

# Calculation of binding energy for nonsymmetric muonic helium hydride ions in the hyperspherical approach

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Symmetric and nonsymmetric muonic three-body systems have been predicted to form in collisions between muonic atoms and hydrogen molecules. The hyperspherical adiabatic expansion is a representation for the investigation of muonic three-body bound states. In this research we have used hyperspherical “surface” functions for muonic helium hydride ions (isotopes of helium-tritium-muon molecules). Through this approach, the binding energy and lowest eigenpotentials for the muonic molecular ions are calculated in an extreme adiabatic approximation. The obtained results are close to the calculations of others.

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## I. INTRODUCTION

In connection with muon-catalyzed fusion, energy levels of muonic molecules have extensively been studied with various calculational methods [1–3]. The hyper spherical harmonics formalism is a powerful approach for bound-state calculations of three-body systems [4–6]. In this work we mainly consider muonic helium hydride ions like  $t\mu$   $^3\text{He}$  and  $t\mu$   $^4\text{He}$ , (helium-tritium-muon nonsymmetric molecules). There are strong indications that these muonic molecules can form molecular three-body resonances. One of these indications is that  $t\mu\text{He}$  resonances were seen in collisions of  $t\mu$  atom with  $^3\text{He}$  and  $^4\text{He}$  [7–9]. Also, in the muon-catalyzed fusion process, helium impurities gradually accumulate in D-T targets. The muon loss process due to muon transfer from muonic hydrogen atoms through the intermediate  $t\mu$   $^3\text{He}$  and  $t\mu$   $^4\text{He}$  muonic molecules to the accumulated helium nuclei is an important factor in understanding actual  $\mu\text{CF}$  process and stripping probability in DT mixtures [10,11]. The role of the formation of a muonic molecule in a charge-exchange reaction was confirmed in a number of experiments [12]. In the  $t\mu\text{He}$  system, a Coulomb interaction is not able to bind the systems under consideration due to the repulsion in the  $\mu\text{He}+t$  channel. Only a three-body resonant state can be formed. States like that are supported by the attractive polarization potential in the  $t\mu+\text{He}$  channel and therefore are clustered.

Our goal in this research is to study systematical calculations of energy levels for  $t\mu$   $^3\text{He}$  and  $t\mu$   $^4\text{He}$  systems in hyperspherical coordinates. In order to do this, the Hamiltonian of the system, interacting only via the Coulomb force, in Jacobi coordinates  $(r, R)$  as shown in Fig. 1, and the nonrelativistic Schrödinger equation for the three particles is written. In practice, for the numerical calculation of this infinite set of coupled equations, they are truncated to a finite set.

The approach, using the hyperspherical “surface” function method [13], has been applied in this paper. The hyperspherical method allows one to separate the hyperradial motion from the angular part. Physical boundary conditions for their solution can be easily formulated. Moreover, coupling of channels turns out to be rather small in our case and allows one to use the decoupled one-level approximation.

The formulation of the problem in hypercoordinates and adiabatic expansion is given in Secs. II and III. In Sec. IV, the behavior of effective potential and surface functions for different hyperradii  $R$  is discussed. Finally, in Sec. V, the numerical results are given, leading to a discussion and conclusions.

## II. THEORETICAL DESCRIPTION OF MUONIC MOLECULES

In this section we explain the treatment of the nonsymmetric three-body Coulomb problem. Since we have two heavy particles and one light particle (helium, tritium, and muon), it seems that the Born-Oppenheimer approach will be reasonable to explain this system. But within the framework

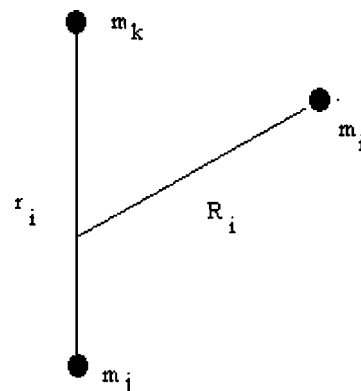


FIG. 1. Jacobi coordinates  $(R_i, r_i)$ ;  $m_i$ ,  $m_j$ , and  $m_k$  are the mass of particles in muonic molecules.

