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NEW EFFECTIVE MASS IN ADIABATIC APPROACH FOR THE MUONIC THREE-BODY PROBLEM

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The method for the construction of the adiabatic equation describing the discrete and continuous spectra of the mesic molecule systems by means of the generalization of the concept of the effective mass is presented.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, JINR.

Новая эффективная масса в адиабатическом подходе для мюонной задачи трех тел

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Предложен метод построения адиабатического уравнения для описания дискретного и непрерывного спектров мезомолекулярных систем путем обобщения понятия эффективной массы.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

In this work we discuss our numerical experiments on calculating the energy levels of mesic molecules and mesic atoms cross sections in the framework of some adiabatic approaches. The performed analysis, first, has to explain the known disagreements between adiabatic and variational calculations of the energy levels of the weakly bound states of $dd\mu$ and $dt\mu$ molecules and, second, to give the basis for the construction of new effective adiabatic equations describing adequately both discrete and continuous spectra of mesic molecular systems. We called the above disagreement «the white hole» in the history of μcF theory [1]. Let us remember this disagreement. In 1984 we obtained the following values of the weakly bound states energy in the three-body adiabatic representation

$-\varepsilon_{11}\ (dd\mu)$	$-\varepsilon_{11}\ (dt\mu)$
1.956 ± 0.001 (eV)	0.656 ± 0.001 (eV).

We used 884 states of the two centers problem, in particular , 52 states of the discrete spectrum and 832 states of the continuous one. Our adiabatic results have stimulated the direct variational calculations [2]. However later in our variational calculations we obtained the more accurate values

$$-\varepsilon_{11}\,(dd\mu) \qquad -\varepsilon_{11}\,(dt\mu)$$
$$1.97475\ (\text{eV}) \qquad 0.6600\ (\text{eV}).$$

In these calculations [3] we used about 2660 variational functions. Since up to now we have «a monopoly» in adiabatic calculations of the binding states of mesic molecules, we suggest the explanation of the disagreements mentioned above. We think that this will be useful for the correct applications of adiabatic approaches in the muonic three-body scattering problem and other problems.

The adiabatic representation [4] is based on the expansion of the Shroedinger three-body wave function $\Psi(\overline{R}, \overline{r})$ over a complete set of two center problem solutions

$$\Psi(\overline{R}, \overline{r}) = \sum_j^{\infty} \Phi_j\,(\overline{r}, \overline{R})\, R^{-1}\chi_j\,(R). \tag{1}$$

Using formally the Kantorovich method for reducing a partial differential equation to a set of ordinary ones we obtain the infinite system of radial equations

$$\left[\frac{d^2}{dR^2} + 2ME - U_{ii}(R)\right]\chi_i(R) = \sum_{i=j}^{\infty} U_{ij}(R)\chi_j(R). \tag{2}$$

Here

$$U_{ii}^{J}\,(R) = 2ME_i\,(R) + \frac{1}{R} + H_{ii}^{AD}\,(R) + \frac{J(J+1) - 2m^2}{R^2},$$

$$H_{ii}^{AD}\,(R) = \langle \frac{\partial}{\partial R}\Phi_i | \frac{\partial}{\partial R}\Phi_i \rangle,$$

$$U_{ij}^{J} = H_{ij}\,(R) + \frac{d}{dR}\,Q_{ij}\,(R) + 2Q_{ij}\frac{d}{dR} + B_{ij}^{J}\,(R).$$

We have proposed the boundary conditions of radial wave functions for bound states and the scattering problem, which allows the same treatment for both problems as a nonlinear functional equation. For solving this equation we have constructed a new numerical method [2], that is a generalization of the continuous Newton method.

