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САМАРСКИЙ УНИВЕРСИТЕТ
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Investigation of energy levels of exotic three-particle systems in the variational approach

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RELEVANCE

There are exotic bound states (muonium, positronium, positronium ion, muonic hydrogen, pionic helium, kaonic helium), which have attracted the attention of both experimenters and theoreticians for decades.

Pionic (kaonic) helium consists of negative pion (kaon), electron and helium nucleus. π^- is in Rydberg state of large principal (n=17) and orbiral angular momentum (l~16,15) quantum numbers. The pionic helium is predicted to have an anomalously long nanosecond-scale lifetime, which could allow laser spectroscopy to be carried out. The study of pionic (kaonic) helium energy levels is important for test of Standard Model and determination fundamental constants such as the pion mass, kaon mass.

In the work [1], a successful experiment has already been carried out, which gave a transition frequency value ((n, l) = (17.16) → (17.15)) of 183760 MHz. From the measurement of pion transitions between states with large values of the principal and orbital quantum numbers ((n, l) = (17.16) → (17.15)) one can try to obtain a more accurate value of the pion mass than can be done by other methods.

Theoretical calculation of energy levels in pionic helium was carried out in [2] using variation approach with exponential basis.

1. M. Hori, H. Aghai-Khozani, A. Soter, A. Dax, D. Barna, Nature 581, 37 (2020).
2. M. Hori, A. Soter, V. I. Korobov, Phys. Rev. A 89, 042515 (2014).

PURPOSE AND TASKS

The purpose of this work is to study the energy spectrum of three-particle pionic helium Heπe and kaonic helium HeKe on the basis of variational approach with Gaussian basis.

Tasks:

1. Analytical calculation of matrix elements for kinetic, potential energies and normalization for ground and excited states.
2. 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 three-particle systems.
3. Calculation of the energy levels bound states on the basis of stochastic variational method [1,2].

Previously, within the framework of the stochastic variational method, the energy levels of mesomolecules of hydrogen, muonic helium, and other systems were studied.

1. K. Varga and Y. Suzuki, Comp. Phys. Comm. 106, 157 (1997).
2. A. V. Eskin, V. I. Korobov, A. P. Martynenko, F. A. Martynenko, Atoms 11, 25 (2023).

STOCHASTIC VARIATIONAL METHOD

A system of three particles with masses m_1, m_2 and m_3 and charges e_1, e_2 and e_3 is described by the Schrödinger equation in Jacobi coordinates and has the form:

$$H\Psi(\boldsymbol{\rho},\boldsymbol{\lambda}) = E\Psi(\boldsymbol{\rho},\boldsymbol{\lambda})$$

$$H = -\frac{\hbar}{2\mu_1}\Delta_\rho - \frac{\hbar}{2\mu_2}\Delta_\lambda + \frac{e_1e_2}{|\boldsymbol{\rho}|} + \frac{e_1e_3}{\left|\boldsymbol{\lambda} + \frac{m_2}{m_1+m_2}\boldsymbol{\rho}\right|} + \frac{e_2e_3}{\left|\boldsymbol{\lambda} - \frac{m_1}{m_1+m_2}\boldsymbol{\rho}\right|}$$

$$\mu_1 = \frac{m_1m_2}{m_1+m_2},\ \mu_2 = \frac{(m_1+m_2)m_3}{m_1+m_2+m_3},\ \boldsymbol{\rho} = \mathbf{r}_1 - \mathbf{r}_2,\ \boldsymbol{\lambda} = \frac{\mathbf{r}_1m_1 + \mathbf{r}_2m_2}{m_1+m_2} - \mathbf{r}_3$$

The upper bound for the energy of the ground state of the system is given by the smallest eigenvalue of the generalized eigenvalue problem

$$\Psi = \sum_{i=1}^{K} c_i\psi_i(\boldsymbol{\rho},\boldsymbol{\lambda},A_i)$$

$$\psi(\boldsymbol{\rho},\boldsymbol{\lambda},A) = e^{-\frac{1}{2}[A_{11}\boldsymbol{\rho}^2 + A_{22}\boldsymbol{\lambda}^2 + 2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})]}$$

