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EXCITED STATES WITH HIGH ORBITAL ANGULAR MOMENTUM OF THE MUON IN MUONIC-ELECTRONIC HELIUM ATOMS

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Motivation

In previous studies, the energy levels of three-body bound states consisting of leptons, pionic helium, and kaonic helium were investigated within the framework of a variational approach in quantum electrodynamics:

1. A.V. Eskin, V.I. Korobov, A.P. Martynenko, F.A. Martynenko, The Energy Spectrum of the Excited States in Mesonic Helium, Phys.Part.Nucl. 56 (2025) 2, 235-241;
2. V.I. Korobov, A.V. Eskin, A.P. Martynenko, F.A. Martynenko, Energy levels of mesonic helium in quantum electrodynamics, Phys.Rev.A 109 (2024) 3, 032802;
3. A.V. Eskin, A.P. Martynenko, F.A. Martynenko, D.K. Pometko, Few-particle lepton bound states in variational approach, Int. J. Mod. Phys. A 41 (2026) 15n16, 2650108, e-Print: 2602.10068;
4. D.K. Pometko, A.P. Martynenko, F.A. Martynenko, A.V. Eskin, Few-Body Lepton Bound States in Quantum Electrodynamics, Bulletin of the Lebedev Physics Institute, 2026, Vol. 53, No. 5, pp. 224–230.

In this work we continue to study the high-angular-momentum muon states in quantum electrodynamics in the case of muonic helium atom.

Goals and tasks of the research

Goals of the research:

- to develop a variational method for the three-particle case in the Jacobi coordinates in quantum electrodynamics using the MATLAB software package;
- to study the excited states energy levels of muonic helium (μeHe) within the framework of the variational approach.

Tasks of the research:

1. to construct the Hamiltonian of a three-particle Coulomb system in quantum electrodynamics in Jacobi coordinates;
2. to perform the analytical calculations of the matrix elements of the Hamiltonian with the Gaussian wave functions;
3. to calculate the energy levels of the excited states ${}^{3}_{2}He - \mu^- - e^-$ and ${}^{4}_{2}He - \mu^- - e^-$ with muon orbital momentum $l = 10,\ 11,\ 12,\ 13$;
4. to calculate the corrections to the energy levels to the relativism, the vacuum polarization and the contact interaction.

Muonic helium formation

The aim of this work is to study excited states of high-angular-momentum muons in muon-electron helium atoms, in which the muon and electron are approximately equidistant from the nucleus. From here on, we refer to such states as the Rydberg muon states, emphasizing that the principal quantum number for the muon orbit is quite large. When a beam of negative muons enters a helium target, it is slowed to a kinetic energy of several tens of eV due to ionization and excitation of target molecules. An exotic muonic helium atom is formed when a muon stops within the target and is captured by the target atom into an outer atomic orbit, replacing one of the electrons in an orbit with $n \leq 14$. The capture is a complex process and depends on the atomic and molecular structure, the range of values of the principal quantum number n, and the angular momentum l. The lifetime of a muonic helium atom is determined by large orbital angular momentum of $l = (10 \div 13)$, at which point the muon is formed. Its transition to the ground state with $l = 0$ is strongly suppressed. After capture, the muon cascades from its high-angular-momentum state through the atom's own series of bound states, located within the electron levels due to its greater mass. The cascade is accompanied by the emission of X-rays and ends when the particle is absorbed by the nucleus. For pionic helium atoms, studies of the Rydberg states allow us to obtain a more accurate pion mass than is known from other sources. M. Hori's group plans to perform laser spectroscopy of the kaonic atom using the kaon beam at DAPHNE, which will improve the accuracy of charged kaon mass determination by 2-3 orders of magnitude compared to the current level.

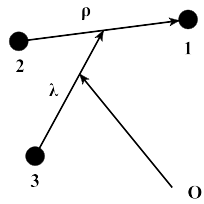


Fig. 1: The Jacobi coordinates for a 3-particle system (the muon-electron helium atom)

The system $He - \mu^- - e^-$ is studied by means of the Schrödinger equation:

$$H\Psi(\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ \boldsymbol{r}_3) = E\Psi(\boldsymbol{r}_1,\ \boldsymbol{r}_2,\ \boldsymbol{r}_3). \qquad (1)$$

