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SAMARA UNIVERSITY

IV international conference on particle physics and astrophysics

Weakly bound states of dtμ muonic molecular ion in quantum electrodynamics

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October 24, Moscow, Russia

INTRODUCTION AND OVERVIEW

The investigation of the energy spectra of hydrogen muonic molecules is important for muonic catalysis of nuclear fusion reactions. A calculation of fine and hyperfine structure of muonic molecular ions as well as of higher order QED corrections allows us to predict the rates of reactions of their formation and other parameters of the μCF cycle.

Note that there are several different approaches to the classification of bound states in mesomolecular ions. One of them originates from adiabatic approach and involves a pair of two quantum numbers J and ν, where J is rotational quantum number and ν is vibrational quantum number.

One can introduce so-called “binding energy”:

$$\epsilon_{binding} = -2\mathrm{Ry}(E_{total} + \frac{m_r}{2n^2})(in\ eV),$$

where m_r is reduced mass of tμ, n is principle quantum number of such bound state. For (0,0), (0,1), (1,0) and (1,1) states n=1, while for the $(-1)^{L+1}$ parity metastable P-state n=2. For a given total energy of a particular state of a mesomolecular ion the sign of binding energy defines whether the state is bound or not.

- *Korobov V.I., Puzynin I.V. and Vinitsky S.I. Physics Letters 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.*

PURPOSE

The aim of this work is to study the energy spectrum of three-particle dtμ muonic molecular ion on the basis of variational approach.

Tasks:

1. Analylical calculation of diagonal and off-diagonal matrix elements of kinetic energy, potential energy and overlap for all basis functions;

2. Writing computer code to solve bound state problem for three particles using stochastic variational method with correlated Gaussian basis;

3. Calculation of the energy of the ground and excited states, including weakly-bound states, of dtμ muonic molecular ion on the basis of variational method.

GENERAL FORMALISM

Let us consider a system of N particles. The Schrodinger equation in Jacobi coordinates has the form:

$$H\Psi = E\Psi$$

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

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

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

An upper bound for the energy of ground and excited states is given by the lowest eigenvalue of the generalized eigenvalue problem:

$$HC = E_K BC$$

$$H_{ij} = \langle \psi(\mathbf{x}, A_i) | H | \psi(\mathbf{x}, A_j) \rangle$$

$$B_{ij} = \langle \psi(\mathbf{x}, A_i) | \psi(\mathbf{x}, A_j) \rangle$$

GAUSSIAN BASIS FUNCTIONS

In variational approach with correlated Gaussian basis wave functions have the form:

$$\Psi(\mathbf{x}, A) = G_A(\mathbf{x})\theta_L(\mathbf{x}),$$

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

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

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

x_N – center of mass coordinate

The angular part of the basis wave function has the following form:

$$\theta_L(\mathbf{x}) = [[[\mathbb{Y}_{l_1}(\mathbf{x}_1)\mathbb{Y}_{l_2}(\mathbf{x}_2)]_{L_{12}}\ \mathbb{Y}_{l_3}(\mathbf{x}_3)]_{L_{123}} \ldots]_{LM} .$$

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

JACOBI COORDINATES

We use the following order of particles:

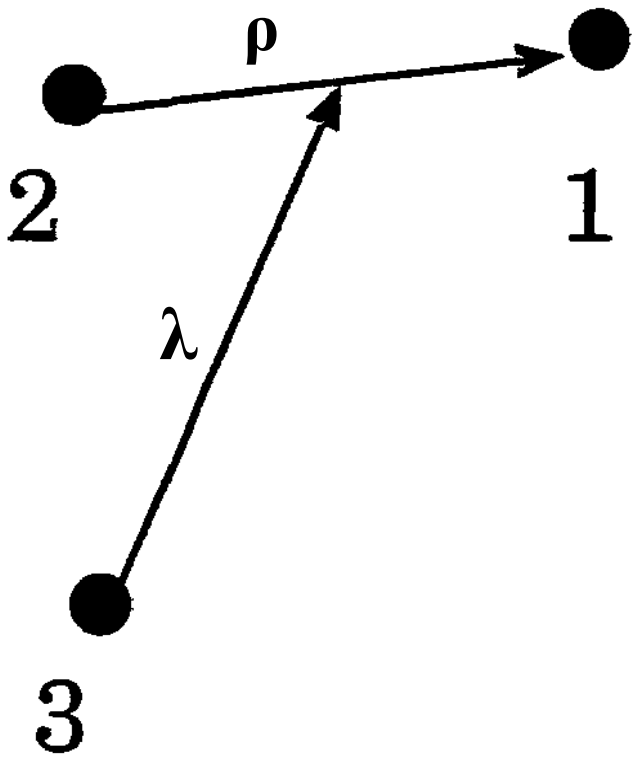
$$\begin{matrix} 1 & 2 & 3 \\ t & d & \mu \end{matrix}$$