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of the Born-Oppenheimer approach, it is very difficult to treat the contribution from the continuum spectra of the two-center problem correctly. Thus, to avoid these difficulties we have used another adiabatic formulation: namely, the hyperspherical adiabatic approach [14]. This method is based on an expansion of the three-body wave function into the so-called surface functions.

The motion of three particles in their center-of-mass system can be described as Jacobi coordinates  $(\vec{r}, \vec{R})$ , as shown in Fig. 1. In this variable the Hamilton operator of the three-body Coulomb system is given by

$$H = T + V_c. \quad (1)$$

The kinetic-energy operator  $T$  and the sum of the three two-body Coulomb interactions,  $V_c$ , are given by

$$T = -\frac{1}{2m}\Delta_{\vec{r}} - \frac{1}{2M}\Delta_{\vec{R}}, \quad (2)$$

$$V_c = -\frac{Ze^2}{r} - \frac{e^2}{|\vec{R} - \beta\vec{r}|} + \frac{e^2}{|\vec{R} - \gamma\vec{r}|}, \quad (3)$$

where

$$m^{-1} = m_{\mu}^{-1} + m_z^{-1}, \quad M^{-1} = m_t^{-1} + (m_{\mu} + m_z)^{-1},$$

$$\beta = \frac{m_z}{m_{\mu} + m_z}, \quad \gamma = 1 - \beta, \quad (4)$$

and  $m_{\mu}$ ,  $m_t$ ,  $m_z$ , and  $Z$  denote the masses of the muon, tritium, helium isotopes, and the charge of the particle, respectively.

Introducing dimensionless variables according to

$$\vec{x} = \frac{\vec{r}}{a}, \quad \vec{y} = \frac{\vec{R}}{\alpha a}, \quad (5)$$

with  $\alpha = \sqrt{m/M}$  and  $a$  being the Bohr radius of the  $(Z\mu)$  subsystem,  $a = (Zme^2)^{-1}$ .

Then the kinetic-energy operator  $T$  and the sum of the three two-body Coulomb interactions,  $V_c$ , are changed,

$$T = - (2ma^2)^{-1} [\Delta_{\vec{x}} + \Delta_{\vec{y}}] \quad (6)$$

and

$$V_c = - (2ma^2)^{-1} \left[ \frac{2}{x} + \frac{2}{Z|\alpha\vec{y} - \beta\vec{x}|} - \frac{2}{Z|\alpha\vec{y} + \gamma\vec{x}|} \right]. \quad (7)$$

Taking  $(2ma^2)^{-1}$  as our energy unit, the Hamiltonian can be read

$$H = -\Delta_{\vec{x}} - \Delta_{\vec{y}} - \frac{2}{x} - \frac{2}{Z|\alpha\vec{y} - \beta\vec{x}|} + \frac{2}{Z|\alpha\vec{y} + \gamma\vec{x}|}, \quad (8)$$

by defining the hyperradius  $\rho$  and the hyperangle  $\omega$  instead of the variables  $x$  and  $y$ , via

$$\vec{x} = \rho \cos \omega, \quad \vec{y} = \rho \sin \omega,$$

$$\hat{x} = \frac{\vec{x}}{|\vec{x}|}, \quad \hat{y} = \frac{\vec{y}}{|\vec{y}|}, \quad (9)$$

the nontations being  $\hat{x}$  and  $\hat{y}$  used for  $\hat{x} \equiv (\theta_x, \varphi_x)$  and for  $\hat{y} \equiv (\theta_y, \varphi_y)$ , respectively, with  $0 \leq \rho < \infty$  and  $0 \leq \omega \leq \pi/2$ . In the hyperspherical coordinates  $(\rho, \Omega) \equiv (\rho, \omega, \hat{x}, \hat{y})$ , the Hamiltonian can be written as