We introduce the Jacobi coordinates $(\boldsymbol{\rho},\ \boldsymbol{\lambda})$:

$$\boldsymbol{\rho} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \qquad (2)$$

$$\boldsymbol{\lambda} = \frac{\boldsymbol{r}_1 m_1 + \boldsymbol{r}_2 m_2}{m_1 + m_2} - \boldsymbol{r}_3. \qquad (3)$$

Relationship between particle coordinates and $(\boldsymbol{\rho},\ \boldsymbol{\lambda})$:

$$\boldsymbol{r}_1 = -\frac{m_2}{m_{12}}\boldsymbol{\rho} - \frac{m_3}{m_{123}}\boldsymbol{\lambda} + \boldsymbol{R}, \qquad (4)$$

$$\boldsymbol{r}_2 = \frac{m_1}{m_{12}}\boldsymbol{\rho} - \frac{m_3}{m_{123}}\boldsymbol{\lambda} + \boldsymbol{R}, \qquad (5)$$

$$\boldsymbol{r}_3 = \frac{m_{12}}{m_{123}}\boldsymbol{\lambda} + \boldsymbol{R}, \qquad (6)$$

where $m_{12} = \frac{m_1+m_2}{m_1\ m_2}$ and $m_{123} = \frac{m_1+m_2+m_3}{m_1\ m_2\ m_3}$ are reduced masses.

Wave function of a three-particle system is taken in the Gaussian form:

$$\Psi(\boldsymbol{\rho},\ \boldsymbol{\lambda},\ A) = \sum_{i=1}^{K} C_i \psi_i(\boldsymbol{\rho},\ \boldsymbol{\lambda},\ A^i), \qquad (7)$$

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

The Schrödinger equation can be reduced to matrix form:

$$H \cdot C = E\mathcal{B} \cdot C. \qquad (8)$$

Matrix elements of the normalization coefficient matrix $\mathcal{B}$ and the Hamiltonian H:

$$\mathcal{B}_{ij} = \langle\psi_j(\boldsymbol{\rho},\ \boldsymbol{\lambda},\ A^j)|\psi_i(\boldsymbol{\rho},\ \boldsymbol{\lambda},\ A^i)\rangle, \quad (9)$$

$$H_{ij} = \langle\psi_j(\boldsymbol{\rho},\ \boldsymbol{\lambda},\ A^j)|\hat{H}|\psi_i(\boldsymbol{\rho},\ \boldsymbol{\lambda},\ A^i)\rangle. \quad (10)$$

When calculating matrix elements, the following notation is introduced:

$$B_{kn} = A^i_{kn} + A^j_{kn}. \quad (11)$$

The variational wave function of the system for muon excited states is chosen as follows:

$$\Psi_{lm}(\boldsymbol{\rho},\boldsymbol{\lambda},A) = \sum_{i=1}^{K} C_i Y_{lm}(\theta_\rho,\phi_\rho)\rho^l \times \quad (12)$$
$$\times e^{-\frac{1}{2}\{(A^i_{11}\boldsymbol{\rho}^2 + 2A^i_{12}\boldsymbol{\rho}\boldsymbol{\lambda} + A^i_{22}\boldsymbol{\lambda}^2)},$$

where $Y_{lm}(\theta_\rho,\ \phi_\rho)$ is a spherical wave function describing muon excited state.

Normalization of the wave function also can be calculated analytically:

$$\langle\Psi|\Psi\rangle = \sum_{i,j=1}^{K} C_i C_j 2^{l+2}\pi^{\frac{3}{2}}\Gamma\left(l+\frac{3}{2}\right)\frac{B_{22}^l}{(\det B)^{l+\frac{3}{2}}}. \quad (13)$$

where the determinant of the matrix B is equal:

$$\det B = B_{11}B_{22}B_{33} - B_{11}B_{23}^2 - \quad (14)$$
$$-B_{12}^2 B_{33} + 2B_{12}B_{13}B_{23} - B_{13}^2 B_{22}.$$

Hamiltonian of three-particle system in the non-relativistic approximation:

$$\hat{H}_0 = -\frac{1}{2\mu_1}\nabla^2_{\boldsymbol{\rho}} - \frac{1}{2\mu_2}\nabla^2_{\boldsymbol{\lambda}} + \frac{e_1e_2}{|\boldsymbol{\rho}|} + \quad (15)$$
$$+\frac{e_1e_3}{|\boldsymbol{\lambda}+\frac{m_2}{m_{12}}\boldsymbol{\rho}|} + \frac{e_2e_3}{|\boldsymbol{\lambda}-\frac{m_1}{m_{12}}\boldsymbol{\rho}|}.$$

