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Самарский УНИВЕРСИТЕТ
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Bound states of tdμ, dpμ and tpμ mesomolecules in quantum electrodynamics

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The purpose of this work is to study the energy spectrum of three-particle mesomolecules tdμ, dpμ and tpμ on the basis of variational approach.

Tasks:

1. Compile computer code to solve problems for bound state of several particles using the stochastic variational method, which uses a correlated Gaussian basis to obtain a very accurate solution for small systems.
2. Calculation of matrix elements for kinetic, potential energies and normalization for excited states.
3. Calculation of the energy of the ground and excited states of mesomolecules tdμ, dpμ and tpμ on the basis of stochastic variational method of Varga-Suzuki and variational method of Korobov.

To calculate the rates of formation of mesomolecules, it is necessary to know the structure of their energy levels in states with different rotational and vibrational quantum numbers, and also the corresponding wave functions. Such calculations were made repeatedly, beginning in 1957, but only in 1973-1977, in Dubna, a general method (an adiabatic representation in the three-body problem) was developed, which made it possible to calculate all of them with reasonable accuracy. In recent years, direct variational methods of calculations have significantly improved the accuracy of previous calculations.

Korobov V.I., Puzynin I.V. and Vinitsky S.I. Physics Letfers B **196** (1987) 272-276

Frolov A.M. and Wardlaw D.M. Eur. Phys. J. D **63** (2011) 339–350

Aznabayev D.T., Bekbaev A. K., Ishmukhamedov I. S., and Korobov V. I. Physics of Particles and Nuclei Letters **12** (2015) 689–694.

Consider a system of 3 particles with masses m_1, m_2 and m_3 and charges z_1, z_2 and z_3 respectively. The Schrodinger equation in the Jacobi coordinates has the form:

$$H\Psi = E\Psi$$

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} - T_{cm} - \sum_{i<j}^{N} V_{ij} \qquad V_{ij} - \text{For central two-body interactions}$$

In stochastic variational approach (Varga-Suzuki) the basis functions are assumed to have the form

$$\Psi_{SM_S TM_T}(\mathbf{x}, A) = A\{G_A(\mathbf{x})\chi_{SM_S}\eta_{TM_T}\}$$

$$G_A(\mathbf{x}) = e^{-\tilde{\mathbf{x}} A\mathbf{x}/2}$$

χ_{SM_S} − is the spin function

η_{TM_T} − is the isospin function of the system

$$-\tilde{\mathbf{x}} A\mathbf{x} = \sum_{i=1}^{N-1}\sum_{j=1}^{N-1} A_{ij} x_i \cdot x_j$$

The diagonal elements of the (N - 1) × (N - 1) dimensional symmetric, positive definite matrix A correspond to the nonlinear parameters of an Gaussian expansion, and the off-diagonal elements connect the different relative coordinates representing the correlations between the particles.

$\mathbf{x} = (x_1, ..., x_{N-1})$ − Jacobi coordinates

x_N − the coordinate of the centre of mass

In the variational method the wave function of the system is presented as follows

$$\Psi = \sum_{i=1}^{K} c_i \psi_{SM_S TM_T}(\mathbf{x}, A_i)$$

$$\psi_{SM_S TM_T} = e^{-\sum_{i<j} \alpha_{ij}(r_i - r_j)^2}$$

In atomic physics the trial function of Hylleraas type or correlated exponential type is often used with success. This function contains the exponential form expressed in terms of the interparticle-distance coordinates. Instead of the exponential function let us consider its Gaussian analogue

an upper bound for the ground and excited state energy of the system is given by the lowest eigenvalue of the generalized eigenvalue problem

$$HC = E_K BC$$

$$H_{ij} = \langle \psi_{SM_S TM_T}(\mathbf{x}, A_i) \mid H \mid \psi_{SM_S TM_T}(\mathbf{x}, A_j) \rangle$$

$$B_{ij} = \langle \psi_{SM_S TM_T}(\mathbf{x}, A_i) \mid \psi_{SM_S TM_T}(\mathbf{x}, A_j) \rangle$$

