# Resonances in muonic systems

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A number of resonances, shape as well as Feshbach type, have been observed in atomic systems. It is expected that similar types of resonances exist in muonic systems. Froelich and Szalewicz [Phys. Lett. A **129**, 321 (1988)] carried out a calculation for $td\mu$ and obtained two resonances, for $J=0$ and 1, just above the $d\mu$ threshold. Our calculation, carried out with large basis sets and different sets of nonlinear parameters, using the complex-rotation method, shows the existence of Feshbach-type resonances below the $n=2$ threshold of $t\mu$ and $d\mu$. Positions of these resonances are in good agreement with the results of Hara and Ishihara [Phys. Rev. A **40**, 4232 (1989)]. The widths of these resonances are calculated.

A number of bound states of muonic systems, $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $tt\mu$, and $td\mu$, have been calculated during the past few years.[1–4] These states are important in the catalysis of nuclear reactions in the presence of a negative muon.[5] The most important of these systems is $td\mu$, in which an energy release of 17.6 MeV takes place in each reaction until $\mu$ gets attached to the $\alpha$ particle, after catalyzing an average of 150 reactions. This attachment, called sticking, could be very small if fusion takes place from a resonance state, which is formed due to the three-body Coulomb interactions between the particles. The resonances could also enhance the formation rates. A number of resonances, shape as well as Feshbach type, have been observed in atomic systems and extensive calculations have been carried out for various systems.[6] It is expected that similar resonances exist in muonic systems. Froelich and Szalewicz[7] carried out a calculation of $td\mu$ by the stabilization method.[8] They observed a stable root for $J=0$, as well as for $J=1$. They calculated the widths of the states by analytic continuation of two nearly crossing levels as a function of the complex parameter. They found resonance parameters, position above $t\mu$ and width, 54.35 and 0.74 eV for $J=0$, and 54.63 and 2.04 eV for $J=1$. We carried out a calculation using Hylleraas-type wave functions, and we find stabilized roots for $J=0$ and 1. We look for roots below the $n=2$ thresholds of $t\mu$ and $d\mu$ by extending our calculation to calculate the complex eigenvalue $E_r - i\Gamma/2$ by the complex-rotation method.[8]

It is well known that $2s$ and $2p$ degeneracy produces an attractive dipole potential,[9–11] which behaves asymptotically as $-\alpha/r^2$ and can support an infinite number of resonances. If the relativistic corrections, e.g., the Lamb shift, are taken into account, the degeneracy is broken and the number of resonances is finite. We do find stabilized roots for $J=0$ and 1 just below the $n=2$ threshold of $t\mu$ and $d\mu$. These roots continue to exist in the calculation carried out using the complex-rotation method and therefore these resonances can be predicted with confidence. These are Feshbach-type or closed-channel resonances and have been obtained in $e^+$-H and $e^-$-H systems in a number of theoretical calculations using different techniques.[6]

A Hylleraas type of wave function used by Hu[2,3] in the calculation of binding energies of the $td\mu$ system has been used in these calculations. The wave function for $J=0$ is

$$\Psi = f_1 , \tag{1}$$

where

$$f_1 = \sum_{l,m,n} C_{lmn} P_{lmn}(a_1,a_2,a_3;b_1,b_2,b_3) + \sum_{\substack{l,m,n \\ m\neq n}} D_{lmn} Q_{lmn}(e_1,e_2,e_3;g_1,g_2,g_3) ,$$

$$P_{lmn}(a_1,a_2,a_3;b_1,b_2,b_3) = r_{12}^l (r_{13}^m r_{23}^n + r_{13}^n r_{23}^m)[\exp(-a_1 r_{12} - a_2 r_{13} - a_3 r_{23}) + \exp(-b_1 r_{12} - b_2 r_{13} - b_3 r_{23})] ,$$

and

$$Q_{lmn}(e_1,e_2,e_3;g_1,g_2,g_3) = r_{12}^l (r_{13}^m r_{23}^n - r_{13}^n r_{23}^m)[\exp(-e_1 r_{12} - e_2 r_{13} - e_3 r_{23}) + \exp(-g_1 r_{12} - g_2 r_{13} - g_3 r_{23})] .$$