$$H = -\rho^{-5/2} \frac{\partial^2}{\partial \rho^2} \rho^{5/2} + \frac{\Lambda^2(\Omega)}{\rho^2} + \frac{\vartheta(\Omega)}{\rho}, \quad (10)$$

where the grand angular momentum operator  $\Lambda(\Omega)$  is given by

$$\Lambda^2(\Omega) = -\frac{1}{\cos \omega \sin \omega} \frac{\partial^2}{\partial \omega^2} \cos \omega \sin \omega + \frac{\vec{L}_{\hat{x}}^2}{\cos^2 \omega} + \frac{\vec{L}_{\hat{y}}^2}{\sin^2 \omega} - \frac{1}{4}, \quad (11)$$

where  $\vec{L}_{\hat{x}}$  and  $\vec{L}_{\hat{y}}$  are the orbital angular momentum operators corresponding to the variables  $\hat{x} = \vec{x}/|\vec{x}|$  and  $\hat{y} = \vec{y}/|\vec{y}|$ , respectively, as

$$\vec{L}_{\hat{x}} = \vec{x} \times \frac{1}{i} \vec{\nabla}_x, \quad \vec{L}_{\hat{y}} = \vec{y} \times \frac{1}{i} \vec{\nabla}_y. \quad (12)$$

The angular part of the three-body Coulomb potential reads

$$\vartheta(\Omega) = -2 \left[ \frac{1}{\cos \omega} + \frac{1}{Z|\alpha\hat{y} \sin \omega - \beta\hat{x} \cos \omega|} - \frac{1}{Z|\alpha\hat{y} \sin \omega + \gamma\hat{x} \cos \omega|} \right]. \quad (13)$$

The five angles symbolized by  $\Omega = (\omega, \hat{x}, \hat{y})$  together with hyperradius  $\rho = \sqrt{x^2 + y^2}$  (a measure for the size of the three-body system) provide a complete set of variables to describe the positions of all three particles.

### III. HYPERSPHERICAL ADIABATIC EXPANSION

The six-dimensional Schrödinger equation in hyperspherical coordinates is

$$\left[ -\rho^{-5/2} \frac{\partial^2}{\partial \rho^2} \rho^{5/2} + \frac{\Lambda^2(\Omega)}{\rho^2} + \frac{\vartheta(\Omega)}{\rho} \right] \Psi(\rho, \Omega) = E \Psi(\rho, \Omega). \quad (14)$$

We are using surface functions as a basis for the solutions  $\Psi(\rho, \Omega)$  of Eq. (14). Then, we consider first the Hamiltonian (10) for fixed values of the hyperradius,

$$H_{\rho}(\Omega) = \frac{\Lambda^2(\Omega)}{\rho^2} + \frac{\vartheta(\Omega)}{\rho}. \quad (15)$$

The corresponding eigenvalue equation

$$H_{\rho}(\Omega) \Phi_n(\rho, \Omega) = U_n(\rho) \Phi_n(\rho, \Omega) \quad (16)$$

is a differential equation containing only the angular part of the Hamiltonian. Therefore, the eigenvalues  $U_n(\rho)$ , referred

to as eigenpotentials, and its eigenfunctions  $\Phi_n(\rho, \Omega)$  are the so-called surface functions. Since the surface functions form a complete set on the sphere of constant values of the hyper-radius, the three-body wave function  $\Psi(\rho, \Omega)$  is expanded in the complete orthogonal set of  $\Phi_n(\rho, \Omega)$  as follows:

$$\Psi(\rho, \Omega) = \rho^{-5/2} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega). \quad (17)$$

Substituting Eq. (17) into Eq. (14) we have

$$\begin{aligned} & \left[ -\rho^{-5/2} \frac{\partial^2}{\partial \rho^2} \rho^{5/2} + H_\rho(\Omega) \right] \left( \frac{1}{\rho^{5/2}} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega) \right) \\ &= \frac{E}{\rho^{5/2}} \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega) \end{aligned} \quad (18)$$

and

$$\begin{aligned} & -\rho^{-5/2} \frac{\partial^2}{\partial \rho^2} \left( \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega) \right) + \rho^{-5/2} \sum_{n=1}^{\infty} f_n(\rho) H_\rho \Phi_n(\rho, \Omega) \\ &= \rho^{-5/2} E \sum_{n=1}^{\infty} f_n(\rho) \Phi_n(\rho, \Omega). \end{aligned} \quad (19)$$

