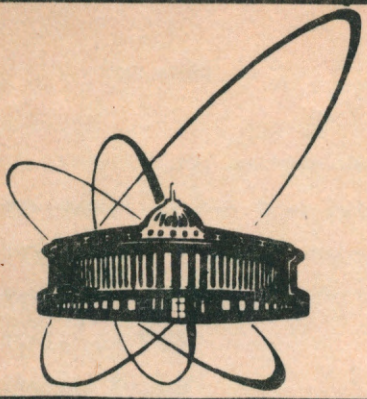

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ON THE CLASSIFICATION SCHEME FOR RESONANT STATES OF MUONIC MOLECULES

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I. Introduction

Recently /1/ we have used the one-state hyperradial-adiabatic approximation and have provided the upper limit for the energy values of the muonic molecular ions $(xy\mu)^+$ in the ground state with total angular momentum J=1 and total parity p=1. As $J \neq (-1)^p$, in this case such states are called abnormal parity bound states. Two systems, $(pd\mu)^+$ and $(pt\mu)^+$, were found to have a loosely bound state of that symmetry. Full variational calculations /2,3/ immediately followed this publication, providing more accurate energy values. They verified the existence of the above-mentioned loosely bound state. The authors of /2/ had also calculated the J = 0,1 normal parity resonances of $(dd\mu)^+$ below the n=2 level of $d\mu$ and of $(dt\mu)^+$ below the n=2 level of $t\mu$. We note that for these resonant states no preliminary adiabatic calculations where made contrary to a usual practice in the muonic molecular physics. To classify the calculated resonant states /2/, the authors used the Born-Oppenheimer (BO) adiabatic potential curves. Their analysis was later supported and worked out in detail /4/. There are two points which look unsatisfactory in this analysis. First, the number of normal parity bound states of $(dd\mu)^+$ and $(dt\mu)^+$ is reported /2/ to increase by one when the total angular momentum of the system is changed from J=0 to J=1. One additional state was suggested to "be related to the even parity bound state". This statement is not clear. Second, in the case of $(dt\mu)^+$, where the dissociation limit can be either a $t\mu$ or $d\mu$ muonic atom with the principal quantum number n=2, they have no regular way to choose a proper one for a given state. In ref. /2/, the $t\mu(n=2)$ limit is used for all nine calculated states of $(dt\mu)^+$, while in /4/ the sixth state of J=0 resonances calculated

in /2/, lying at 11.41 eV below the level $t\mu(n=2)$, or at 22.42 eV below the level $d\mu(n=2)$, is attributed to the expected series of resonances converging to the limit $d\mu(n=2)$. It was also stated that the ninth state cannot be properly classified within the proposed scheme /4/.

It is well-known and has lately been discussed in detail /5/, that the BO adiabatic method has two principal defects: 1) adiabatic potential curves do not provide proper atomic energy spectra for heteronuclear systems when internuclear distance is going to infinity ,and 2) BO adiabatic states (and the corresponding potential curves) do not have exact symmetry properties of a total three-body system. As we have shown /5/, the first problem can be resolved by transforming out the so-called mass polarization operator in the total Hamiltonian, and the second one is easily overcome by the partial wave (symmetry) analysis. The adiabatic idea should be introduced at the next step. As a result, we arrive at the adiabatic hyperradial method in which adiabatic states are labelled by the exact quantum numbers and the corresponding eigenvalues (potential curves) produce exact two-body (atomic) threshold energies in the asymptotic region.

If is clear that with this adiabatic analysis being at hand the classification problem of the results of the full variational calculation /2/ should be much easier. One can expect that the classification scheme used in the BO method will not survive in this way and a new scheme should appear. In what follows we use the results of the variational calculation of resonant states of $(dd\mu)^+$ and $(dt\mu)^+$ muonic molecules below the n=2 level of muonic atoms /2/ to demonstrate how it works. The organisation of the paper is chosen to be similar to that in ref./2/ in order to simplify the comparison between two papers.