The variational exponential expansion for arbitrary L, using the relative coordinates (r_{31}, r_{32} and r_{21}), was given in the form:

$$\psi_{L0} = \sum_{l=0} \sum_{i=1} c_{il} Y_{L0}^{l,L-l}(\mathbf{r}_{31}, \mathbf{r}_{32}) \exp(-\alpha_{1l}^{(i)} r_{32} - \alpha_{2l}^{(i)} r_{31} - \alpha_{3l}^{(i)} r_{21})$$

where the c_{il} are linear parameters and $\alpha_{jl}^{(i)}$ are the nonlinear parameters. The notation $Y_{LM}^{l,L-l}(x,y)$ is customary:

$$Y_{LM}^{l_1,l_2}(\mathbf{x},\mathbf{y}) = x^{l_1} y^{l_2} [Y_{l_1 m_1}(\mathbf{n}_x) Y_{l_2 m_2}(\mathbf{n}_y)]_{LM}$$

For L = 1, there are two systems of angular functions:

$$Y_{10}^{10}(\mathbf{r}_{31}, \mathbf{r}_{32}) = \mathbf{k} \cdot \mathbf{r}_{31}$$
$$Y_{10}^{01}(\mathbf{r}_{31}, \mathbf{r}_{32}) = \mathbf{k} \cdot \mathbf{r}_{32}$$

where $\mathbf{k}$ is the unit vector along the Z axis.

In these expressions, $\mathbf{k}$ is again the unit vector along the Z axis. The formulas for averaging the matrix elements over the orientations of the Z axis are as follows:

$$\oint (\mathbf{a} \cdot \mathbf{b}) d\Omega_k = 4\pi (\mathbf{a} \cdot \mathbf{b})$$

$$\oint (\mathbf{a} \cdot \mathbf{k})(\mathbf{b} \cdot \mathbf{k}) d\Omega_k = \frac{4\pi}{3}(\mathbf{a} \cdot \mathbf{b})$$

$$\oint (\mathbf{a} \cdot \mathbf{k})(\mathbf{b} \cdot \mathbf{k})(\mathbf{c} \cdot \mathbf{k})(\mathbf{d} \cdot \mathbf{k}) d\Omega_k = \frac{4\pi}{15}[(\mathbf{a} \cdot \mathbf{b})(\mathbf{c} \cdot \mathbf{d}) + (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) + (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c})]$$

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We use the following order of particles:

$$\underset{1\ 2\ 3}{t\,d\,\mu}, \quad \underset{1\ 2\ 3}{d\,p\,\mu} \quad \text{and} \quad \underset{1\ 2\ 3}{p\,t\,\mu}.$$

The Jacobi coordinates are related to the particle radiuses-vectors as follows:

$$\boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2$$

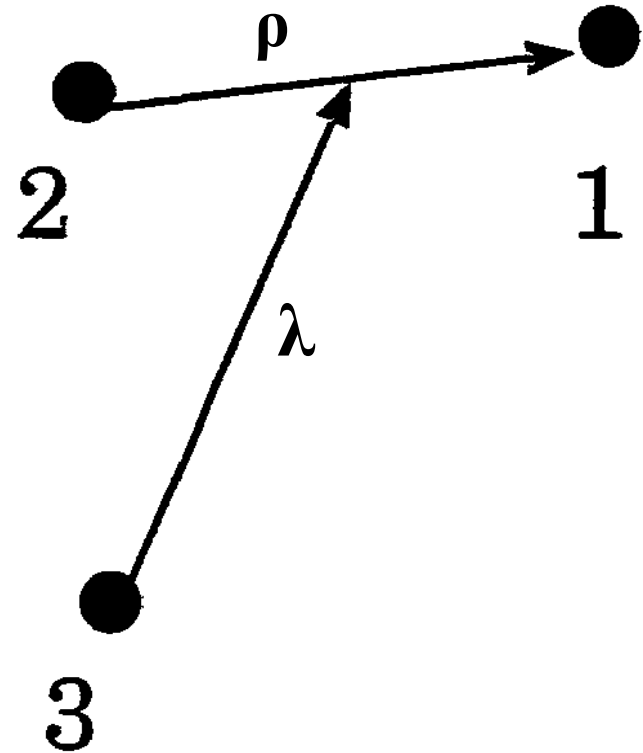$$\boldsymbol{\lambda} = \frac{\mathbf{r}_1 m_1 + \mathbf{r}_2 m_2}{m_1 + m_2} - \mathbf{r}_3$$