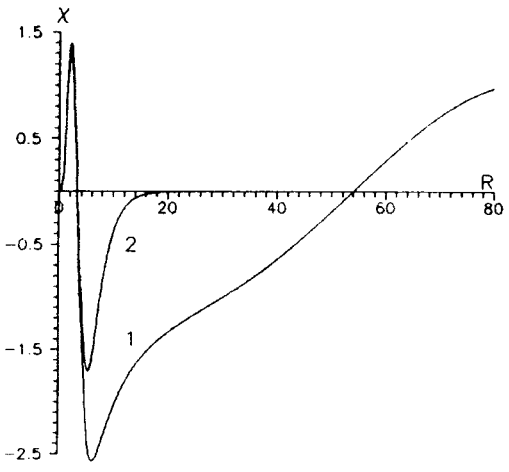


Fig. 1. The radial wave functions 1 — $\chi_1^{(1)}$ for the open and 2 — $\chi_2^{(1)}$ for the closed channels in the reaction of the resonant scattering $(t\mu)_{n=1} + d \rightarrow (t\mu)_{n=1} + d$ with orbital momentum $J = 1$

Our first adiabatic calculations were performed in the two level approximation. In 1975 first we obtained the quasy-stationary state of the $dt\mu$ molecule with the total orbital momentum $J = 1$ and $M = 10.894$ (in this units of reduced mass $m^* = 202.024 m_e$). For this mass we found the energy

$$-\varepsilon = E = 0.68 \text{ eV} \quad (E \equiv \widetilde{E} - E_1(\infty))$$

and the width

$$\Gamma = 10.87 \text{ eV}.$$

The radial wave functions $\chi_1^{(1)}(R)$ for the open channel and $\chi_2^{(1)}(R)$ for the closed channel in the case of the elastic scattering

$$(t\mu)_{1s} + d \rightarrow (t\mu)_{1s} + d$$

are displayed in fig.1.

This result however was not published in ref.[5]. Now we have reproduced the transformation of this state to the weakly bound state when the

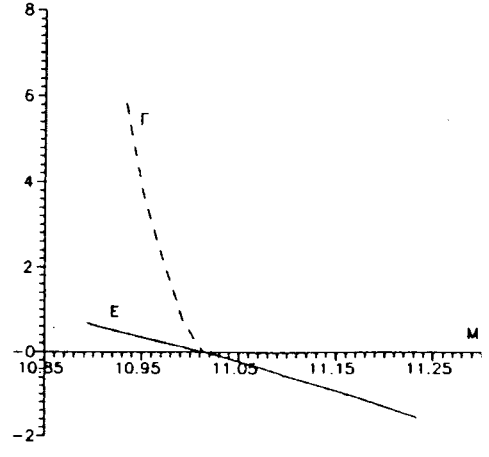


Fig. 2. The dependence of the energy E (eV) and width Γ (eV) of the $dt\mu$ -mesic molecule ($J = 1$, $v = 1$) on the effective mass M

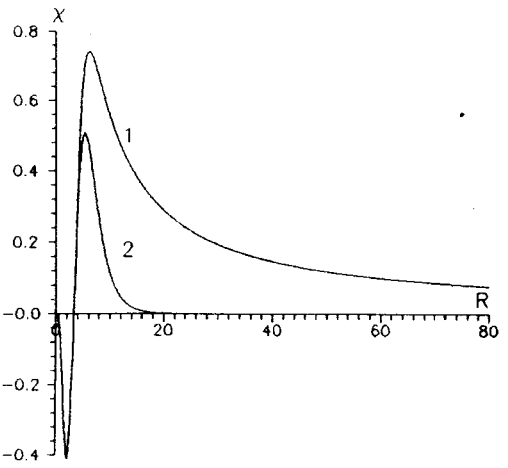


Fig. 3. The radial wave functions 1 — $\chi_1^{(1)}$ and 2 — $\chi_2^{(1)}$ for the $J = 1$ and the zero collision energy $\varepsilon = 0$,$(t\mu)_{n=1} + d \to (t\mu)_{n=1} + d$

effective mass M increases as parameter.