Then,

$$\begin{aligned} & -\sum_{n=1}^{\infty} \left[ \Phi_n(\rho, \Omega) \frac{\partial^2}{\partial \rho^2} f_n(\rho) + f_n(\rho) \frac{\partial^2}{\partial \rho^2} \Phi_n(\rho, \Omega) \right. \\ & \quad \left. + 2 \frac{\partial}{\partial \rho} f_n(\rho) \frac{\partial}{\partial \rho} \Phi_n(\rho, \Omega) \right] + \sum_{n=1}^{\infty} U_n(\rho) f_n(\rho) \Phi_n(\rho, \Omega) \\ &= \sum_{n=1}^{\infty} E f_n(\rho) \Phi_n(\rho, \Omega), \end{aligned} \quad (20)$$

and by multiplying Eq. (20) in  $\Phi_m^*(\rho, \Omega)$  and integrating over  $\Omega$  we have

$$\begin{aligned} & -\sum_{n=1}^{\infty} \frac{\partial^2}{\partial \rho^2} f_n(\rho) \int \Phi_n(\rho, \Omega) \Phi_m^*(\rho, \Omega) d\Omega \\ & -\sum_{n=1}^{\infty} f_n(\rho) \int \Phi_m^*(\rho, \Omega) \frac{\partial^2}{\partial \rho^2} \Phi_n(\rho, \Omega) d\Omega \\ & -2 \sum_{n=1}^{\infty} \frac{\partial}{\partial \rho} f_n(\rho) \int \Phi_m^*(\rho, \Omega) \frac{\partial}{\partial \rho} \Phi_n(\rho, \Omega) d\Omega \\ & + \sum_{n=1}^{\infty} U_n(\rho) f_n(\rho) \int \Phi_n(\rho, \Omega) \Phi_m^*(\rho, \Omega) d\Omega \\ &= -\sum_{n=1}^{\infty} f_n(\rho) \int \Phi_n(\rho, \Omega) \Phi_m^*(\rho, \Omega) d\Omega. \end{aligned} \quad (21)$$

Then we have a system of coupled differential equations as

$$\left[ -\frac{\partial^2}{\partial \rho^2} + U_n(\rho) - E \right] f_n(\rho) = \sum_{m=1}^{\infty} \left[ Q_{nm} + 2P_{nm} \frac{\partial}{\partial \rho} \right] f_m(\rho). \quad (22)$$

The coupling matrix elements are given by

$$Q_{nm}(\rho) = \int d\Omega \Phi_n^*(\rho, \Omega) \frac{\partial^2}{\partial \rho^2} \Phi_m(\rho, \Omega) \quad (23)$$

and

$$P_{nm}(\rho) = \int d\Omega \Phi_n^*(\rho, \Omega) \frac{\partial}{\partial \rho} \Phi_m(\rho, \Omega). \quad (24)$$

From the normalization condition of the wave function  $\langle \Psi | \Psi \rangle$ , we have

$$\langle \Phi_n(\rho, \Omega) | \Phi_m(\rho, \Omega) \rangle = \int d\Omega \Phi_n^* \Phi_m(\rho, \Omega) = \delta_{nm} \quad (25)$$

and the bound-state solution of Eq. (14) is reduced to

$$\sum_{m=1}^{\infty} \int_0^{\infty} d\rho |f_m(\rho)|^2 = 1. \quad (26)$$

Up to this point we have introduced no approximations. In a practical numerical integration, Eq. (22), the infinite set of coupled equations must be truncated to a finite set. Instead of solving the coupled system of differential equation (22), we have only treated the so-called extreme adiabatic approximation (EAA), which is given by ignoring the derivatives of the surface functions with respect to the hyperradius. For this mean, each of the eigenfunctions  $\Phi_n(\rho, \Omega)$  can be expand for any given value of  $\rho$  in the complete set of hyperspherical harmonics  $P_{k\alpha}(\Omega)$ :

$$\Phi_n(\rho, \Omega) = \sum_{k\alpha} \chi_{k\alpha, n}(\rho) P_{k\alpha}(\Omega). \quad (27)$$