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

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

$$HC = E_KBC$$

ORDER OF PARTICLES

We use the following order of particles:

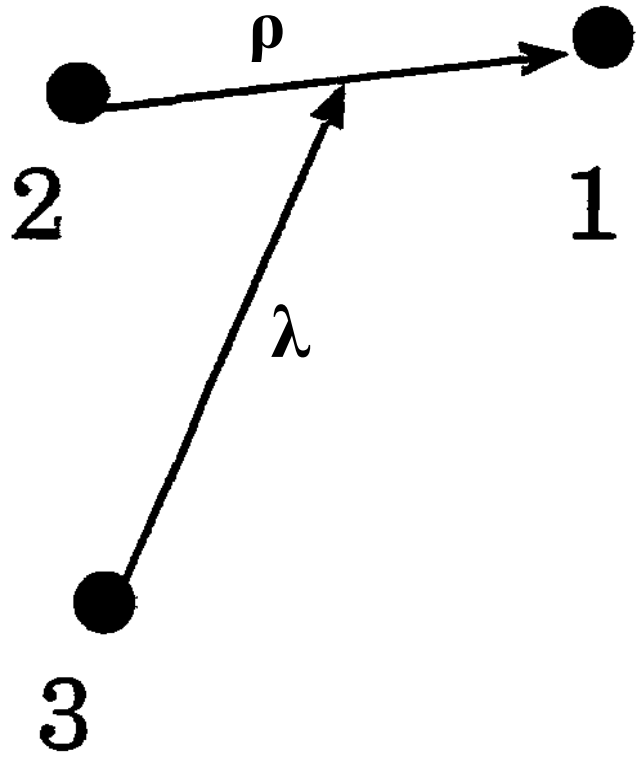
$$\overset{1}{He}\,\overset{2}{\pi}\,\overset{3}{e} \qquad \overset{1}{He}\,\overset{2}{K}\,\overset{3}{e}$$

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

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

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

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

MATRIX ELEMENTS

Since the π, K−-meson is in an orbital excited state l in the problem under consideration, the variational wave function of the system is chosen in the form:

$$\psi_{lm}(\boldsymbol{\rho},\boldsymbol{\lambda},A)=\sum_{l=1}^{K}C_i Y_{lm}(\theta_\rho,\varphi_\rho)\rho^l e^{-\frac{1}{2}\left[A_{11}\boldsymbol{\rho}^2+A_{22}\boldsymbol{\lambda}^2+2A_{12}(\boldsymbol{\rho}\cdot\boldsymbol{\lambda})\right]}$$

The kinetic energy operator contains two terms. The matrix element of the Laplace operator with respect to **λ** is calculated analytically and has the form:

$$\left\langle\Psi\left|\nabla_\lambda^2\right|\Psi\right\rangle=\sum_{i,j=1}^{K}C_iC_j 2^{l+2}\pi^{3/2}\Gamma(l+3/2)\frac{B_{22}^{l-1}}{(\det B)^{l+5/2}}\left[3A_{22}^i(A_{22}^i-B_{22})\det B+(2l+3)(A_{22}^iB_{12}-A_{12}^iB_{22})^2\right]$$

The analogous matrix element with the Laplace operator in **ρ** is equal to

$$\left\langle\Psi\left|\nabla_\rho^2\right|\Psi\right\rangle=\sum_{i,j=1}^{K}C_iC_j 2^{l+2}\pi^{3/2}\Gamma(l+1/2)\frac{B_{22}^{l-1}}{(\det B)^{l+5/2}}\times$$

$$\times\left[(2l+1)\det B(-(2l+3)A_{11}^iB_{22}+3(A_{12}^i)^2+2lA_{12}^iB_{12})+(2l+1)(2l+3)(A_{12}^iB_{12}-A_{11}^iB_{22})^2\right]$$

The normalization of the wave function is determined by the following expression:

$$\left\langle\Psi\left|\Psi\right\rangle\right.=\sum_{i,j=1}^{K}C_iC_j 2^{l+2}\pi^{3/2}\Gamma(l+3/2)\frac{B_{22}^{l}}{(\det B)^{l+3/2}},\quad B_{kn}=A_{kn}^i-A_{kn}^j,\quad \det B=B_{11}B_{22}-B_{12}^2$$