II. The outline of the method

The hyperradius R for a system of two nuclei x and y and a negative muon μ is defined by

$$MR^2=MX^2+mx^2 \ , \tag{1}$$

where M and m are the reduced masses of the systems (x,y) and (x+y)+μ, respectively,

$$1/M=1/m_x+1/m_y \ , \tag{2}$$

$$1/m=1/m_\mu+1/(m_x+m_y), \tag{3}$$

X is the position vector of y relative to x and x is that of μ with respect to the center of mass of (x+y).

The Hamiltonian of the system is given by

$$H = -\frac{1}{2M}\frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R} + h(\hat{o};R), \tag{4}$$

where h is the adiabatic Hamiltonian operator which includes R as a parameter, and $\hat{o}$ represents five dimensionless variables. Following /1,5,6/ we use the set $\hat{o}=(\alpha,\beta,\gamma,\xi,\eta)$, where (α,β,γ) define the Euler rotation specifying the body-fixed frame with its unit vectors to coincide with the principal axes of the inertia tensor of a three-body problem. The hyperspheroidal coordinates ξ and η are easily given by muon-nucleus distances $r_{\mu x}$, $r_{\mu y}$ and internuclear distance X

$$\xi=(r_{\mu x}+ r_{\mu y})/ X \ , \ \eta=(r_{\mu x}- r_{\mu y})/ X. \tag{5}$$

A physical solution of the Schroedinger equation

$$(H -E) \psi (R,\xi,\eta) = 0 \tag{6}$$

with the well-defined total angular momentum J and total parity p

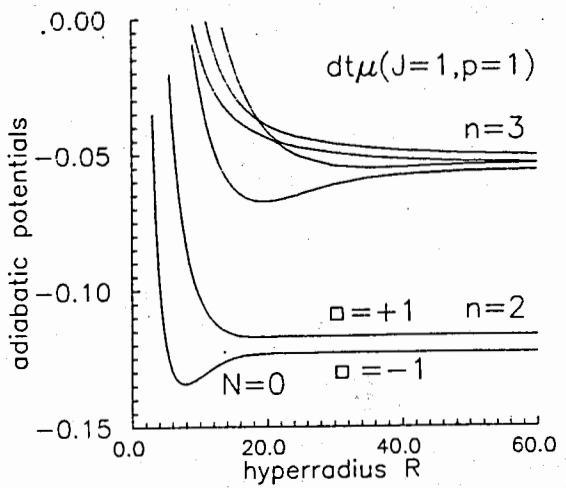

Fig. 1 Six lowest hyperradial adiabatic potential curves for $(dt\mu)^+$. The exact quantum numbers of total angular momentum J and total parity p are given in parentheses. The grand radial quantum number N is given only for the lowest curve. The fragmentation quantum number □ = −1 for the lowest curve indicating that it converges to tμ (n=2) state of muonic atom. The next curve converges to dμ,(□=+1), atom with principal quantum number n=2. The energy scale is given by the dμ(n=2)-tμ(n=2) energy difference which ≃ 12 eV.

provide the physically meaningful approximation for the bound energy of the of (J=1, p=1)-spectrum of $(dt\mu)^+$ below the n=2 state of the tμ-atom. As we have shown /1/, the corresponding potential (12) supports just one bound state so that the quantum numbers of the adiabatic potential curve completely define this state. The next potential curve (N=1, n=2, □=1) converging to the dμ

(n =2)-atom is repulsive; thus the upper series should not appear. The classification of the abnormal parity bound states of $(dt\mu)^+$ below n=2 levels of muonic atom is completed. The situation is the same for $(pd\mu)^+$ and $(pt\mu)^+$. It is similar for homonuclear systems $(xx\mu)^+$ where the □-quantum number disappears but the nucleus exchange symmetry provides the usual BO gerade/ungerade exact quantum number. This question is discussed in subsequent sections.

