Bound and resonant states of muonic molecules below the $n=2$ level of muonic atoms

S. Hara
Institute of Physics, University of Tsukuba, Ibaraki 305, Japan
and Atomic Processes Laboratory, Institute of Physical and Chemical Research (RIKEN), Wako-shi 351-01, Japan

T. Ishihara
Institute of Applied Physics, University of Tsukuba, Ibaraki 305, Japan
(Received 1 May 1989)

We calculate, by a variational procedure, the bound-state energies of the even-parity muonic molecules with total angular momentum $J=1$ and the energies of the $(dd\mu)^+$ and $(dt\mu)^+$ resonant states below the $n=2$ energy level of muonic atoms. We have found 11 resonant states with $J=0$ and 12 with $J=1$ for $(dd\mu)^+$ and 9 states with $J=0$ and 10 with $J=1$ for $(dt\mu)^+$. Some of the resonant energies, relative to the $n=2$ level of the muonic atoms, are less than the dissociation energy of D_2, and therefore these states may play some role in muon-catalyzed fusion.

I. INTRODUCTION

Energy levels of muonic molecules $(pp\mu)^+$, etc., composed of a negative muon μ and proton p or its isotopes deuteron d and triton t in the ground muonic molecular states ($1s\,\sigma_g$, in the notation referring to the states of the united atoms) have been studied extensively[1-4] since the weakly bound states of muonic molecules play an important role in the muon-catalyzed fusion. For example, the muon-catalyzed dt fusion is considered to occur through the so-called Vesman mechanism[5]

$$t\mu(1s)+D_2\rightarrow[(dt\mu)^+dee]^*\ ,$$

where the small excess energy in forming a $(dt\mu)^+$ molecule is absorbed by the rotational and vibrational motion of the electronic molecule $[(dtu)^+dee]$. Carter[6] demonstrated the existence of the total angular momentum $J=1$ even-parity bound state of muonic molecules related to the $2p\pi_u$ potential curve. Although this state is embedded in the continuum $t\mu(1s)+d$ and $d\mu(1s)+t$, it is a real bound state because it has the abnormal parity $(-1)^{J+1}$, while the continuum states are in the normal parity $(-1)^J$. Further, he suggested the existence of the $J=1$ odd-parity resonant state associated with this potential curve. This is resonance since it is in the normal parity and couples with the continuum through nonadiabatic interactions. The bound states and resonances related to the $n=2$ atomic level are of interest. They may contribute to the formation of muonic molecules through the Vesman mechanism in the collision of the metastable $t\mu(2s)$ atom

$$t\mu(2s)+D_2\rightarrow\{[(dt\mu)^+]^*dee\}^*\ ,$$

if the binding energies are very small or if the resonant energies are close to that of $t\mu$ ($n=2$). The approximation adopted by Carter was, however, very crude. He used the lowest-order Born-Oppenheimer (BO) approximation without nonadiabatic couplings among different muonic states. Moreover, he did not take account of correct angular momentum symmetries. Thus his numerical values are not accurate enough. Recently, Matveenko[7] estimated the energy level of the even-parity bound state using the hyper-radial adiabatic potential curves.[8]

Here, we solve the three-body problem without approximation and present, for the first time, reliable results for the binding energies of the even-parity muonic molecules with $J=1$. We also investigate, for $(dd\mu)^+$ and $(dt\mu)^+$, resonant states which lie below the $n=2$ level of muonic atoms. We have found 11 resonant states with $J=0$ and 12 with $J=1$ for $(dd\mu)^+$ and 9 resonant states with $J=0$ and 10 with $J=1$ for $(dt\mu)^+$. There exist several resonant states within the dissociation energy of the D_2 molecule, and therefore, they may play some role, either positive or negative, in muon-catalyzed fusion reaction. For these states, the energy values presented in this paper may not be very accurate. However, our main purpose is not to give the very accurate energies, but to show the existence of the shallow muon-molecular resonant levels whose binding energies relative to the $2s$ and $2p$ states of muonic atoms are less than the dissociation energy of D_2.

All of our calculation is carried out variationally without separation of vibrational and rotational motions. Though we frequently use the terminology of the BO approximation, it is only for illustrative purposes. In fact, the BO results[6] for energies of the $J=1$ even-parity bound states differ from the present variational results by more than 10 eV in some cases.