MATRIX ELEMENTS

The potential energy operator in the nonrelativistic Hamiltonian consists of pairwise Coulomb interactions U_{ij} (i, j=1, 2, 3). The convenience of using the Gaussian basis in this case also lies in the fact that all matrix elements of the potential energy operator are calculated analytically (in electronic atomic units):

$$\langle \Psi | U_{12} | \Psi \rangle = \langle \Psi | \frac{e_1 e_2}{|\boldsymbol{\rho}|} | \Psi \rangle = -Z \sum_{i,j=1}^{K} C_i C_j \, 2^{l+3/2} \pi^{3/2} \Gamma(l+1) \frac{B_{22}^{l-1/2}}{(\det B)^{l+1}}$$

$$\langle \Psi | U_{13} | \Psi \rangle = -Z \sum_{i,j=1}^{K} C_i C_j \, 2^{l+5/2} \pi \, \Gamma(l+3/2) \frac{B_{22}^{l+1/2}}{(\det B)^{l+3/2}} \, {}_2F_1\left(\frac{1}{2}, l+\frac{3}{2}, \frac{3}{2}, -\frac{\left(F_2^{23}\right)^2}{\det B} \right)$$

$$\langle \Psi | U_{23} | \Psi \rangle = \sum_{i,j=1}^{K} C_i C_j \, 2^{l+5/2} \pi \, \Gamma(l+3/2) \frac{B_{22}^{l+1/2}}{(\det B)^{l+3/2}} \, {}_2F_1\left(\frac{1}{2}, l+\frac{3}{2}, \frac{3}{2}, -\frac{\left(F_2^{13}\right)^2}{\det B} \right)$$

$$F_2^{13} = B_{12} + \frac{m_1}{m_{12}} B_{22}, \quad F_2^{23} = B_{12} - \frac{m_2}{m_{12}} B_{22},$$

All these matrix elements are expressed in terms of variational parameters A_{ij}, B_{ij}. These matrix elements are used below for solution of equation $HC = E_K BC$.

MATRIX ELEMENTS

The obtained wave functions make it possible to calculate the radial distribution densities in ρ and λ and root mean square values $\sqrt{\langle \rho^2 \rangle}, \sqrt{\langle \lambda^2 \rangle}$, which are determined by the expressions:

$$W(\rho) = \frac{(2\pi)^{3/2}}{\langle \psi | \psi \rangle} \sum_{i,j=1}^{K} \frac{C_i C_j}{B_{22}^{3/2}} \rho^{2l+2} e^{-\frac{1}{2}\frac{\det B}{B_{22}}\rho^2},$$

$$W(\lambda) = \frac{2^{l+5/3}\pi}{\langle \psi | \psi \rangle} \sum_{i,j=1}^{K} \frac{C_i C_j \Gamma\left(l+\frac{3}{2}\right)}{B_{11}^{l+3/2}} \lambda^2 e^{-\frac{1}{2}B_{22}\lambda^2} {}_1F_1\left(l+\frac{3}{2}, \frac{3}{2}, \frac{B_{12}^2 \lambda^2}{2B_{11}}\right),$$

$$\langle \rho^2 \rangle = \frac{\pi^{3/2} 2^{l+3} \Gamma\left(l+\frac{5}{2}\right)}{\langle \psi | \psi \rangle} \sum_{i,j=1}^{K} \frac{C_i C_j B_{22}^{l+1}}{(\det B)^{l+5/2}},$$

$$\langle \lambda^2 \rangle = \frac{\pi^{3/2} 2^{l+2} \Gamma\left(l+\frac{3}{2}\right)}{\langle \psi | \psi \rangle} \sum_{i,j=1}^{K} \frac{C_i C_j B_{22}^{l-1}}{(\det B)^{l+5/2}} \left(3B_{11}B_{22} - 2B_{12}^2 l\right),$$

These distributions are used after the numerical solution of the problem to analyze the characteristic distances at which our particles are located. They are illustrated in the graphs below.

PROGRAM

To solve the problem, the code was written in Matlab. The program was based on the program of K. Varga and J. Suzuki, which was implemented in the Fortran language.