The indices $i=1,2,3$ refer to triton, deuteron, and muon, respectively, and $r_{ij}$ are interparticle distances. The $a$'s, $b$'s, $e$'s, and $g$'s are the nonlinear parameters and the $a$'s and $b$'s are subjected to cusp constraints described by Hu.[12]

The wave function for $J=1$ is

$$\Psi = f_1 \mathbf{r}_{12} + f_2 \mathbf{r} , \tag{2}$$

 

TABLE I. Nonlinear parameters[a] used in $J=0$ states. The units are the inverse muon Bohr radius.

| | $a_1=b_1$ | $b_2$ | $b_3$ | $e_1=g_1$ | $e_2$ |
|---|---|---|---|---|---|
| Set[a] I | 0.301 | 0.7265 | 1.183 | 0.757 | 0.491 |
| Set II | 0.43 | 0.7265 | 1.183 | 0.457 | 0.975 |
| Set III | 0.53 | 0.7265 | 1.183 | 0.557 | 0.973 |
| Set IV | 0.63 | 0.7265 . | 1.163 | 0.657 | 0.975 |
| Set V | 0.73 | 0.732 | 1.163 | 0.657 | 0.975 |
| Set VI | 0.83 | 0.7265 | 1.183 | 0.657 | 0.973 |
| Set[b] VII | 0.93 | 0.7265 | 1.183 | 0.657 | 0.973 |
| Set VIII | 1.23 | 0.7265 | 1.183 | 0.657 | 0.973 |

[a]The other parameters are the same for the seven sets and they are $a_2=1.201$, $a_3=0.71$, $e_2=0.975$, $e_3=0.39$, $g_2=0.491$, and $g_3=1.221$.
[b]$a_3=0.73$, $g_1=1.09$.

where $f_1$ is of the same form as $f_1$ in $\Psi$ for $J=0$ and

$$f_2=\sum_{l,m,n} E_{lmn}P_{lmn}(c_1,c_2,c_3;d_1,d_2,d_3) + \sum_{\substack{l,m,n\\ m\neq n}} F_{lmn}Q_{lmn}(p_1,p_2,p_3;q_1,q_2,q_3) \; .$$

$c$'s, $d$'s, $p$'s, and $q$'s are the additional nonlinear parameters, and $\mathbf{r}$ is the distance of $\mu$ from the center-of-mass of $t$ and $d$.

Eigenvalues are calculated by diagonalizing the expression

$$E=\langle \Psi H \Psi\rangle / \langle \Psi\Psi\rangle \; , \tag{3}$$

where $H$ is the Hamiltonian of the system.

In addition to bound states of the system, we obtain roots in the scattering region. The eigenvalues have been scaled to 206.768 262 Ry (1 Ry = 13.605 698 eV), the binding energy of $t\mu$ with $m_t=\infty$. Consequently, $E(t\mu)=-0.963\,748$ and $E(d\mu)=-0.946\,671$. If a root indicates a real resonance, then it should continue to exist when the coordinates are rotated through an angle $\theta$ using the transformation $r_{ij}=r_{ij}\exp(i\theta)$, and the Hamiltonian is continued analytically in the complex energy plane. The kinetic and potential parts scale as $\exp(-2i\theta)$ and $\exp(-i\theta)$, respectively, and the Hamiltonian can be written as

$$H=T\exp(-2i\theta)+V\exp(-i\theta) \; . \tag{4}$$

Again the eigenvalues are obtained by diagonalizing the expression given in Eq. (3), wherein now the eigenvalue and eigenvectors are complex. Since the rotated Hamiltonian is complex, complex eigenvalues are obtained. In this complex-rotation method, a resonance, if it exists, is "uncovered" for $\theta>\arg(E)/2$ and stays at the same place, while the other roots follow the branch cut, as the cut associated with the threshold is rotated through various angles. The eight sets of nonlinear parameters used in the calculation are given in Table I. The angle $\theta$'s used in the calculations for $J=0$ and 1, and the labels in the curves, are given in Table II.