$$\mathbf{R} = 0$$

and back

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2 = \boldsymbol{\rho}$$

$$\mathbf{r}_{13} = \mathbf{r}_1 - \mathbf{r}_3 = \boldsymbol{\lambda} + \frac{m_2}{m_1 + m_2}\boldsymbol{\rho}$$

$$\mathbf{r}_{23} = \mathbf{r}_2 - \mathbf{r}_3 = \boldsymbol{\lambda} - \frac{m_1}{m_1 + m_2}\boldsymbol{\rho}$$

The wave function of the ground state is represented as follow:

$$\psi_{00}(\boldsymbol{\rho},\boldsymbol{\lambda},A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}$$

Wave function of ground state (0,0) and excited state (0,1)

The wave function of the excited state:

$$\psi_{10}(\boldsymbol{\rho},\boldsymbol{\lambda},A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}(\boldsymbol{\varepsilon}\boldsymbol{\rho})$$ Wave function of excited state (1,0)

$$\psi_{01}(\boldsymbol{\rho},\boldsymbol{\lambda},A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}(\boldsymbol{\varepsilon}\boldsymbol{\lambda})$$

$$\psi_{11}^{*}(\boldsymbol{\rho},\boldsymbol{\lambda},A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}(\boldsymbol{\varepsilon}[\boldsymbol{\rho}\times\boldsymbol{\lambda}])$$ Wave function of excited state (1,1)*

The wave function of the excited state with orbital angular momentum L = 1 is a superposition of Ψ_{10} and Ψ_{01}. In our work we obtain for this state the approximation Ψ_{10}.

$$\psi_{00}(\boldsymbol{\rho}, \boldsymbol{\lambda}, A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\boldsymbol{\rho} \cdot \boldsymbol{\lambda})]}$$

The operator of kinetic energy:

$$\hat{T} = -\frac{\hbar^2}{2\mu_1}\nabla_{\boldsymbol{\rho}}^2 - \frac{\hbar^2}{2\mu_2}\nabla_{\boldsymbol{\lambda}}^2$$

where:

$$\mu_1 = \frac{m_1 m_2}{m_1 + m_2}, \qquad \mu_2 = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}$$

Matrix elements of kinetic energy:

$$< \phi' \mid \hat{T} \mid \phi >^{00} = \frac{24\pi^3}{\det B^{2.5}} \{ \frac{\hbar^2}{2\mu_1} I_\rho^{00} + \frac{\hbar^2}{2\mu_2} I_\lambda^{00} \}$$

$$I_\rho^{00} = A_{12}^2 B_{11} - 2A_{11}A_{12}B_{12} + A_{11}(B_{12}^2 + (A_{11} - B_{11})B_{22})$$

$$I_\lambda^{00} = A_{12}^2 B_{22} - 2A_{22}A_{12}B_{12} + A_{22}(B_{12}^2 + (A_{22} - B_{22})B_{11})$$

$$B_{ij} = A_{ij} + A_{ij}'$$

The operator of potential energy:

$$V = \frac{e_1 e_2}{|\boldsymbol{\rho}|} + \frac{e_1 e_3}{|\boldsymbol{\lambda} + \dfrac{m_2}{m_1 + m_2}\boldsymbol{\rho}|} + \frac{e_2 e_3}{|\boldsymbol{\lambda} - \dfrac{m_2}{m_1 + m_2}\boldsymbol{\rho}|}$$