The work of the program begins with reading the input file, which contains the masses of particles, charges, and the boundaries of the intervals for the generation of nonlinear variational parameters.

Matrix elements of normalization, kinetic and potential energies, calculated analytically, are included in the program.After generating nonlinear variational parameters and calculating the normalization and energies from them, the standard MATLAB function is called to solve the eigenvalue problem.

The result of the program operation is the numerical values of the energies of the ground and excited states, as well as the matrix of nonlinear variational parameters and the vector of expansion coefficients of the wave function in terms of the basis states, which can be used to calculate the radial distribution densities in ρ and λ and root mean square values $\sqrt{\langle \rho^2 \rangle}, \sqrt{\langle \lambda^2 \rangle}$ and corrections.

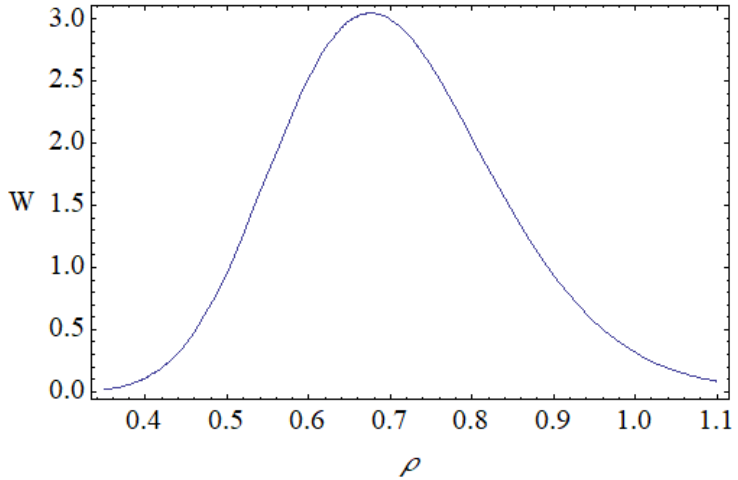
K. Varga, Y. Suzuki Computer Physics Communications **106** (1997) 157-168

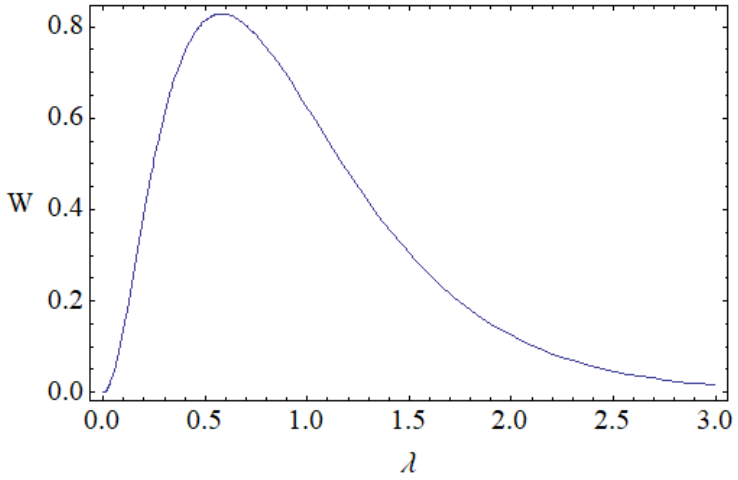
PROGRAM

```
Step 51 Energy1= -2.8081066215309773 Energy2= -2.6587193483232556
Step 52 Energy1= -2.8081285749218612 Energy2= -2.6588471626999364
Step 53 Energy1= -2.8081720719486762 Energy2= -2.6617218665731222
Step 54 Energy1= -2.8082120588126767 Energy2= -2.6618746228798771
Step 55 Energy1= -2.8082547436763878 Energy2= -2.6620515046881614
Step 56 Energy1= -2.8082689638245486 Energy2= -2.6621353838264219
Step 57 Energy1= -2.8082947124410991 Energy2= -2.6621562704249331
Step 58 Energy1= -2.8083084601128099 Energy2= -2.6624636715689713
Step 59 Energy1= -2.8083431910775878 Energy2= -2.6625436538251024
Step 60 Energy1= -2.8083595193690818 Energy2= -2.6625521145429638
Step 61 Energy1= -2.8083752801752633 Energy2= -2.6625798687037405
Step 62 Energy1= -2.8083957350452429 Energy2= -2.662764817235491
Step 63 Energy1= -2.808418834609983 Energy2= -2.6634817743639729
Step 64 Energy1= -2.8084344261507446 Energy2= -2.6636046694208781
Step 65 Energy1= -2.8084377894163084 Energy2= -2.6636082204717733
Step 66 Energy1= -2.8084508104731016 Energy2= -2.6636731612366606
Step 67 Energy1= -2.8084575743951481 Energy2= -2.6636935787052609
Step 68 Energy1= -2.8084650058552221 Energy2= -2.6651184386439422
Step 69 Energy1= -2.8084787079656452 Energy2= -2.6651200113925886
Step 70 Energy1= -2.808483860329591 Energy2= -2.6651247926748809
Step 71 Energy1= -2.8084962929609776 Energy2= -2.6660913381163907
Step 72 Energy1= -2.8085171374970961 Energy2= -2.6662476967443056
Step 73 Energy1= -2.8085287055830457 Energy2= -2.6663778415930639
Step 74 Energy1= -2.8085316347333915 Energy2= -2.6663806451116949
Step 75 Energy1= -2.8085352299683497 Energy2= -2.6663879584185581
Step 76 Energy1= -2.8085414391138421 Energy2= -2.667095882738006
Step 77 Energy1= -2.8085444518964819 Energy2= -2.6671032786393409
Step 78 Energy1= -2.8085541454485274 Energy2= -2.6671164473699061
Step 79 Energy1= -2.8085711724918054 Energy2= -2.6671165185029948
Step 80 Energy1= -2.8085861300383259 Energy2= -2.667140064529415
Step 81 Energy1= -2.8085917176255553 Energy2= -2.6671451178581522
Step 82 Energy1= -2.8085998221259696 Energy2= -2.6671624170305499
```