The  $\chi_{k\alpha}$  are real numbers which for a given  $n$  constitute the coordinates of a vector  $\Phi_n(\rho, \Omega)$  in the Hilbert space and fulfill the orthonormalization conditions

$$\sum_{k\alpha} \chi_{k\alpha, n}(\rho) \chi_{k\alpha, n'}(\rho) = \delta_{n, n'}. \quad (28)$$

For the coupling matrix elements  $Q_{nm}(\rho)$  and  $P_{nm}(\rho)$  we have

$$Q_{nm}(\rho) = \int d\Omega P_{k\alpha}(\Omega) P_{k\alpha}^*(\Omega) \sum_{k\alpha} \chi_{k\alpha, n}(\rho) \frac{\partial^2}{\partial \rho^2} \chi_{k\alpha, m}(\rho) \quad (29)$$

by considering

$$\int d\Omega P_{k\alpha}(\Omega) P_{k\alpha}^*(\Omega) = 1. \quad (30)$$

Then,

$$\Phi_{nm}(\rho) = \sum_{k\alpha} \chi_{k\alpha,n}(\rho) \frac{\partial^2}{\partial \rho^2} \chi_{k\alpha,m}(\rho) \quad (31)$$

and also

$$P_{nm}(\rho) = \sum_{k\alpha} \chi_{k\alpha,n}(\rho) \frac{\partial}{\partial \rho} \chi_{k\alpha,m}(\rho). \quad (32)$$

Differentiating Eq. (28) with respect to  $\rho$  once, one obtains

$$\sum_{k\alpha} \left[ \chi_{k\alpha,n}(\rho) \frac{\partial}{\partial \rho} \chi_{k\alpha,m}(\rho) + \chi_{k\alpha,m}(\rho) \frac{\partial}{\partial \rho} \chi_{k\alpha,n}(\rho) \right] = 0. \quad (33)$$

Differentiating once again for  $n=m$  leads to

$$\sum_{k\alpha} \chi_{k\alpha,n}(\rho) \frac{\partial^2}{\partial \rho^2} \chi_{k\alpha,n}(\rho) = - \sum_{k\alpha} \left| \chi_{k\alpha,n}(\rho) \frac{\partial}{\partial \rho} \chi_{k\alpha,m}(\rho) \right|^2. \quad (34)$$

Substituting Eqs. (33) and (34) into Eq. (22), then Eq. (22) is simplified to [15]

$$\frac{\partial^2}{\partial \rho^2} f_n(\rho) = [U_n(\rho) + \langle \Phi'_n | \Phi'_n \rangle - E] f_n(\rho). \quad (35)$$

Neglecting the derivatives of the surface functions with respect to the hyperradius (called the EAA), we shall have

$$\frac{\partial^2}{\partial \rho^2} f_n(\rho) = [U_n(\rho) - E] f_n(\rho). \quad (36)$$

For the calculation of the binding energies, we restrict ourselves to the EAA, and the lower bound for the exact energies are determined [16].

#### IV. BEHAVIOR OF THE EFFECTIVE POTENTIAL AND SURFACE FUNCTIONS FOR DIFFERENT HYPERRADII

The main task is the determination of eigenpotentials from Eq. (16). As can be seen from Eq. (16), for small hyperradii, the grand angular momentum term  $\Lambda^2/\rho^2$  dominates over the Coulomb potential  $\vartheta/\rho$ . Hence, Eq. (16) is reduced to

$$[\Lambda^2(\Omega) - \rho^2 U_n(\rho, \Omega)] \Phi_n(\rho, \Omega) = 0, \quad \text{for } \rho \rightarrow 0. \quad (37)$$