In Fig. 1, we plot complex eigenvalues for $J=0$, using 1101 terms in the wave function for nonlinear parameters of set III given in Table I, and we see clearly that the curve has a loop giving an average value of $(-0.318\,382-i0.64\times10^{-5})$ for $E_r-i\Gamma/2$. The other sets of nonlinear parameters give curves crossing in the same region, but for clarity only one curve is shown. This certainly indicates a Feshbach-type resonance at 1815.560 eV above the $t\mu$ ground state and $\Gamma=0.036$ eV. The average relative distances for this resonance are $r_{td}=10.19$, $r_{t\mu}=6.29$, and $r_{d\mu}=6.44$ in muonic units of length.

In Fig. 2, we plot complex eigenvalues for $J=1$, using 1070 terms in the wave function for nonlinear parameters of set IV given in Table III and we see that the curve has a loop giving an average value $(-0.316\,477\,8-i0.125\times10^{-5})$ for the resonance parameters. Again, for clarity only one curve is shown even though the other curves have crossings in the same region. This indicates a Feshbach-type resonance at 1820.920 eV above the $t\mu$ ground state and $\Gamma=0.007$ eV. The positions for the lowest resonances in $J=0$ and 1

TABLE II. Angles ($\theta=45/A$ in degrees) used in Eq. (4).

| $J=0$ | | | | $J=1$ | | | |
|---|---|---|---|---|---|---|---|
| $A$ | Label | $A$ | Label | $A$ | Label | $A$ | Label |
| $\infty$ | $a$ | 6 | $h$ | $\infty$ | $a$ | 7 | $i$ |
| 90 | $b$ | 5 | $i$ | 90 | $b$ | 6.6 | $k$ |
| 45 | $c$ | 4.8 | $j$ | 45 | $c$ | 6 | $l$ |
| 24 | $d$ | 4 | $k$ | 24 | $d$ | 5.4 | $m$ |
| 12 | $e$ | 3.43 | $l$ | 12 | $e$ | 5 | $n$ |
| 9 | $f$ | 3 | $m$ | 10 | $f$ | 4.8 | $o$ |
| 8 | $g$ | 2 | $n$ | 9 | $g$ | 4 | $p$ |
| | | | | 8 | $h$ | 3.43 | $q$ |
| | | | | | | 3 | $r$ |