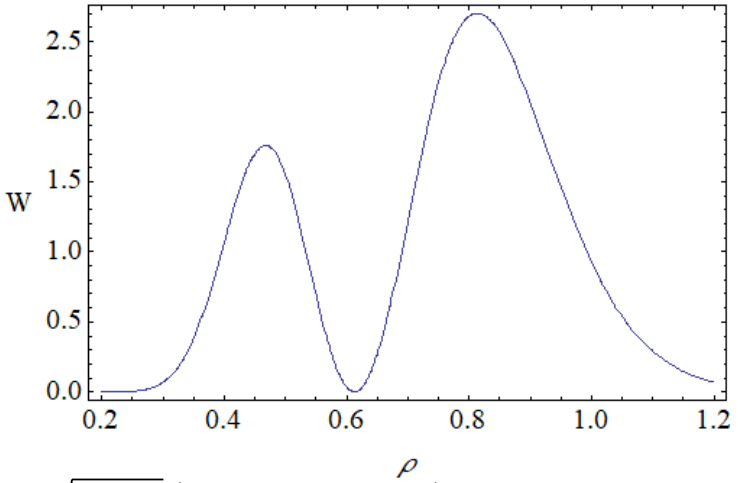
RESULTS

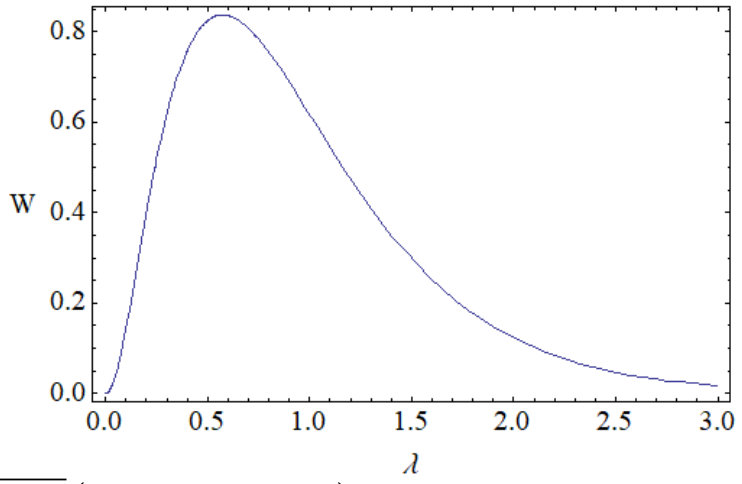
^{3}Heπe (17,16)