Comparing this relation with the eigenvalue equation of the grand angular momentum operator

$$[\Lambda^2 - \ell(\ell+1)] Y_\ell(\Omega) = 0, \quad (38)$$

we obtain

$$U_n \rightarrow \frac{\ell(\ell+1)}{\rho^2}, \quad \Phi_n(\rho, \Omega) \rightarrow Y_\ell, \quad \text{for } \rho \rightarrow 0. \quad (39)$$

Therefore, the surface functions in this region should be proportional to eigenfunctions of  $\Lambda^2$ , which are the well-known hyperspherical harmonics  $Y_\ell(\Omega)$ ,

$$Y_\ell(\Omega) = N_\ell \cos^{l_x} \omega \sin^{l_y} \omega P_k^{(l_x+1/2, l_y+1/2)}(\cos 2\omega) \mathbf{Y}_{l_x, l_y}^{L, M}(\hat{x}, \hat{y}), \quad (40)$$

where  $P_k^{(i,j)}(x)$  is a Jacobi polynomial,

$$P_k^{i,j}(x) = \frac{(x-1)^{-i}(x+1)^{-j}}{2^k k!} \frac{d^k}{dx^k} [(x-1)^{k+i}(x+1)^{k+j}], \quad (41)$$

and  $\mathbf{Y}_{l_x, l_y}^{L, M}(\hat{x}, \hat{y})$  is an eigenfunction of the squared total momentum operator  $\vec{L}^2$ , the so-called bispherical harmonic,

$$\mathbf{Y}_{l_x, l_y}^{L, M}(\hat{x}, \hat{y}) = \sum_{m_x, m_y} \langle l_x, m_x, l_y, m_y | LM \rangle Y_{l_x, m_x}(\hat{x}) Y_{l_y, m_y}(\hat{y}), \quad (42)$$

with the Clebsch-Gordan coefficients  $\langle l_x, m_x, l_y, m_y | LM \rangle$  and the usual spherical harmonic  $Y_{lm}(\hat{x})$ . The normalization constant  $N_\ell$  is

$$N_\ell = \sqrt{\frac{2k!(l_x + l_y + 2k + 2)\Gamma(l_x + l_y + k + 2)}{\Gamma\left(l_x + k + \frac{3}{2}\right)\Gamma\left(l_y + k + \frac{3}{2}\right)}}. \quad (43)$$

The index  $[l]$  of the hyperspherical harmonic collectively denotes the set of quantum numbers  $[l] = \{k, l_x, l_y, L, M\}$ . The eigenvalue in Eq. (38) is given by  $l = l_x + l_y + 2k + \frac{3}{2}$ . In case of degeneracy, instead of a single  $Y_l(\Omega)$  in Eq. (39), we have a linear combination of hyperspherical harmonics for this value of  $l$ .

At large hyperradii and at negative energies, the muon is bound by one of the positive charges. The surface function goes over to channel functions—i.e., to products of muonic two-body states and a free wave function describing the motion of responding two-body binding energies  $\varepsilon_m$ . That is,

$$U_n(\rho) \rightarrow \varepsilon_m, \quad \text{for } \rho \rightarrow \infty, \quad (44)$$

and

$$\begin{aligned} \Phi_n(\rho, \Omega) &\rightarrow \Theta_{[m_i]}(\rho, \Omega) \\ &= \rho^{3/2} R_{n, l_x}(\rho \cos \omega) \sin^{l_y} \omega \mathbf{Y}_{l_x, l_y}^{L, M}(\hat{x}, \hat{y}), \quad \text{for } \rho \rightarrow \infty. \end{aligned} \quad (45)$$