The kinetic energy operator in the Jacobi coordinates can be transformed to the form:

$$\hat{T} = -\frac{1}{2\mu_1}\nabla_\rho^2 - \frac{1}{2\mu_2}\nabla_\lambda^2, \tag{16}$$

where $\mu_1 = \frac{m_1 m_2}{m_{12}}$ and $\mu_2 = \frac{m_{12} m_3}{m_{123}}$ are the reduced masses of particles (1,2) and (1,2,3) respectively.

The matrix elements of the Laplace operators are expressed in terms of non-linear variational parameters:

$$\langle\Psi|\nabla_{\boldsymbol{\lambda}}^2|\Psi\rangle = \sum_{i,j=1}^{K} \frac{C_i C_j 2^{l+2}\pi^{\frac{3}{2}}}{\langle\Psi|\Psi\rangle}\Gamma\left(l+\frac{3}{2}\right)\frac{B_{22}^{l-1}}{(\det B)^{l+\frac{5}{2}}}\times \tag{17}$$

$$\times\left[3A_{22}^i(A_{22}^i - B_{22})detB + (2l+3)(A_{22}^i B_{12} - A_{12}^i B_{22})^2\right],$$

$$\langle\Psi|\nabla_{\boldsymbol{\rho}}^2|\Psi\rangle = \sum_{i,j=1}^{K} \frac{C_i C_j 2^{l+1}\pi^{\frac{3}{2}}}{\langle\Psi|\Psi\rangle}\Gamma\left(l+\frac{1}{2}\right)\frac{B_{22}^{l-1}}{(\det B)^{l+\frac{5}{2}}}\times \tag{18}$$

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

The potential energy operator in the Jacobi coordinates consists of pair Coulomb interactions:

$$\hat{U} = \frac{e_1 e_2}{|\boldsymbol{\rho}|} + \frac{e_1 e_3}{|\boldsymbol{\lambda} + \frac{m_2}{m_{12}}\boldsymbol{\rho}|} + \frac{e_2 e_3}{|\boldsymbol{\lambda} - \frac{m_1}{m_{12}}\boldsymbol{\rho}|}. \tag{19}$$

Matrix elements of the potential energy of Coulomb interactions are determined by the expressions:

$$\langle\Psi|U_{12}|\Psi\rangle = -Z\sum_{i,j=1}^{K}\frac{C_i C_j 2^{l+\frac{3}{2}}\pi^{\frac{3}{2}}}{\langle\Psi|\Psi\rangle}\Gamma(l+1)\frac{B_{22}^{l-1}}{(\det B)^{l+1}}, \tag{20}$$

$$\langle\Psi|U_{13}|\Psi\rangle = -Z\sum_{i,j=1}^{K}\frac{C_i C_j 2^{l+\frac{5}{2}}\pi}{\langle\Psi|\Psi\rangle}\Gamma\left(l+\frac{3}{2}\right)\frac{B_{22}^{l+\frac{1}{2}}}{(\det B)^{l+\frac{3}{2}}}\,{}_2F_1\left(\frac{1}{2}, l+\frac{3}{2}, \frac{3}{2}, -\frac{(F_2^{23})^2}{\det B}\right), \tag{21}$$

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

where ${}_2F_1$ is the hypergeometric function. We introduce additional designations:

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

The energy values of $(^3_2He - \mu^- - e^-)$ atom

As the result of solution of variational task, we obtain the follows energy values:

1. First column represents a non-relativistic energy;
2. In the next columns we present some important corrections.

State	E_{nr}	$-\frac{\alpha^2}{8}\mathbf{p}_e^4$	ΔU_{vp}	ΔU_{cont}
(14,13)	-2.81111089	-0.00030330	-0.00000033	0.00000361
(14,12)	-2.84289819	-0.00031998	-0.00000035	0.00000380
(13,12)	-3.07090707	-0.00025213	-0.00000028	0.00000303
(13,11)	-3.10157048	-0.00027561	-0.00000030	0.00000324
(12,11)	-3.42617315	-0.00020518	-0.00000024	0.00000247
(12,10)	-3.45844905	-0.00019336	-0.00000023	0.00000233

Table 1: Energy levels of the high-angular-momentum muon states of muonic helium $(^3_2He - \mu^- - e^-)$ atom in electron atomic units (e.a.u.)