IV. (J=0, p=1, q=ungerade)- resonant states of $(dd\mu)^+$

These states have three exact quantum numbers of the total angular momentum J, total parity p and muonic-coordinate parity quantum number q that corresponds to the ungerade label in this section. There is one adiabatic potential curve (N=0) which correlates to the 1s state of the dμ-atom and two of them correlate to n=2 states of dμ in the separated-atom limit. The N=1-5 calculated hyperradial adiabatic potential curves are given in Fig.2. They are very similar to the corresponding ungerade σ-terms of the usual BO classification scheme. The N=1 potential curve that corresponds to the 4fσ BO-term and the diagonal matrix element were used in eq.(11) to calculate the spectrum of $(dd\mu)^+$. The results of our one-state hyperradial adiabatic approximation and the results of the full variational calculation /2/ are given in Table I. One-to-one correspondence of the calculated spectra is clear. The accuracy of our results is rather good. The classification of states is trivial if the hyperradial vibrational quantum number v= 0,1,... is added to the already mentioned grand radial quantum number N=1 and principal

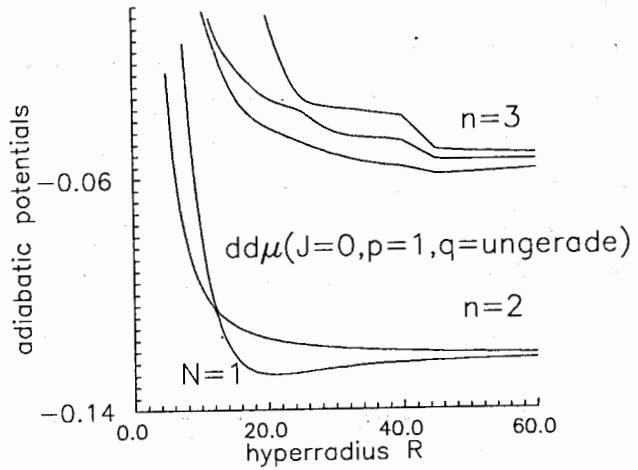

Fig. 2 Five (N= 1-5) hyperradial adiabatic potential curves for $(dd\mu)^+$. The exact quantum numbers are given in parentheses. The depth of the first curve ≃ 30.5 eV. This potential curve supports an infinite series of states.

quantum number n=2 of the threshold state of the dμ-atom. It can be checked that the calculated resonant energies converge at the threshold according to the geometric progression law /4/

$$E_v \simeq A\ \gamma^v, \qquad (13)$$

where A can be deduced from the calculated energies and γ is defined by the coefficient-c > 0 of the effective potential from the Schroedinger eq.(12) in a large R-limit, $V_\sim -c / R^2$ /4/.

V. (J=0, p=1, q=gerade)- resonant states of $(dd\mu)^+$

These states again have three exact quantum numbers. Five, N=1-5, hyperradial adiabatic potential curves of this symmetry

TABLE 1 Resonant energies (in eV) of the (q=ungerade, J=0, p=1) resonant states of $(dd\mu)^+$, relative to the n=2 level of $d\mu$.

v	ref./2/	this paper
0	-21.156	-20.0
1	-9.415	-8.7
2	-4.080	-3.7
3	-1.603	-1.6
4	—	-0.65

TABLE 2 Resonant energies (in eV) of the (q= gerade, J=0, p=1) resonant states of $(dd\mu)^+$, relative to the n=2 level of $d\mu$.

v	ref./2/	this paper
0	-218.113	-217.2
1	-135.278	-134.2
2	-72.962	-71.8
3	-31.884	-31.0
4	-12.606	-12.2
5	-5.304	-5.1
6	-2.210	-2.2
7	—	-0.85

are shown in Fig.3. In this case the corresponding gerade σ-terms of the BO classification scheme are also very similar to those from Fig.3. The powerful potential N=2 ,that corresponds to the BO 3dσ potential curve, was used to calculate the spectrum of $(dd\mu)^+$ below the n=2 state of the dμ-atom. The presentation of the results of the calculation is the same as in the previous secti-

on, they are listed in Table 2. The agreement of the results of two papers is clear. This proves reliability of the presented adiabatic approximation. It should be also stated that the proposed classification scheme is consistent with the BO scheme used in /2,4/ as far as J=0 states discussed above are concerned.