Here,  $R_{n, l_x}(\rho \cos \omega)$ ,  $m$ , and  $l_x$  represent the hydrogenlike wave function and quantum and angular quantum numbers, respectively. The index  $i$  specifies by which of the two nuclei the muon is bound. To represent the surface functions in the whole space of  $\rho$  we use the ansatz

$$\Phi_n(\rho, \Omega) = \sum_{i=1}^2 \sum_m a_{n[m_i]}(\rho) \Theta_{[m_i]}(\rho, \Omega) + \sum_{[l]} b_{n[l]}(\rho) Y_{[l]}(\Omega), \quad (46)$$

which [inserted into Eq. (16)] yields a generalized eigenvalue problem for the determination of the coefficients  $a_{n[m_i]}$  and  $b_{n[l]}$  and eigenpotentials  $U_n(\rho)$ . In this framework we treated the systems  ${}^3\text{Het}\mu$  and  ${}^4\text{Het}\mu$  in the states with the total angular momentum  $L=0$ . In calculations, we use 120

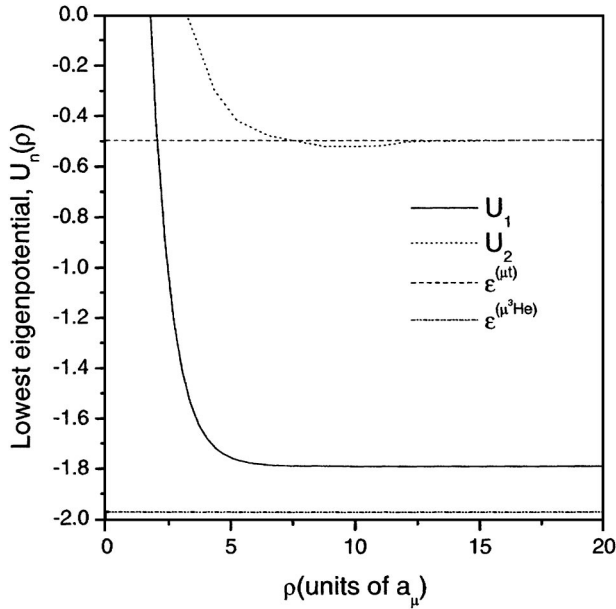


FIG. 2. The lowest eigenpotentials  $U_1(\rho)$  and  $U_2(\rho)$  of the  $t\mu^3\text{He}$  system. For  $L=0$  they converge towards the ground-state energies  $\varepsilon^{(\mu^3\text{He})}$  and  $\varepsilon^{(\mu t)}$ , respectively.

hyperspherical functions [Eq. (40)] and take 10 channel functions (46) for muonic molecules.

## V. DISCUSSION AND CONCLUSION

In this research we employed the method of hyperspherical surface functions to calculate the nonsymmetric three-body Coulomb problem. The hyperspherical method allows one to separate hyperradial motion from the angular part. The eigenpotentials and eigenfunctions are calculated for isotopes of helium and tritium from the angular equation—in

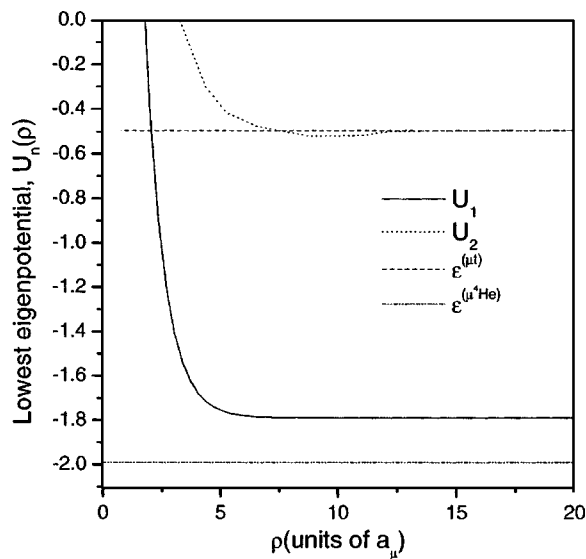


FIG. 3. The lowest eigenpotentials  $U_1(\rho)$  and  $U_2(\rho)$  of the  $t\mu^4\text{He}$  system. For  $L=0$  they converge towards the ground-state energies  $\varepsilon^{(\mu^4\text{He})}$  and  $\varepsilon^{(\mu t)}$ , respectively.