Matrix elements of potential energy:

$$<\phi' | \hat{V} | \phi> = e_1 e_2 I_{12}^{00} + e_1 e_3 I_{13}^{00} + e_2 e_3 I_{23}^{00}$$

$$I_{12}^{00} = \frac{8\sqrt{2}\pi^{2.5}}{\sqrt{B_{22} \det B}}$$

$$F_1^{13,23} = B_{11} + B_{22}(\frac{m_{2,1}^{13,23}}{m_1 + m_2})^2 \mp 2B_{12}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

$$I_{13,23}^{00} = \frac{8\sqrt{2}\pi^{2.5}}{\sqrt{F_1^{13,23}(B_{22}F_1^{13,23} - (F_2^{13,23})^2)}}$$

$$F_2^{13,23} = B_{12} \mp 2B_{22}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

Matrix elements of normalization:

$$<\phi' | \phi>^{00} = \frac{8\pi^3}{\det B^{1.5}}$$

$$\psi_{10}(\boldsymbol{\rho}, \boldsymbol{\lambda}, A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}(\boldsymbol{\varepsilon\rho})$$

The operator of kinetic energy:

$$\hat{T} = -\frac{\hbar^2}{2\mu_1}\nabla^2_{\boldsymbol{\rho}} - \frac{\hbar^2}{2\mu_2}\nabla^2_{\boldsymbol{\lambda}}$$

where:

$$\mu_1 = \frac{m_1 m_2}{m_1 + m_2}, \qquad \mu_2 = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}$$

Matrix elements of kinetic energy:

$$<\phi'|\hat{T}|\phi>^{10} = -\frac{6\pi^2}{\det B^{3.5}}\{\frac{\hbar^2}{2\mu_1}I^{10}_\rho + \frac{\hbar^2}{2\mu_2}I^{10}_\lambda\}$$

$$I^{10}_\rho = 5A_{11}B_{22}[B^2_{12} + (A_{11} - B_{11})B_{22}] - 2A_{12}B_{12}(B^2_{12} + 5A_{11}B_{22} - B_{11}B_{22}) + A^2_{12}(2B^2_{12} + 3B_{11}B_{22})$$

$$I^{10}_\lambda = 5A^2_{12}B^2_{22} + A_{22}B_{22}(-10A_{12}B_{12} + 3B^2_{12} - 3B_{11}B_{22}) + A^2_{22}(2B^2_{12} + 3B_{11}B_{22})$$

$$B_{ij} = A_{ij} + A'_{ij}$$

The operator of potential energy:

$$V = \frac{e_1 e_2}{|\boldsymbol{\rho}|} + \frac{e_1 e_3}{|\boldsymbol{\lambda} + \dfrac{m_2}{m_1 + m_2} \boldsymbol{\rho}|} + \frac{e_2 e_3}{|\boldsymbol{\lambda} - \dfrac{m_2}{m_1 + m_2} \boldsymbol{\rho}|}$$

Matrix elements of potential energy:

$$< \phi' | \hat{V} | \phi >= e_1 e_2 I_{12}^{10} + e_1 e_3 I_{13}^{10} + e_2 e_3 I_{23}^{10}$$

$$I_{12}^{10} = \frac{4\sqrt{2}\pi^{1.5}\sqrt{B_{22}}}{(\det B)^2}$$

$$I_{13,23}^{10} = \frac{2\sqrt{2}\pi^{1.5}(3B_{22}F_1^{13,23} - (F_2^{13,23})^2)}{(F_1^{13,23})^{1.5}(B_{22}F_1^{13,23} - (F_2^{13,23})^2)^2}$$

$$F_1^{13,23} = B_{11} + B_{22}(\frac{m_{2,1}^{13,23}}{m_1 + m_2})^2 \mp 2B_{12}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

$$F_2^{13,23} = B_{12} \mp 2B_{22}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