II. EVEN-PARITY BOUND STATES WITH $J=1$

As was discussed by Carter,[6] the even-parity bound state with $J=1$ is, in the BO approximation, related to the $2p\pi_u$ adiabatic potential curve which has a minimum at the internuclear distance $R\approx 8.0$. This minimum is 0.0095 ($\simeq 53$ eV) below the dissociation limit, the $2p$ state of muonic atoms. A schematic diagram for the bound state is given in Fig. 1. We use the units, unless otherwise stated,

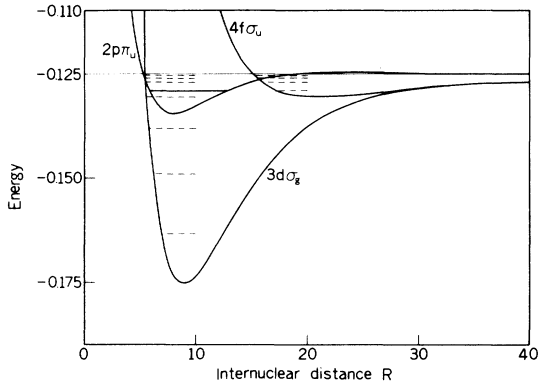

FIG. 1. Schematic diagram for the adiabatic potential curves, bound (solid curve) and resonant (dashed curve) states of the muonic molecules $(dd\mu)^+$ below the $n=2$ atomic level. Units are defined in Eq. (1).

$$e=\hbar=m_\mu=1 \tag{1}$$

and the following physical constants: the muon mass $m_\mu=206.7686m_e$, with m_e being the electron mass, the proton mass $=1836.151m_e$, the deuteron mass $=3670.481m_e$, the triton mass $=5496.899m_e$, and 1 Ry $=13.605\,804$ eV.

To calculate the bound-state energies, we utilize the variational procedure[1] which was once employed to the ground states. The wave function for the even-parity state with $J=1$ can be written as[9]

$$\Psi(\mathbf{r},\mathbf{R})=\sum_i B_i g_i(\xi,\eta,R)\sin\Theta\sin\Phi\ , \tag{2}$$

$$g_i(\xi,\eta,R)=[(\xi^2-1)(\eta^2-1)]^{1/2} \times R^{a_i}\xi^{b_i}\eta^{c_i}\exp(-\alpha_i R-\beta_i R\xi)\ , \tag{3}$$

where Θ is the polar angle of the internuclear distance vector $\mathbf{R}$ from the space-fixed z axis, a set of variables $\mathbf{r}(\xi,\eta,\Phi)$ is spheroidal coordinates for the muon,[1] and a_i, b_i, and c_i are integers. For homonuclear molecules, $(dd\mu)^+$, etc., c_i is even corresponding to the π_u symmetry.

For all the muonic molecules, there exists one (vibrational quantum numbers $v=0$) even-parity bound state with $J=1$. The results for the binding energies are given in Table I. Energies are measured relative to the $n=2$ state of heavier muonic atoms. We have adopted 280 terms of basis functions for the homonuclear molecules and up to 500 terms for the heteronuclear ones $(dt\mu)^+$, etc.

The binding energies of the even-parity bound state of $(dd\mu)^+$ and $(dt\mu)^+$ are larger than the dissociation energy of D_2 and therefore they may not be important in the muon-catalyzed dd and dt fusion.

TABLE I. Energies (in eV) of the even-parity bound states with $J=1$.

Isotopes	Energy (eV)
$(pp\mu)^+$	−13.542
$(dd\mu)^+$	−22.595
$(tt\mu)^+$	−27.413
$(pd\mu)^+$	−3.684
$(pt\mu)^+$	−1.566
$(dt\mu)^+$	−19.124

III. UNGERADE RESONANT STATES OF $(dd\mu)^+$

The $4f\sigma_u$ adiabatic potential curve, which is correlated to the metastable $2s$ and the $2p$ states in the separated atom limits, has a shallow ($0.006\approx 32$ eV) but long-tailed minimum (see Fig. 1). There is a possibility of existing, below the $n=2$ atomic level, resonant states which are closely related to the bound states for the $4f\sigma_u$ potential curve in the BO approximation.