TABLE I. Binding energies (eV) of  $t\mu^3\text{He}$  for  $L=0$ .

| System            | State | Ref. [17] | Present |
|-------------------|-------|-----------|---------|
| $t\mu^3\text{He}$ | (0,0) | -72.296   | -72.59  |
|                   | (0,1) | -53.330   | -53.54  |
|                   | (0,2) | -19.379   | -19.48  |

particular, the eigenpotentials which play the role of effective potentials in the radial equation. The characteristic features of the respective problem—e.g., the occurrence of bound states and resonances as well as polarizability effects—can be inferred immediately from these potential curves. A further advantage is that, by solving the radial equation, the lower bound is obtained for the binding energy of muonic molecules. The corresponding eigenpotentials of the  $t\mu^3\text{He}$  and  $t\mu^4\text{He}$  systems for  $L=0$  are shown in Figs. 2 and 3. The improved potential curves ( $L=0$ ) dissociating to  $\mu^3\text{He}+t$  [ $U_1(\rho)$ ] and  $t\mu+^3\text{He}$  [ $U_2(\rho)$ ] for  $t\mu^3\text{He}$  are shown in Fig. 2. Also the improved potential curve ( $L=0$ ) for  $t\mu^4\text{He}$  is shown in Fig. 3. The lowest potential is purely repulsive, as expected in view of the Coulomb repulsion between the tritium and  $\mu\text{He}$  subsystems. The attractive character of the second eigenpotential is a consequence of the polarization of the  $t\mu$  atom in the Coulomb field of the He nucleus. With the calculated eigenpotential, by using 120 hyperspherical functions [Eq. (40)], the nonrelativistic energy  $\varepsilon_{J\nu}$ (eV) of the rotational-vibrational states ( $J, \nu$ ) of muonic helium hydride ( $t\mu^3\text{He}$  and  $t\mu^4\text{He}$ ) appearing below the  $t\mu(1s)$  threshold are calculated as  $\varepsilon_{00}=-72.59$ ,  $\varepsilon_{01}=-53.54$ ,  $\varepsilon_{02}=-19.48$  and  $\varepsilon_{00}=-81.67$ ,  $\varepsilon_{01}=-64.28$ ,  $\varepsilon_{02}=-32.29$  respectively. The values of  $\varepsilon_{J\nu}$  are in agreement with those in Ref. [17]. The calculated bound-state energies are listed in Tables I and II. The method of this research gives the lower bound of the eigenenergy if derivatives of the surface functions with respect to the hyperradius (the coupling of channels) is neglected. One can conclude that this fact supports the validity of the one-level approximation in our approach. The calculated errors are reduced by considering the coupling of channels and increasing the number of hyperspherical functions. The results show that this approach is very appropriate for studying muonic molecule systems.

It is obvious that this paper treats only three-body systems without electrons. To extend the discussion to systems of one or two electrons the Born-Oppenheimer approximation is good. We know that the lower channel, asymptotically ( $\mu\text{He}+t$ ) should be bound by either one or two electrons, since the hydrogen molecule ion and the hydrogen molecule are bound by energies in the eV range. Of course, both en-

TABLE II. Binding energies (eV) of  $t\mu^4\text{He}$  for  $L=0$ .

| System            | State | Ref. [17] | Present |
|-------------------|-------|-----------|---------|
| $t\mu^4\text{He}$ | (0,0) | -81.335   | -81.67  |
|                   | (0,1) | -63.958   | -64.28  |
|                   | (0,2) | -32.063   | -32.29  |

ergy and distance scales of the electron-free system will differ from that of the systems with electrons by the ratio of muon and electron masses. We should mention that  $t\mu\text{He}$  makes a strong screening on the formed  $[(t\mu\text{He})e]$  and the large distance of atomic electron will have ignorable effect on the  $t\mu\text{He}$  nucleus. This means that the atomic electron in formed systems does not have an important role in fusion of  $[(t\mu\text{He})e]$ , and four- or five-body resonant states in the men-

tioned screened low-energy region do not have practical importance in muon-catalyzed fusion.

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