact means that the calculation scheme in Jacobi coordinates using the Kantorovich expansion can be applied to solving the scattering problems below the three-body threshold.

The proposed approach and software can be adapted and applied to the analysis of quantum transparency effect, quantum diffusion of molecules, bound and metastable states, and the resonance scattering in triatomic systems.

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