^{3}Heπe (17,15)



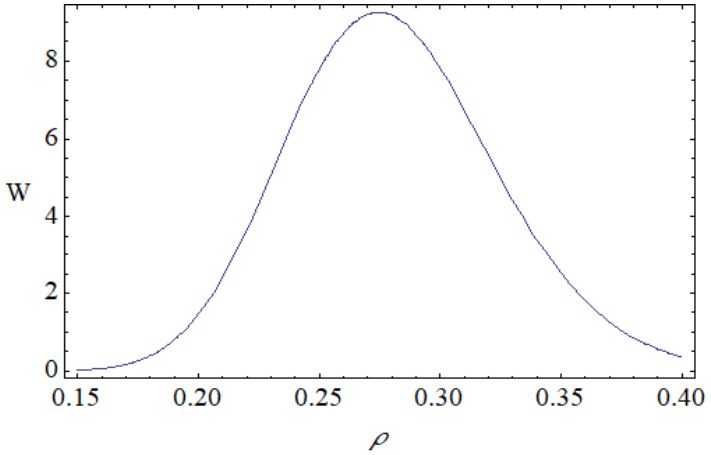


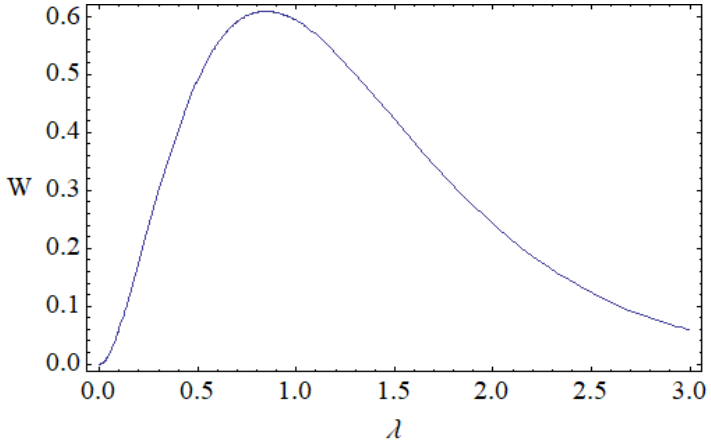
$$\sqrt{\langle \rho^2 \rangle}\left({}^3He\pi e(17,16)\right) = 37921\,\text{fm}, \quad \sqrt{\langle \lambda^2 \rangle}\left({}^3He\pi e(17,16)\right) = 59736.3\,\text{fm}$$

$$\sqrt{\langle \rho^2 \rangle}\left({}^3He\pi e(17,15)\right) = 40828\,\text{fm}, \quad \sqrt{\langle \lambda^2 \rangle}\left({}^3He\pi e(17,15)\right) = 59724.8\,\text{fm}$$