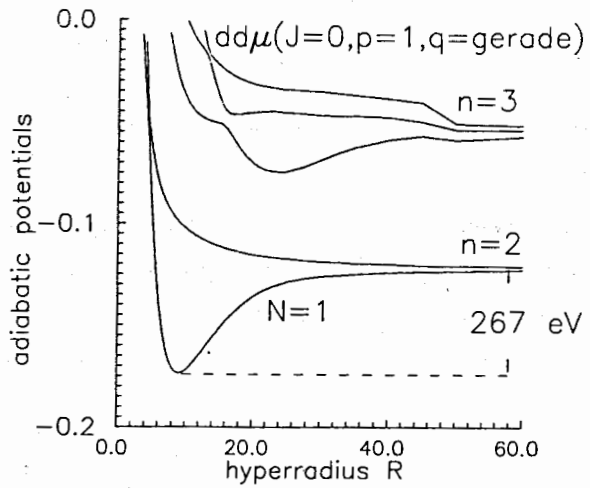

Fig. 3 The same as in Fig 2 but for q = gerade.

VI. (J=0, p=1)-resonant states of $(dt\mu)^+$

Only two exact quantum numbers, those of total angular momentum J and total parity p, are available for this system. The already discussed fragmentation quantum number □ should be added to make a difference between adiabatic potential curves of lower series (□ = -1),converging to the n=2 level of tμ, and those from the upper series (□ = +1) converging to the n=2 level of dμ. The BO potential curves are not sensitive to this physical effect ; thus heteronuclear systems are better candidates for demonstrating the reasons for introducing a new classification scheme.

All hyperradial adiabatic potential curves (N=2-5) converging to the n=2 level of the tμ (N=2,3) or dμ-atom (N=4,5) are given in Fig.4. The lowest one (N=2) is similar to the N=1 curve from the

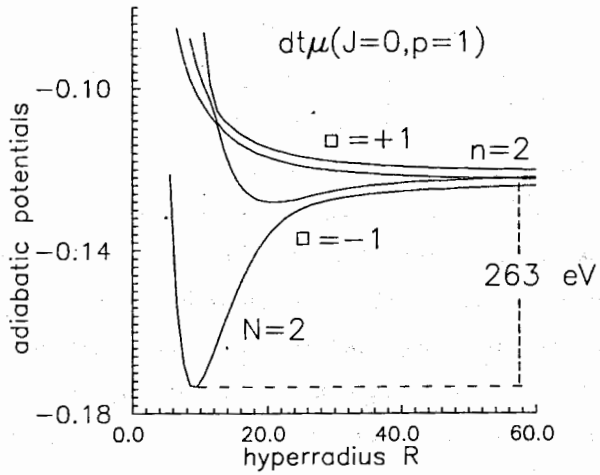

Fig. 4 Two lower curves converge to the tμ(n=2) state. The other two converge to the dμ(n=2) one. The depth of the N=3 curve ≃ 23 eV. The N=4 curve has a shallow minimum at R ≃ 53 and a long-range attractive tail supporting an infinite series of states. Triple avoided-crossing at R ≃ 12.5 should be separately noted.

gerade series for $(dd\mu)^+$, see Fig.3. Both have a powerful long-range attractive tail ($\sim 1/R^2$) in the large R limit. The second (N=3,□=-1)-curve looks like the N=1 ungerade potential curve from Fig.2 for all but large R, where it exhibits a long-range repulsion $\sim 1/R^2$,while the corresponding $(dd\mu)^+$-ungerade curve has a long-range attractive tail of the same order in R. This means that in the $(dt\mu)^+$ case the N=2 curve supports infinitely many states, while the N=3 one can support only a limited number of

resonances. We have calculated eight resonances corresponding to the N=2 potential curve and have found that the N=3 curve can support only one state. This is, of course, a very different situation as compared with the infinite series of (J=0, p=-1, q=ungerade)-symmetry for $(dd\mu)^+$. The breakdown of the symmetry property of the system results in the qualitative change of its spectrum.