The expression for the vacuum polarization potential in e.a.u. (the δ-approximation for the Uehling-Serber potential) has the following form:

$$\Delta U_{vp} = \Delta U_{vp}(r_{13}) + \Delta U_{vp}(r_{23}) = -\frac{4}{15}\alpha^2(Z\alpha)\delta(\boldsymbol{\lambda} + \frac{m_2}{m_{12}}\boldsymbol{\rho}) + \frac{4}{15}\alpha^2(Z\alpha)\delta(\boldsymbol{\lambda} - \frac{m_1}{m_{12}}\boldsymbol{\rho}). \tag{24}$$

The matrix elements of such potentials are calculated analytically in closed form:

$$< \Psi|\Delta U_{vp}(r_{13})|\Psi >= -\frac{4}{15}\alpha^2(Z\alpha)\sum_{i,j=1}^{K}\frac{C_i C_j 2^{l+\frac{1}{2}}}{\langle\Psi|\Psi\rangle}\Gamma\left(l+\frac{3}{2}\right)\frac{1}{(F_1^{13})^{l+\frac{3}{2}}}, \tag{25}$$

$$< \Psi|\Delta U_{vp}(r_{23})|\Psi >= -\frac{4}{15}\alpha^2(Z\alpha)\sum_{i,j=1}^{K}\frac{C_i C_j 2^{l+\frac{1}{2}}}{\langle\Psi|\Psi\rangle}\Gamma\left(l+\frac{3}{2}\right)\frac{1}{(F_1^{23})^{l+\frac{3}{2}}}, \tag{26}$$

$$F_1^{13} = B_{11} + \frac{m_2^2}{m_{12}^2}B_{22} - 2\frac{m_2}{m_{12}}B_{12}, \quad F_1^{23} = B_{11} + \frac{m_1^2}{m_{12}^2}B_{22} + 2\frac{m_1}{m_{12}}B_{12}. \tag{27}$$

The contact interaction potential (e.a.u.):

$$\Delta U_{cont} = \frac{\pi Z \alpha^2}{2}\delta(\boldsymbol{\lambda} + \frac{m_2}{m_{12}}\boldsymbol{\rho}) - \frac{\pi\alpha^2}{2}\delta(\boldsymbol{\lambda} - \frac{m_1}{m_{12}}\boldsymbol{\rho}). \tag{28}$$

Relativistic corrections are defined by following expression in the Hamiltonian of the system:

$$\Delta U_{rel} = -\frac{\alpha^2}{8}\left(\frac{\mathbf{p}_1^4}{m_1^3} + \frac{\mathbf{p}_2^4}{m_2^3} + \frac{\mathbf{p}_3^4}{m_3^3}\right). \tag{29}$$

The main contribution to the relativistic correction in the energy spectrum (e.a.u.) is connected with the electron motion:

$$\langle\Psi| - \frac{\alpha^2}{8}\nabla_{\boldsymbol{\lambda}}^4|\Psi\rangle = -\alpha^2 \sum_{i,j=1}^{K} \frac{C_i C_j 2^{l-1}\pi^{\frac{3}{2}}}{\langle\Psi|\Psi\rangle}\Gamma\left(l+\frac{3}{2}\right)\frac{B_{22}^{l-2}}{(\det B)^{l+\frac{7}{2}}}\Big[15(A_{22}^i)^2(\det B)^2(A_{22}^i - B_{22})^2 + \tag{30}$$

$$10(2l+3)A_{22}^i(A_{22}^i - B_{22})\det B(A_{22}^i B_{12} - A_{12}^i B_{22})^2 + (2l+3)(2l+5)(A_{22}^i B_{12} - A_{12}^i B_{22})^4\Big].$$

State	E_{nr}	$-\frac{\alpha^2}{8}\mathbf{p}_e^4$	ΔU_{vp}	ΔU_{cont}
(14,13)	-2.82505929	-0.00030182	-0.00000033	0.00000361
(14,12)	-2.85670449	-0.00031536	-0.00000034	0.00000370
(13,12)	-3.08873955	-0.00019461	-0.00000023	0.00000245
(13,11)	-3.11916631	-0.00027631	-0.00000029	0.00000309
(12,11)	-3.44854579	-0.00019806	-0.00000024	0.00000242
(12,10)	-3.48181792	-0.00021110	-0.00000025	0.00000235

Table 2: Energy levels of the high-angular-momentum muon states of muonic helium $(^4_2He - \mu^- - e^-)$ atom in e.a.u.