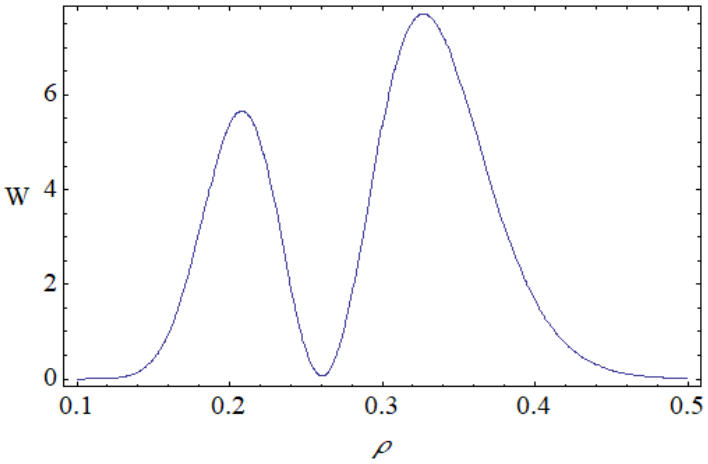
RESULTS

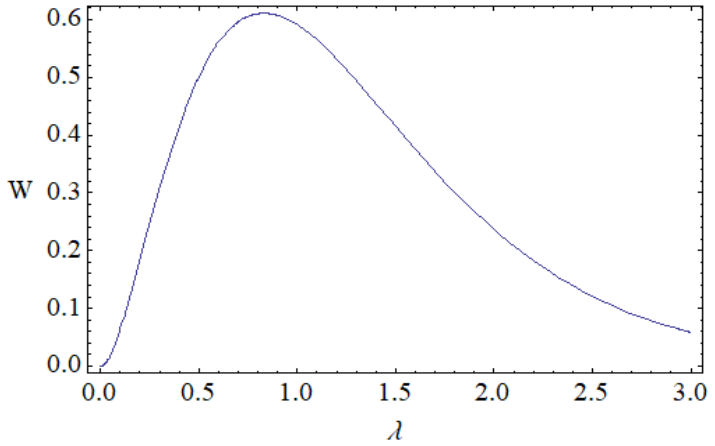
^{3}HeKe (21,20)





^{3}HeKe (21,19)





$$\sqrt{\langle \rho^2 \rangle}\left({}^3HeKe(21,20)\right) = 15040\,\text{fm}, \qquad \sqrt{\langle \lambda^2 \rangle}\left({}^3HeKe(21,20)\right) = 80359\,\text{fm}$$

$$\sqrt{\langle \rho^2 \rangle}\left({}^3HeKe(21,19)\right) = 15997\,\text{fm}, \qquad \sqrt{\langle \lambda^2 \rangle}\left({}^3HeKe(21,19)\right) = 81700\,\text{fm}$$

RESULTS

In this work, the following numerical values were obtained:

State (n,l)	E(^{3}Heπe),eau	E(^{4}Heπe),eau
(17,16), eau	-2.642382215	-2.656768966
(17,15) , eau	-2.669828479	-2.684242202

$$E(17,16) - E(17,15) = 183760 \text{ MHz (experiment [1] for } {}^4\text{He}\,\pi\text{e)}$$

$$E(17,16) - E(17,15) = 180588 \text{ MHz (theory for } {}^3\text{He}\,\pi\text{e)}$$

$$E(17,16) - E(17,15) = 180765 \text{ MHz (theory for } {}^4\text{He}\,\pi\text{e)}$$

1. In the experiment, there is a frequency shift due to the collision of pion helium atoms. This shift is analyzed by a separate group of experimenters [1].
2. For a more accurate comparison of theory with experiment, it is necessary to take into account corrections: relativistic corrections, corrections for vacuum polarization, and the structure of the nucleus.

1. M. Hori, H. Aghai-Khozani, A. Soter, A. Dax, D. Barna, Nature 581, 37 (2020).

RESULTS

In this work, the following numerical values for kaonic helium were obtained:

State (n,l)	E(^{3}HeKe),eau	E(^{4}HeKe),eau
(19,18)	-5. 11167212	-5. 28178268
(20,18)	-4. 69322183	-4. 85784789
(20,19)	-4. 68062221	-4. 83289366
(21,19)	-4. 32386298	-4. 46016857
(21,20)	-4.31336107	-4. 44998430
(22,20)	-4.01034272	-4. 13254880

RESULTS

In this work, the following numerical values were obtained:

State (n,l)	E(^{3}Heπe),eau	E(^{4}Heπe),eau
(21,19), eau	-4. 32386298	-4. 46016857
(21,20), eau	-4.31336107	-4. 44998430

$$E(21,20) - E(21,19) = \quad 69099\,\text{MHz (theory for } {}^3\text{He}Ke)$$

$$E(21,20) - E(21,19) = \quad 67009\,\text{MHz (theory for } {}^4\text{He}Ke)$$

1. Our theoretical results can be regarded as an estimate for an experimental search for transition frequencies.
2. For a more accurate comparison of theory with experiment, it is necessary to take into account corrections: relativistic corrections, corrections for vacuum polarization, and the structure of the nucleus.

THANK YOU
FOR YOUR ATTENTION