The resonant energies of the (J=0, p=+1)-symmetry of $(dt\mu)^+$ obtained in our one-level hyperradial adiabatic calculation are listed in Table 3 and compared with the results of the full variational calculation /2/. All the energy values but that for the fifth and sixth states, are close to each other. Contrary to the classification suggested in /2,4/, we conclude that the wave function of the sixth state has no nodes in the R variable. This conclusion is exact only in the framework of the one-state hyperradial adiabatic approach. As it follows from Fig.3, the adiabatic potential curves with N=2-4 are strongly interacting at R=12.5 ; thus our approximation does not work in that region. On the other hand, the wave function should be small in that classically forbidden region and we can expect that the exact wave function of the sixth state has no nodes in the R variable in the physically important region. This is a valueable information which easily follows from our analysis and proves the importance of the presented classification scheme.

The N=5 potential curve of the same symmetry has a very weak minimum at R ≃ 53 which converts into a $1/R^2$ attractive tail supporting one more infinite series of resonances. This is a $\Box$ = +1 (upper) series in our classification. It is interesting to note that these states cannot be detected in the course of any direct variational calculation as they are located above the $\Box$= -1 infi-

TABLE 3 Resonant energies (in eV) of the (J=0,p=1) resonant states of $(dt\mu)^+$, relative to the n=2 level of $t\mu$. Lower series.

v	ref./2/	v	N	this paper
0	-217.892	0	3	-217.0
1	-139.724	1	3	-138.8
2	-79.095	2	3	-78.6
3	-36.567	3	3	-35.9
4	-17.443	4	3	-14.9
5	-11.414	0	4	-12.9
6	-7.225	5	3	-6.7
7	-3.565	6	3	-3.1
8	-1.600	7	3	-1.3

TABLE 4 Resonant energies (in eV) of the (J=0,p=1) resonant states of $(dt\mu)^+$, relative to the n=2 level of $t\mu$. Upper series. The estimates of the (J=1,p=-1) states are also given.

v	J = 0	J = 1
0	-4.02	-3.85
1	-1.78	-1.68
2	-0.82	-0.76
3	-0.38	-0.35

nite series of the resonant states. The energies of the first four states from this series are given in Table 4. The one-state adiabatic estimates of the (J=1, p=-1)-symmetry states from this series are also given there.

VII. (J=1, p=-1, q=ungerade)-states of $(dd\mu)^+$ and (J=1, p=-1)-states of $(dt\mu)^+$

To estimate resonant energies of the states with J=1, we have used the same Schroedinger Eq. (11) with the $J(J+1)/R^2$ term added to the effective potential (12). The same classification scheme including exact quantum numbers {J,p,q(for homonuclear systems)}, the additional quantum numbers {N, n, m, v, □ (for heteronuclear systems)} are used. Our results for $(dd\mu)^+$ and the results of the full variational calculation /2/ are listed in Table 5. The ground state from ref./2/ does not appear in our calculation, all other energy values from two papers are in good agreement with each other. One possibility is that this additional state has a purely numerical origin as the rotational part of the Hamiltonian is positive definite and being added to the J=0 part of the Hamiltonian just pushes the spectrum up. The statement from /2/ that this state is "related to the even parity bound state" is not helpful as formally it means that parity violation takes place. The problem is naturally solved if one more attractive adiabatic potential curve of the (J=1,p=-1,q=ungerade)-symmetry with additional quantum numbers n=2,m=1 exists /7/. As it follows from the analysis of/2/ this curve should be close to the ground abnormal-parity adiabatic potential curve discussed in Section III.

In this case the total wave function (7) has two components with m=0,1. The two-component hyperradial adiabatic Hamiltonian for this case was recently discussed in detail /8/. Then, with classical rotator model being introduced /5,8/, it can be directly shown that the decoupled equation for m=1 component of the related eigenfunction just coinsides with the Shroedinger equation that produces (J=1,p=1)-symmetry potential curve from /1/ plus small at -

TABLE 5 Resonant energies (in eV) of the (q=ungerade ,J=1,p=-1) resonant states of $(dd\mu)^+$,relative to the n=2 level of $d\mu$.

v	ref./2/	v	this paper
0	-22.648		
1	-20.122	0	-20.0
2	-8.805	1	-8.7
3	-3.749	2	-3.7
4	-1.395	3	-1.6
5	——	4	-0.65