We use the stabilization method[10,11] to search the energy position of the ungerade(u)-type resonant states of $(dd\mu)^+$ by increasing the number of basis functions in the variational procedure. For $J=0$, we adopt the following trial function of the σ_u symmetry:

$$\Psi=\sum_i A_i f_i(\xi,\eta,R)\ , \tag{4}$$

$$f_i(\xi,\eta,R)=R^{a_i}\xi^{b_i}\eta^{c_i}\exp[-\alpha_i R-\beta_i R\xi]\ \ (\text{for } c_i \text{ odd})\ . \tag{5}$$

By using up to 936 terms of basis functions, we have found 4 resonant states (v from 0 to 3) below the $n=2$ level of the $d\mu$ atom. Variation of the resonant energies as functions of numbers of trial functions is given in Table II. Throughout this computation, orbital exponents α_i and β_i in Eq. (5) are fixed (not optimized) and only numbers of polynomials of R, ξ, and η are changed. The numbers of polynomials are given by $(a\times b\times c)$ in this table. Although the resonant energy for the $v=3$ state is not converged completely, the existence of this state may be concluded. A schematic diagram for the u-type resonant states with $J=0$ are given in Fig. 1. Probability distributions

TABLE II. Variation of the resonant energies (in eV) of the u type $(dd\mu)^+$ with $J=0$. Resonant energies are measured relative to the $n=2$ level of $d\mu$. Numbers in parentheses denote numbers of a_i, b_i, and c_i in Eq. (5).

No. of terms	$v=0$	1	2	3
441 (9×7×7)	−21.154	−9.406	−3.819	
630 (10×7×9)	−21.155	−9.414	−4.061	−0.906
756 (12×7×9)	−21.156	−9.415	−4.077	−1.451
936 (13×8×9)	−21.156	−9.415	−4.078	−1.608

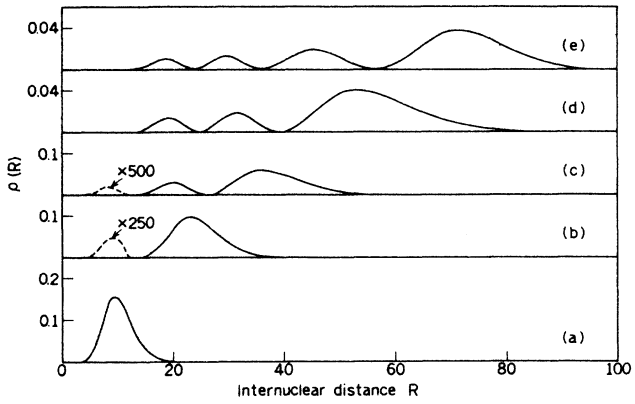

FIG. 2. (a) Probability distribution for the $(dd\mu)^+$ even-parity bound state with $J=1$, (b)–(e): the probability distributions for the $(dd\mu)^+$ u-type resonant states with $J=0$ ($v=0$–3). The probability distribution for the u-type resonant state with $J=1$ ($v=0$) is indistinguishable from (a), and those for $J=1$ ($v=1$–4) are very close to (b)–(e) with an additional small peak at $R \leq 10$ [examples are given by dashed curves in (b) and (c)]. Units are defined in Eq. (1).

$$\rho(R)=\int |\Psi(\mathbf{r},\mathbf{R})|^2 d\mathbf{r}\, 2\pi \sin\Theta\, d\Theta \tag{6}$$

for these resonant states are plotted in Fig. 2, together with that for the even-parity bound state.

For $J=1$, the π_u state mixes with the σ_u state. Thus our trial function is

$$\Psi=\sum_i A_i f_i(\xi,\eta,R)\cos\Theta+\sum_i B_i g_i(\xi,\eta,R)\sin\Theta\cos\Phi\ . \tag{7}$$

The forms of g_i and f_i are the same as Eqs. (3) and (5). We have added up to 350 terms of π_u-type basis function to the σ_u wave functions (maximum number of basis functions is 1286). We have found five resonant states for $(dd\mu)^+$ with $J=1$.

In the BO picture, the $2p\pi_u$ potential curve couples with the $4f\sigma_u$ curve. Since the $2p\pi_u$ potential curve supports one bound state, the σ_u-π_u coupling produces one extra resonant state in addition to those corresponding to the $J=0$ case. Thus, the additional resonant state for $J=1$ is mainly in π_u character and is strongly related to the even-parity bound state, while other four states are mainly in σ_u character. The probability distribution

TABLE III. Resonant energies (in eV) of the u type $(dd\mu)^+$, relative to the $n=2$ level of $d\mu$.

v	$J=0$	v	v_{σ_u}	v_{π_u}	$J=1$
0[a]	−22.595[a]	0		0	−22.648
0	−21.156	1	0		−20.122
1	−9.415	2	1		−8.805
2	−4.080[b]	3	2		−3.749
3	−1.603	4	3		−1.395

[a]Even-parity bound state with $J=1$.
[b]Obtained by $(13\times7\times10)$ term trial function.