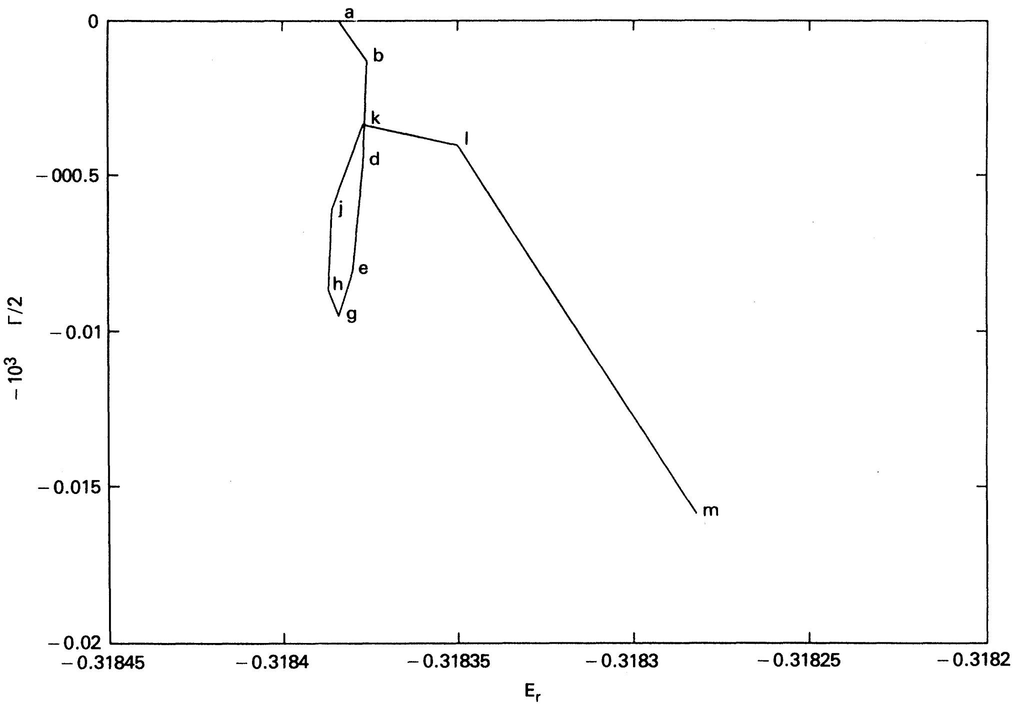


FIG. 1. $J=0$ rotation paths through various angles for the complex eigenvalue below $n=2$ thresholds. The curve is for set III, which is given in Table I. The labels refer to angles of rotation (cf. Table II).

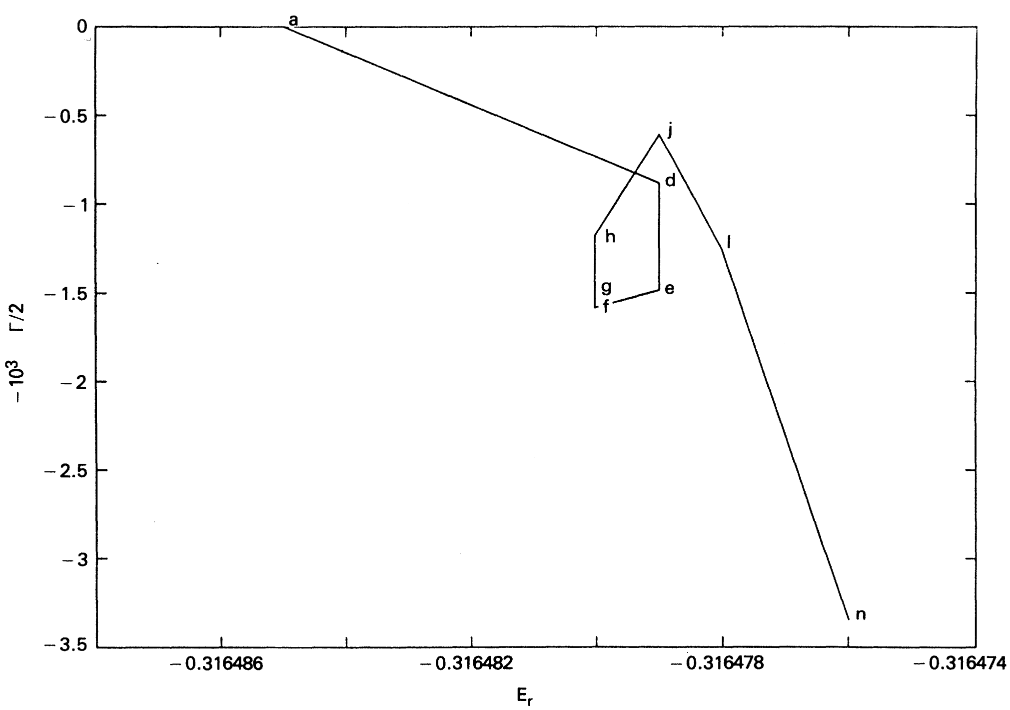


FIG. 2. $J=1$ rotation paths through various angles for the complex eigenvalue below $n=2$ thresholds. The curve is for set IV given in Table II. The labels refer to the angles of rotation (cf. Table II).