TABLE 6 Resonant energies (in eV) of the (J=1,p=-1) resonant states of $(dt\mu)^+$,relative to the n=2 level of $t\mu$. Lower series.

v	ref./2/	v	N	this paper
0	-212.547	0	3	-211.6
1	-135.375	1	3	-134.4
2	-75.674	2	3	-74.7
3	-34.233	3	3	-33.1
4	-19.161	...	...	...
5	-16.351	4	3	-13.7
6	-10.505	0	4	-11.8
7	-6.485	5	3	-6.1
8	-3.185	6	3	-2.8
9	-1.346	7	3	-1.2

tractive term which pushes the energy down. This analysis is supported by the results of the full variational calculation /2/. The resonant energies of $(dt\mu)^+$ with (J=1,p=-1)-symmetry are given in Table 6. Again the additional state declared in /2/ to be "related to the even-parity bound state" does not appear in our calculation. This state is supported by the potential curve that was not calculated in this paper, it can be easily classified as it was discussed above in the $(dd\mu)^+$-case. The most interesting state is that supported by the N=4 potential curve. It has practically no zeros in R and is well localized in the space, as discussed in section VI.

VIII. Conclusion

In this paper, we have performed the hyperradial one-state-adiabatic calculation of the resonant states of $(dd\mu)^+$ and $(dt\mu)^+$ muonic molecules below the n=2 level of muonic atoms. The hyperradial adiabatic potential curves that are by-products of our work are used to produce a new classification scheme of the molecular states in a three-body system. We conclude that for heteronuclear systems like $(dt\mu)^+$ this classification is very useful. It allows one to separate definitely the upper $\Box$=+1 and the lower $\Box$=-1 series of the spectra. Thus, for example, we demonstrated that among the nine resonances with J=0 reported in /2/ the sixth (lying at 11.41 eV below the level $t\mu$(n=2)) should really be referred to this level, contrary to what was suggested in /4/ using arguments based on the BO classification procedure. We also predicted important physical features of this state. We were able for the first time to calculate the upper series of resonances in $(dt\mu)^+$ and showed that this series cannot be detected by a direct

variational procedure as it lies above the infinite lower series of the same symmetry. The other important characteristic of the proposed classification scheme is that of labelling of hyperradial adiabatic potential curves by exact quantum numbers of a three-body system. By using this scheme we easily demonstrate that $2p\pi$ BO adiabatic potential curve which does not account for any real symmetry of heteronuclear systems, like $(dt\mu)^+$, is actually splitted into two hyperradial adiabatic potential curves with exact symmetry properties. This fact can be of special interest for spectroscopy of the so-called $2p\pi$-electronic states /9/. We agree with the authors of /2/ that a detailed study of these resonant states should be very interesting, see also a new paper /10/. An informative discussion of these states can be found in /4,11/.

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References

1. Ishihara, T., Fukuda, H., Hara, S., Matveenko, A. V. : Preprint JINR, E4-88-849, Dubna(1988).
2. Hara, S., Ishihara, T. :Phys. Rev. A40, 4332(1989).
3. Korobov, V. I.,Vinitsky, S. I. : Phys. Lett. 288B, 21(1989) ; 255B, 7(1991).
4. Isao Shimamura : Phys. Rev. A40, 4863(1989).
5. Matveenko, A. V. :Phys. Lett. 129B, 11(1983).; Kaschiev, M., Matveenko, A. V., Revai, J. : Phys. Lett. 162B, 18(1985) ; Matveenko, A. V., Abe, Y. : Few-body.Systems 2, 127(1987).
6. Hara, S.,Fukuda, H., Ishihara, T., Matveenko, A. V. : Phys. Lett. 130A, 22(1988).
7. Ishihara, T.: private communication.
8. Matveenko, A. V. : Few-body Systems 4, 103(1988).
9. Beckel, C. L., Shafi, M., Peek, J. M.: J. Chem. Phys. 59, 5228(1973).
10. Hu, C. Y., Bhatia, A. K.: Phys. Rev. A43, 1229(1991).
11. Landau, L. D., Lifshitz, E. M. : Quantum Mechanics, 3rd ed. (Pergamon, Oxford, 1977), Sec. 35.

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