Matrix elements of normalization:

$$< \phi' | \phi >^{10} = \frac{6\pi^2 B_{22}}{\det B^{2.5}}$$

$$\psi_{11}^{*}(\boldsymbol{\rho},\boldsymbol{\lambda},A) = e^{-\frac{1}{2}[A_{11}\rho^2 + A_{12}\lambda^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}(\boldsymbol{\varepsilon}[\boldsymbol{\rho}\times\boldsymbol{\lambda}])$$

The operator of kinetic energy:

$$\hat{T} = -\frac{\hbar^2}{2\mu_1}\nabla_{\boldsymbol{\rho}}^2 - \frac{\hbar^2}{2\mu_2}\nabla_{\lambda}^2$$

where:

$$\mu_1 = \frac{m_1 m_2}{m_1 + m_2}, \qquad \mu_2 = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}$$

Matrix elements of kinetic energy:

$$<\phi' | \hat{T} | \phi>^{11} = -\frac{60\pi^2}{\det B^{3.5}}\{\frac{\hbar^2}{2\mu_1}I_{\rho}^{11} + \frac{\hbar^2}{2\mu_2}I_{\lambda}^{11}\}$$

$$I_{\rho}^{11} = A_{12}^2 B_{11} - 2A_{11}A_{12}B_{12} + A_{11}(B_{12}^2 + (A_{11} - B_{11})B_{22})$$

$$I_{\lambda}^{11} = A_{12}^2 B_{22} - 2A_{22}A_{12}B_{12} + A_{22}(B_{12}^2 + (A_{22} - B_{22})B_{11})$$

$$B_{ij} = A_{ij} + A_{ij}'$$

The operator of potential energy:

$$V = \frac{e_1 e_2}{|\boldsymbol{\rho}|} + \frac{e_1 e_3}{|\boldsymbol{\lambda} + \dfrac{m_2}{m_1 + m_2}\boldsymbol{\rho}|} + \frac{e_2 e_3}{|\boldsymbol{\lambda} - \dfrac{m_2}{m_1 + m_2}\boldsymbol{\rho}|}$$

Matrix elements of potential energy:

$$<\phi' | \hat{V} | \phi> = e_1 e_2 I_{12}^{11} + e_1 e_3 I_{13}^{11} + e_2 e_3 I_{23}^{11}$$

$$I_{12}^{11} = \frac{8\sqrt{2}\pi^{1.5}}{\sqrt{B_{22}}(\det B)^2}$$

$$F_1^{13,23} = B_{11} + B_{22}(\frac{m_{2,1}^{13,23}}{m_1 + m_2})^2 \mp 2B_{12}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

$$I_{13,23}^{11} = \frac{8\sqrt{2}\pi^{1.5}}{\sqrt{F_1^{13,23}}(B_{22}F_1^{13,23} - (F_2^{13,23})^2)^2}$$

$$F_2^{13,23} = B_{12} \mp 2B_{22}\frac{m_{2,1}^{13,23}}{m_1 + m_2}$$

Matrix elements of normalization:

$$<\phi' | \phi>^{11} = \frac{12\pi^2}{\det B^{2.5}}$$

In the stochastic variational method, there are two options for solving the problem. Create a new basis, or increase an existing one.

1. Assuming that the basis already contains N-1 elements, we will create K new elements and find the energy values for all new N-dimensional bases containing the i-th new element and N-1 of the previously specified elements. The basic element for which the lowest energy value was obtained is selected as the new Nth element of the basis, and is retained in it. The dimension of the basis becomes equal to N. Due to the fact that the basis of (N-1) elements is orthogonal, there is no need to diagonalize.