TABLE IV. Variation of the bound- and resonant-state energies (in eV) of the g type $(dd\mu)^+$ with $J=0$. Resonant energies are measured relative to the $n=2$ level of $d\mu$. Except for the first row, number of basis functions are $(9\times6\times3)+(a\times b\times c)$. For a, b, and c, see Table II.

No. of terms	Bound states $v=0$	$v=1$	Resonant states $v=4$	$v=5$	$v=6$
720	−325.073	−35.844	−12.046	−2.982	
648 $(9\times6\times9)$	−325.072	−35.843	−12.457	−5.209	−1.069
862 $(10\times7\times10)$	−325.072	−35.843	−12.536	−5.270	−1.865
932 $(11\times7\times10)$	−325.072	−35.843	−12.563	−5.284	−2.059
1072 $(13\times7\times10)$	−325.072	−35.843	−12.594	−5.300	−2.210
1170 $(14\times8\times9)$	−325.072	−35.843	−12.606	−5.304	−2.156
Best values[a]	−325.074	−35.844			

[a]Reference 3.

TABLE V. Resonant energies (in eV) of the g type $(dd\mu)^+$, relative to the $n=2$ level of $d\mu$.

v	$J=0$	$J=1$
0	−218.113	−211.926
1	−135.278	−130.348
2	−72.962	−69.225
3	−31.884	−29.504
4	−12.606	−11.478
5	−5.304	−4.758
6	−2.210[a]	−1.913

[a]Result by 1072-term trial function.

$\rho(R)$ for the $J=1$ ($v=0$) resonant state is almost indistinguishable from that for the even-parity bound state. The distributions $\rho(R)$ for the $J=1$ ($v=1$–4) states are very close to those for the $J=0$ ($v=0$–3) states except for an additional small peak at $R \leq 10$ (see dashed curve in Fig. 2). Therefore, we classify five $J=1$ resonant states as $v_{\pi u}=0$ ($v=0$) and $v_{\sigma u}=0$–3 ($v=1$–4). The resonant energies of the u type $(dd\mu)^+$ with $J=0$ and 1, relative to the $n=2$ level of $d\mu$, are presented in Table III.

IV. GERADE RESONANT STATES OF $(dd\mu)^+$

The $3d\sigma_g$ adiabatic potential curve has a deep ($0.05 \approx 280$ eV) minimum. This curve, like the $4f\sigma_u$ potential curve, has a long tail and is correlated to the metastable $2s$ and the $2p$ states in the separated atom limits (see Fig. 1). We repeat the stabilization procedure to search the gerade(g)-type resonance of $(dd\mu)^+$ with $J=0$ and 1 which are closely related to the bound states for the $3d\sigma_g$ potential curve.

For $J=0$, the form of the trial function is the same as Eqs. (4) and (5), except that c_i is even because of the σ_g symmetry. By using up to 1170 terms of basis functions, we have found 7 resonant states ($v=0$–6). Variation of several resonant energies as functions of numbers of trial functions is given in Table IV together with that of the bound states. In this table, 720-term trial function is composed of $(8\times5\times6)$ polynomials with three sets of orbital exponents α_i and β_i. Other trial functions are composed of $(9\times6\times3)$ terms whose orbital exponents are adjusted so as to represent the bound state, plus $(a\times b\times c)$ terms with diffuse orbital exponents, where integers a, b, and c are given in Table IV. It should be noted that the 720-term calculation gives better results for the bound states, while the resonant energies are rather poor. It is difficult, in our computer program, to add an extra large number of basis functions to the 720-term basis set since our basis functions are not mutually orthogonal and bound states become overcomplete. As our main purpose is to show the existence of the resonant states, we have chosen basis functions which give better resonant energies at the cost of the bound-state energies. From Table IV we can confirm, for the g state of $(dd\mu)^+$, the existence of at least one shallow resonant state whose resonant energy is less than the dissociation energy of D_2. The resonant energies of the g type $(dd\mu)^+$ with $J=0$, relative to the $n=2$ level of $d\mu$, are listed in Table V. We present a schematic diagram for the g-type resonant states with $J=0$ in Fig. 1.