The Jacobi coordinates are related to the relative particle coordinates as follows:

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

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

$$\mathbf{R} = 0$$



For the interparticle coordinates:

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

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

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

GAUSSIAN BASIS FUNCTIONS

The wave function of the ground state (L=0):

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

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

In the case of three nonidentical particles in P-state (L=1, where L is total angular momentum of particles) there are three possible wave functions:

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

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

Wave functions of (1,0) and (1,1) states

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

Wave function of $(-1)^{L+1}$ parity state

First two wave functions have "normal" spacial parity $(-1)^L$ while the third one has the "odd" parity $(-1)^{L+1}$. We investigate both of these cases.

The wave function of the excited state with total orbital angular momentum L = 1 is a superposition of Ψ_{10} and Ψ_{01}.

KOROBOV'S (EXPONENTIAL) APPROACH

The variational exponential expansion for arbitrary L, using the relative coordinates (r_{31}, r_{32} and r_{21}) is 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 c_{il} are linear parameters and $\alpha_{jl}^{(i)}$ are 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 **k** is the unit vector along the Z axis.

In these expressions, **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:

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

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

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

GROUND STATE L=0

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

Kinetic energy operator:

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

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:

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

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

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

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

GROUND STATE L=0

Potential energy operator:

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

Matrix elements of potential energy:

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

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

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

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

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

Overlap matrix elements:

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

EXCITED STATE L=1

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

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

Matrix elements of kinetic energy:

$$<\phi'|\hat{T}|\phi>^{10,01,11,(01|10)}=-\frac{6\pi^2}{(\det B)^{7/2}}\left\{\frac{\hbar^2}{2\mu_1}I_\rho^{10,01,11,(01|10)}+\frac{\hbar^2}{2\mu_2}I_\lambda^{10,01,11,(01|10)}\right\},$$

$$I_\rho^{10}=5A_{11}B_{22}[B_{12}^2+(A_{11}-B_{11})B_{22}]-2A_{12}B_{12}(B_{12}^2+5A_{11}B_{22}-B_{11}B_{22})+A_{12}^2(2B_{12}^2+3B_{11}B_{22}),$$

$$I_\lambda^{10}=5A_{12}^2B_{22}^2+A_{22}B_{22}(-10A_{12}B_{12}+3B_{12}^2-3B_{11}B_{22})+A_{22}^2(2B_{12}^2+3B_{11}B_{22}),$$

$$I_\rho^{01}=5A_{12}^2B_{11}^2+A_{11}B_{11}(-10A_{12}B_{12}+3B_{12}^2-3B_{22}B_{11})+A_{11}^2(2B_{12}^2+3B_{22}B_{11}),$$

$$I_\lambda^{01}=5A_{22}B_{11}[B_{12}^2+(A_{22}-B_{22})B_{11}]-2A_{12}B_{12}(B_{12}^2+5A_{22}B_{11}-B_{22}B_{11})+A_{12}^2(2B_{12}^2+3B_{22}B_{11}),$$

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

$$I_\rho^{(01|10)}=-B_{12}[-2A_{12}B_{12}(4A_{11}+B_{11})+5A_{11}B_{12}^2+5A_{12}^2B_{11}]-B_{22}(A_{11}-B_{11})(5A_{11}B_{12}-2A_{12}B_{11}),$$

$$I_\lambda^{(01|10)}=5A_{12}^2B_{12}B_{22}-A_{22}(2A_{12}B_{11}B_{22}+8A_{12}B_{12}^2+3B_{11}B_{12}B_{22}-3B_{12}^3)+5A_{22}^2B_{11}B_{12}.$$

Overlap matrix elements:

$$<\phi'|\phi>^{01}=\frac{6\pi^2B_{11}}{(\det B)^{5/2}},\ <\phi'|\phi>^{11}=\frac{12\pi^2}{(\det B)^{5/2}},\ <\phi'|\phi>^{(01|10)}=-\frac{6\pi^2B_{12}}{(\det B)^{5/2}}.$$