1) several sets of $A_K^n, n = 1,...,N$ are generated randomly;

2) by solving the eigenvalue problem, the corresponding energies $E_K^1,...,E_K^N$ are determined;

3) by choosing the parameter (A_K^n) belonging to the lowest energy E_K^n as a basis parameter and by adding it to the previous basis states, the parameters of the new basis become $A_1,...,A_{K-1}, A_K = A_K^n$;

4) the basis dimension is increased to K + 1.

In the stochastic variational method, there are two options for solving the problem. Create a new basis, or increase an existing one.

2. "Stripping" the given basis, to improve the energy values. In this case, the dimension of the basis remains fixed, but a certain k-th element is replaced by a new one, by analogy with the first method. Simultaneously, it is checked whether new elements give better energy in comparison with the initial state. Such a substitution can be made for all elements of the basis.

1) several sets of ($A_1^n,...,A_K^n, n = 1,...,N$) are generated randomly;

2) by solving the eigenvalue problem, the corresponding energies ($E_K^1,...,E_K^N$) are determined;

3) the parameter set ($A_1^n,...,A_K^n$) belonging to the lowest energy E_K^n are chosen as basis parameters.

To solve this problem was written the code in Matlab. The program was based on the fortran program of K.Varga and Y.Suzuki.

In the program of Varga, Suzuki we made a number of changes. In particular, the matrix elements of the kinetic energy, potential energy and normalization condition were calculated analytically and included to the program code.

The main results of the calculation are the energies of the ground and excited states. The wave function is calculated at each step of the program.

The energy is recorded in the file "ener.txt". Each step to refine the energy can be found in the files "fbs.txt" and "fbs2.txt" after the calculation is completed.

K. Varga, Y. Suzuki Computer Physics Communications **106** (1997) 157-168

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Bound state energy (0,0) tdµ :

- 0.53855183546243 (svm1)

- 0.538591760656226 (svm2)

- 0.538593976205724 (5 svm2)

- 0.53859497087932082507 (Korobov)

The number of excited states: 1

Bound state energy (0,1) tdµ :

- 0.486564423416966 (svm1)

- 0.487265261345949 (svm2)

- 0.487977237559981 (5 svm2)

- 0.48806535322284823806 (Korobov)

Bound state energy (0,0) tpµ :

- 0.51979447100426 (svm1)

- 0.51986559694429 (svm2)

- 0.51987798832482 (5 svm2)

Bound state energy (0,0) dpµ :

- 0.512496673445515 (svm1)

- 0.512695447627241 (svm2)

- 0.512709837201390 (5 svm2)

Bound state energy (1,0) tdμ :

- 0.52296780112542 (svm1)

- 0.52310122781941 (svm2)

- 0.52311978760520 (5 svm2)

- 0.52319145093410217939 (Korobov)

Bound state energy (1,0) dpμ :

- 0.49033236515962 (svm1)

- 0.49046513131319056 (svm2)

- 0.490470566438299 (5 svm2)

Bound state energy (1,1) tdμ :

- 0.48025122820694 (svm1)

- 0.48031862915565 (svm2)

- 0.48043608551941 (5 svm2)

- 0.481991526590075978397226660 (Korobov)

Bound state energy (1,0) tpμ :

- 0.49924435859375 0 (svm1)

- 0.49928288414580 6 (svm2)

- 0.499289503090621 (5 svm2)

Bound state energy tdμ :

- 0.123855852053679 (svm1)

- 0.123866827488976 (svm2)

- 0.123867561755999 (5 svm2)

- 0.123867812559127201 69 (Korobov)

Bound state energy dpμ :

- 0.118985919349536 (svm1)

- 0.118988462402906 (svm2)

- 0.118989205304850 (5 svm2)

Bound state energy tpμ :

- 0.120467219084781 (svm1)

- 0.120467553327225 (svm2)

- 0.120467665186657 (5 svm2)

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