When J is equal to 1, the π_g state mixes with the σ_g state. Thus the form of trial function is the same as Eqs. (3), (5), and (7), except that c_i is even for f_i and c_i is odd for g_i. We have added up to 350 terms of π_g-type basis functions to the σ_g trial function (the largest σ_g-type basis function is 1098 term). The resonant energies of the g type $(dd\mu)^+$ with $J=1$ are given in Table V. Since the $3d$ π_g potential curve is repulsive in the BO picture, the σ_g-π_g coupling does not produce any extra resonant state in addition to the $J=0$ case.

In Table VI, we give the bound-state energies of $(dd\mu)^+$ obtained by our trial functions which are used in search of the resonances.

TABLE VI. Bound-state energies (in eV) of $(dd\mu)^+$ and $(dt\mu)^+$ obtained by the trial functions which are used in search of the resonances.

(J,v)	$(dd\mu)^+$	$(dt\mu)^+$
(0,0)	−325.072	−319.138
(0,1)	−35.843	−34.831
(1,0)	−226.681	−232.470
(1,1)	−1.975	−0.658

TABLE VII. Variation of bound- and resonant-state energies (in eV) of the $(dt\mu)^+$ with $J=0$. Resonant energies are measured relative to the $n=2$ level of $t\mu$.

No. of terms	Bound states		Resonant states		
	$v=0$	$v=1$	$v=6$	$v=7$	$v=8$
1513	−319.131	−34.817	−7.178	−3.322	−0.440
1618	−319.136	−34.826	−7.116	−3.499	−1.093
1828	−319.136	−34.827	−7.202	−3.555	−1.483
2008	−319.138	−34.830	−7.205	−3.557	−1.561
2200	−319.138	−34.831	−7.225	−3.565	−1.600
Best values[a]	−319.140	−34.834			

[a]References 3 and 4.

V. RESONANT STATES OF $(dt\mu)^+$

For heteronuclear molecules, the center of symmetry no longer exists and the g and u property is lost. Therefore, we have to use nearly twice larger basis set for $(dt\mu)^+$. For $J=0$, we have performed a stabilization procedure by using maximum number of 2200 (1264 σ_g and 936 σ_u terms) basis functions. We have found nine ($v=0$–8) resonant states below the $n=2$ level of the $t\mu$ atom. Variation of some of the resonant energies as functions of numbers of trial functions is given in Table VII together with that of the bound states. From this table, we can conclude the existence of at least two shallow resonant states. The resonant energies of $(dt\mu)^+$ with $J=0$, relative to the $n=2$ level of $t\mu$, are given in Table VIII.

For $J=1$, we have carried out the stabilization procedure by using up to 2600-term trial functions which are composed of 2200 σ and 400 π-type basis functions. We have found 10 resonant states. One additional state for $J=1$ is, like the u-type resonance of $(dd\mu)^+$ with $J=1$, related to the even-parity bound state. The resonant energies of $(dt\mu)^+$ with $J=1$ are given in Table VIII. The bound-state energies for $(dt\mu)^+$ obtained by the present trial functions are also listed in Table VI.

TABLE VIII. Resonant energies (in eV) of $(dt\mu)^+$, relative to the $n=2$ level of $t\mu$.

v	$J=0$	v	$J=1$
0	−217.892	0	−212.547
1	−139.724	1	−135.375
2	−79.095	2	−75.674
3	−36.567	3	−34.233
0[a]	−19.124[a]	4	−19.161
4	−17.443	5	−16.351
5	−11.414	6	−10.505
6	−7.225	7	−6.485
7	−3.565	8	−3.185
8	−1.600	9	−1.346

[a]Even-parity bound state with $J=1$.

VI. CONCLUSION

In this paper, we have performed a variational calculation for the energies and wave functions of the even-parity bound states with $J=1$ and the resonant states with $J=0$ and 1 of the muonic molecules which are correlated to the metastable $2s$ and the $2p$ states of muonic atoms. We have confirmed the existence of shallow resonant states for $(dd\mu)^+$ and $(dt\mu)^+$ with $J=0$ and 1, though the calculated energies may not be very accurate. Shallow resonant states may also exist for $J\geq 2$. There is a possibility that the metastable $t\mu(2s)$ atoms and the resonant states related to the $n=2$ atomic levels play some positive or negative role in the muon-catalyzed fusion reaction. A detailed study of these resonant states should be very interesting.

ACKNOWLEDGMENTS

We are grateful to Dr. A. V. Matveenko for helpful discussions, and to Dr. T. Shirai and Dr. T. Kato for their assistance in the computation.

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