EXCITED STATE L=1

Matrix elements of potential energy:

$$<\phi'|\hat{V}|\phi>^{10,01,11,(01|10)} = e_1e_2I_{12}^{10,01,11,(01|10)} + e_1e_3I_{13}^{10,01,11,(01|10)} + e_2e_3I_{23}^{10,01,11,(01|10)},$$

$$I_{12}^{10} = \frac{4\sqrt{2}\pi^{3/2}\sqrt{B_{22}}}{(\det B)^2},\ I_{13,23}^{10} = \frac{2\sqrt{2}\pi^{3/2}(3B_{22}F_1^{13,23} - (F_2^{13,23})^2)}{(F_1^{13,23})^{3/2}[B_{22}F_1^{13,23} - (F_2^{13,23})^2]^2},$$

$$I_{12}^{01} = \frac{2\sqrt{2}\pi^{3/2}(3B_{11}B_{22} - B_{12}^2)}{(B_{22})^{3/2}(\det B)^2},\ I_{13,23}^{01} = \frac{2\sqrt{2}\pi^{3/2}}{[B_{22}F_1^{13,23} - (F_2^{13,23})^2]^2}\Big\{2\sqrt{F_1^{13,23}} +$$

$$+\frac{(3B_{22}F_1^{13,23} - (F_2^{13,23})^2)}{(F_1^{13,23})^{3/2}}\frac{(m_{2,1}^{13,23})^2}{m_{12}^2} \pm \frac{4F_2^{13,23}}{\sqrt{F_1^{13,23}}}\frac{m_{2,1}^{13,23}}{m_{12}}\Big\},$$

$$I_{12}^{11} = \frac{8\sqrt{2}\pi^{3/2}}{\sqrt{B_{22}}(\det B)^2},\ I_{13,23}^{11} = \frac{8\sqrt{2}\pi^{3/2}}{\sqrt{F_1^{13,23}}[B_{22}F_1^{13,23} - (F_2^{13,23})^2]^2},\ I_{12}^{(01|10)} = -\frac{4\sqrt{2}\pi^{3/2}B_{12}}{\sqrt{B_{22}}(\det B)^2},$$

$$I_{13,23}^{(01|10)} = -\frac{2\sqrt{2}\pi^{3/2}}{[B_{22}F_1^{13,23} - (F_2^{13,23})^2]^2}\Big\{2\frac{F_2^{13,23}}{\sqrt{F_1^{13,23}}} \mp \frac{m_{2,1}^{13,23}}{m_{12}}\frac{(3B_{22}F_1^{13,23} - (F_2^{13,23})^2)}{(F_1^{13,23})^{3/2}}\Big\}.$$

$$F_1^{13,23} = B_{11} + B_{22}\left(\frac{m_{2,1}^{13,23}}{m_1+m_2}\right)^2 \mp 2B_{12}\frac{m_{2,1}^{13,23}}{m_1+m_2},\ F_2^{13,23} = B_{12} \mp 2B_{22}\frac{m_{2,1}^{13,23}}{m_1+m_2}.$$

EXCITED STATE WITH $(-1)^{L+1}$ PARITY

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

Matrix elements of kinetic energy:

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

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

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

Matrix elements of potential energy:

$$<\varphi'|\hat{V}|\varphi> = e_1e_2I_{12}^{11} + e_1e_3I_{13}^{11} + e_2e_3I_{23}^{11},$$

$$I_{12}^{11} = \frac{8\sqrt{2}\pi^{1.5}}{\sqrt{B_{22}}(\det B)^2},\ I_{13,23}^{11} = \frac{8\sqrt{2}\pi^{1.5}}{\sqrt{F_1^{13,23}}(B_{22}F_1^{13,23} - (F_2^{13,23})^2)^2}.$$

Overlap matrix elements:

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

THE PROGRAM

- For the numerical calculation of energy levels of three-particle Coulomb bound states the code in MATLAB is written. The program uses stochastic variational approach with random optimization procedure for nonlinear variational parameters;
- The program is based on the Fortran program by K.Varga and Y.Suzuki;
- A number of changes were made compared to the Fortran program, including the ability to calculate states with nonzero L, more convenient variational parameters generation and various optimization changes;
- The main results of the calculation include energies of ground and excited states along with variational wave functions for each state. The program is capable of calculating L=0 and L=1;
- We are now working on improved calculation of (1,1) state and the ability to calculate various QED corrections such as relativistic and vacuum polarization corrections.

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

RESULTS AND COMPARISON

Bound state energy (0,0) tdμ :
-0.53859497048 (svm)
-0.53859497088 (Korobov)
-0.53859497170 (Frolov)

Bound state energy (0,1) tdμ :
-0.48805628731 (svm)
-0.48806535340 (Korobov)
-0.48806535421(Frolov)

Bound state energy (1,0) tdμ :
-0.52319145028 (svm)
-0.52319145093 (Korobov)
-0.52319145200 (Frolov)

Bound state energy (1,1) tdμ :
-0.48197043950 (svm)
-0.48199152659 (Korobov)
-0.48199152705 (Frolov)

Bound state energy L=1, $(-1)^{L+1}$parity tdμ :
-0.12386781229 (svm)
-0.12386781255 (Korobov)

(all energies are in muon atomic units)

- A.M. Frolov, D.M. Wardlaw, Bound state spectra of three-body muonic molecular ions. // Eur. Phys. J. D, 2011, v. 63, p. 339-350.

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