To study the internal structure of three-particle bound states, we calculate the mean-square distances between particles. Corresponding matrix elements are calculated analytically:

$$\langle(\mathbf{r}_1-\mathbf{r}_2)^2\rangle=\sum_{i,j=1}^{K}\frac{C_iC_j}{\langle\Psi|\Psi\rangle}2^{(l+3)}\pi^{\frac{3}{2}}\Gamma(l+\frac{5}{2})\frac{B_{22}^{(l+1)}}{(\det B)^{(l+\frac{5}{2})}}, \tag{31}$$

$$\langle(\mathbf{r}_1-\mathbf{r}_3)^2\rangle=\sum_{i,j=1}^{K}\frac{C_iC_j}{\langle\Psi|\Psi\rangle}2^{(l+2)}\pi^{\frac{3}{2}}\Gamma(l+\frac{3}{2})\frac{B_{22}^{(l-1)}}{(\det B)^{(l+\frac{5}{2})}}\Big[(2l+3)\big(B_{12}-\frac{m_2}{m_{12}}B_{22}\big)^2+3\det B\Big], \tag{32}$$

$$\langle(\mathbf{r}_2-\mathbf{r}_3)^2\rangle=\sum_{i,j=1}^{K}\frac{C_iC_j}{\langle\Psi|\Psi\rangle}2^{(l+2)}\pi^{\frac{3}{2}}\Gamma(l+\frac{3}{2})\frac{B_{22}^{(l-1)}}{(\det B)^{(l+\frac{5}{2})}}\Big[(2l+3)\big(B_{12}+\frac{m_1}{m_{12}}B_{22}\big)^2+3\det B\Big], \tag{33}$$

$$\delta_{12}=\sqrt{\langle(\mathbf{r}_1-\mathbf{r}_2)^2\rangle}=1.34\ (0.71\times10^{-8}\ cm), \tag{34}$$

$$\delta_{13}=\sqrt{\langle(\mathbf{r}_1-\mathbf{r}_3)^2\rangle}=0.47\ (0.25\times10^{-8}\ cm), \tag{35}$$

$$\delta_{23}=\sqrt{\langle(\mathbf{r}_2-\mathbf{r}_3)^2\rangle}=1.08\ (0.57\times10^{-8}\ cm). \tag{36}$$

Some details of the internal structure of bound states can also be obtained by constructing the radial distribution densities for ρ and λ and calculating the root-mean-square values of $\langle\rho^2\rangle$ and $\langle\lambda^2\rangle$, which are determined by the expressions:

$$\langle\rho^2\rangle = \frac{\pi^{\frac{3}{2}}2^{l+3}\Gamma\left(l+\frac{5}{2}\right)}{\langle\Psi|\Psi\rangle}\sum_{i,j=1}^{K} C_iC_j\frac{B_{22}^{l+1}}{(\det B)^{l+5/2}}, \tag{37}$$

$$\langle\lambda^2\rangle = \frac{\pi^{\frac{3}{2}}2^{l+2}\Gamma\left(l+\frac{3}{2}\right)}{\langle\Psi|\Psi\rangle}\sum_{i,j=1}^{K} C_iC_j\frac{B_{22}^{l-1}}{(\det B)^{l+\frac{5}{2}}}(3B_{11}B_{22}+2B_{12}^2l), \tag{38}$$

$$W(\rho) = \frac{(2\pi)^{\frac{3}{2}}}{\langle\Psi|\Psi\rangle}\sum_{i,j=1}^{K}\frac{C_iC_j}{B_{22}^{3/2}}\rho^{(2l+2)}e^{-\frac{1}{2}\frac{\det B}{B_{22}}\rho^2}, \tag{39}$$

$$W(\lambda) = \frac{2^{l+\frac{5}{2}}\pi}{\langle\Psi|\Psi\rangle}\sum_{i,j=1}^{K}\frac{C_iC_j\Gamma\left(l+\frac{3}{2}\right)}{B_{11}^{l+\frac{3}{2}}}\lambda^2e^{-\frac{1}{2}B_{22}\lambda^2}{}_1F_1\left(l+\frac{3}{2},\frac{3}{2},\frac{B_{12}^2\lambda^2}{2B_{11}}\right), \tag{40}$$

$$W(\rho,\lambda) = \frac{4\pi}{\langle\Psi|\Psi\rangle}\sum_{i,j=1}^{K}\frac{C_iC_j}{B_{12}}\rho^{2l+1}\lambda e^{-\frac{1}{2}[B_{11}\rho^2+B_{22}\lambda^2]}sh(B_{12}\rho\lambda),\ B_{lk}=A_{lk}^i+A_{lk}^j. \tag{41}$$