TABLE III. Nonlinear parameters used in $J=1$ states (the other parameters are the same for the three sets and they are $a_2=0.627$, $a_3=0.599$, $b_3=1.294$, $e_1=g_1=p_1=q_1=0.197$, $e_2=0.801$, $e_3=0.205$, $g_2=0.801$, $g_3=0.205$, $c_2=0.871$, $c_3=0.189$, $d_2=0.0998$, $d_3=0.7731$, $p_2=1.121$, $p_3=0.145$, $q_2=0.541$, and $q_3=0.731$). The units are the inverse Bohr radius.

| | $a_1=b_1$ | $b_2$ | $c_1=d_1$ |
|---|---|---|---|
| Set I | 0.302 | 1.303 | 0.508 |
| Set II | 0.402 | 1.303 | 0.508 |
| Set III | 0.602 | 1.303 | 0.508 |
| Set IV | 0.702 | 1.303 | 0.508 |
| Set V | 0.802 | 1.300 | 0.588 |
| Set VI | 0.902 | 1.303 | 0.708 |
| Set VII | 0.902 | 1.303 | 0.588 |

TABLE IV. Resonance parameters and their comparison with the results of Hara and Ishihara (Ref. 14).

| $J$ | Resonance | Position[a] | Width | Hara and Ishihara |
|---|---|---|---|---|
| 0 | 1 | 1815.561 | 0.036 | 1815.539 |
| | 2 | 1893.929 | 0.076 | 1893.707 |
| | 3 | 1955.046 | 1.125 | 1954.336 |
| 1 | 1 | 1820.920 | 0.007 | 1820.884 |
| | 2 | 1898.285 | 0.084 | 1898.056 |
| | 3 | 1958.491 | 0.284 | 1957.757 |
| | 4 | 2000.036 | | 1999.198 |

[a]Resonance positions are with respect to the $n=1$ threshold of $t\mu$. The units are eV.

agree with those obtained by Hara and Ishihara.[13] The higher resonances in $J=0$ and 1 have also been calculated and our final results are given in Table IV along with those obtained by Hara and Ishihara.[13] The agreement for the positions between the two calculations is very good, but there is no other calculation for widths available at present for comparison. The positions of the higher resonances can be determined from[9–11]

$$E_{n+1}=E_n\exp(-2\pi/\alpha), \quad n=1,2,3,\ldots \tag{5}$$

where $E_n$'s are defined with respect to the $n=2$ threshold of $t\mu$. A similar relation[14] is expected to hold for widths:

$$\Gamma_{n+1}=\Gamma_n\exp(-2\pi/\alpha), \quad n=1,2,3,\ldots . \tag{6}$$

The above relations are strictly valid for higher resonances that do not penetrate deep and when the $\alpha/r^2$ potential is the dominant potential. It should be noticed that higher resonances for $J=0$ and 1 get wider compared to the lower ones. This is contrary to what is seen for atomic systems.[6] This could be due to the coupling with $3s,4s,\ldots,3p,4p,\ldots,$ states, the coupling with $1s$ being weak,[11] and the first few resonances are not strictly due to the $-\alpha/r^2$ potential, or the results have not yet converged for the number of terms used in the wave function for $J=0$ and 1.

The complex-rotation method has the advantage that the total widths are obtained along with the positions, though partial widths cannot be obtained without calculating the continuum functions. However, a better approach for calculating these Feshbach-type or closed-channel resonances would be the use of the Feshbach projection operator formalism, which has been very successfully applied to three-particle systems,[6] and in this approach partial widths can also be calculated, provided scattering functions are known. But one of the problems, which is also encountered in $e^+$-H, is the nonorthogonality of the $t\mu$ and $d\mu$ ground-state wave functions. This makes it difficult to write a projection operator to project out the lower states from the wave function. However, Dirks and Hahn[15] tried to overcome this difficulty and we hope to apply their method in the near future to the resonances in the $td\mu$ system and also to other muonic systems.

The wave functions given here have the capability, with appropriate nonlinear parameters, to provide accurate results for the bound states[12] and predict resonances. We conclude that there are resonances below the $n=2$ threshold of $d\mu$ and $t\mu$. We hope this paper will encourage further investigation, using different methods, as to why widths of the Feshbach resonances get larger as we go to the higher ones.

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