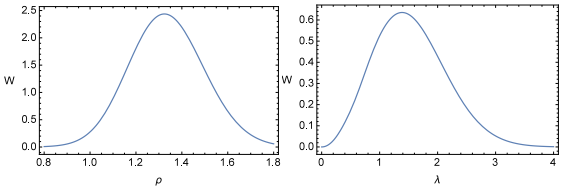


Fig. 2: Radial distribution densities $W(\rho)$, $W(\lambda)$ for the $(14, 13)$ state of $(^4_2He - \mu^- - e^-)$. The values of the variables ρ and λ are expressed in electron atomic units.

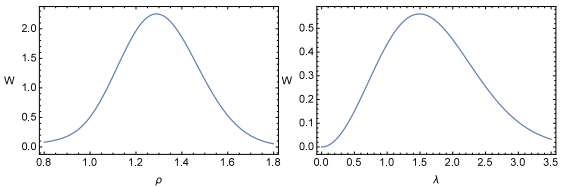


Fig. 3: Radial distribution densities $W(\rho)$, $W(\lambda)$ for the $(13, 12)$ state of $(^4_2He - \mu^- - e^-)$.

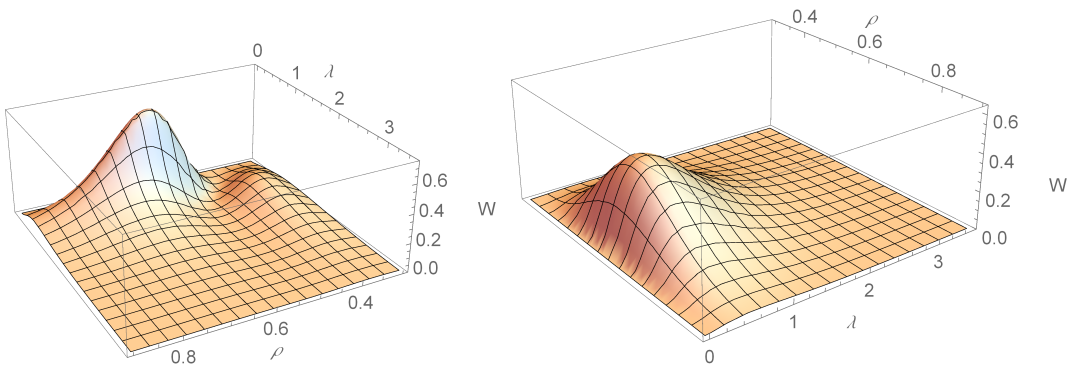


Fig. 4: Radial distribution density $W(\rho, \lambda)$ for the states (14,13) $({}^4_2He - \mu^- - e^-)$ (right) and (14,12) $({}^3_2He - \mu^- - e^-)$ (left). The values of the variables ρ and λ are expressed in electron atomic units.

Conclusions

We study the energy levels of muonic helium for states in which the muon has such a large orbital angular momentum that it is approximately at the same distance from the nucleus as the electron. Calculations are performed in leading order using the variational method with a Gaussian basis, and several key corrections determined by the Breit Hamiltonian (relativism, vacuum polarizations and contact interactions) are calculated in first-order perturbation theory. When calculating the energy of a specific state, we perform an initial run of the program 10 times with a minimum basis of K=200 functions, varying the interval boundaries to generate nonlinear variational parameters. Having chosen these boundaries so that the minimum energy is achieved at this stage, we run several calculation programs with the same parameters, increasing the basis in the expansion to approximately K=800 functions. At each step of the program, the basis is incremented by one, and refinement cycles are performed. The number of such cycles (usually 1000) is specified in the input file at the beginning of the program. Previous studies using a basis of Gaussian wave functions show that it yields results consistent with previous results obtained using other approaches. The results obtained for muonic helium can be used in the analysis of new experimental data.