Figure 2 shows the dependence of the energy E and the width Γ on such a mass. For the mass value $M \approx 11.01$ we have the state with the zero energy and the zero width. The radial functions of such case are presented in fig.3. The function 1 of the open channel is decreasing slowly in comparison with the function 2 of the closed channel. As the mass M increases, the $dt\mu$ system is transferred to the bound state. For the value $M \approx 11.12$ eV we have obtained the «symmetrical» value of the energy $E = -0.68$ eV. Therefore we can expect that the weakly bound state ($J = 1$, $v = 1$) exists and the value of the binding energy is similar to this one if we take into account all the non-adiabatic corrections to the energy level. Indeed, our adiabatic and variational results are near to this value. We have the function $E = E(M)$ and we can find for the «exact» value $E = -0.66$ eV the corresponding value of the effective mass $M \approx 11.11$. The radial functions of this state are presented in fig.4.

Thus we have reproduced the variational energy level by choosing the effective mass M in the two level adiabatic approximation.

We have performed the calculations of the cross-section of the reaction

$$(t\mu)_{1s} + d \to (t\mu)_{1s} + d$$

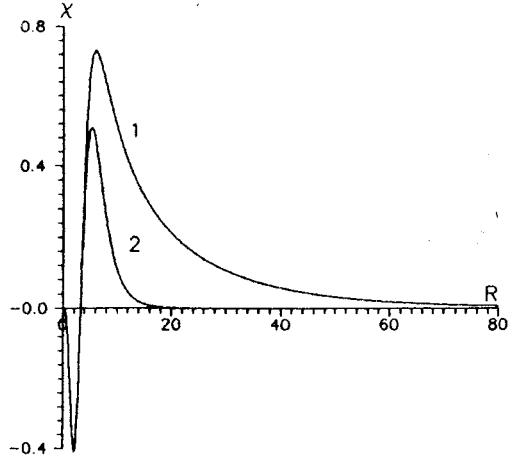


Fig. 4. The radial wave functions 1 — $\chi_1^{(1)}$ and 2 — $\chi_2^{(1)}$ of the bound state ($J = 1$, $v = 1$) of the $dt\mu$-mesic molecule

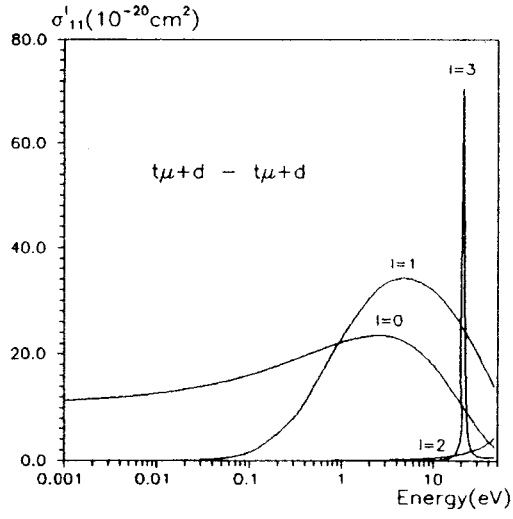


Fig. 5. Partial eleastic scattering cross sections of $t\mu$-atoms on deuterium nuclei

using corresponding value of M. Our results of calculating partial (σ^J_{11}) and total (σ_{11}) elastic scattering cross sections of $t\mu$ - atoms on deuterium nuclei d (see figs.5,6) agree with other multichannel calculations [6] and reproduce the known form resonance for $J = 3$ and $E \approx 21$ eV. The radial wave functions $\chi^{(1)}_1$, $\chi^{(1)}_2$ and $\chi^{(2)}_1$, $\chi^{(2)}_2$ corresponding to the reactions

$$(t\mu)_1 s + d \to (t\mu)_{1s} + d$$

and

$$(d\mu)_{1s} + t \to d + (t\mu)_{1s}$$

are presented in figs.7—8.

A natural generalization of effective mass as a variable parameter appeared in the new effective two level approximation when we take into account non-adiabatic corrections truly. We have obtained them by means of a canonical operator transformation $T = T(R, d/dR)$. This transformation excludes nondiagonal terms in the right-hand side of the equation (2), including the operator terms $2Q(R)\, d/dR$. Thus, the above transformation

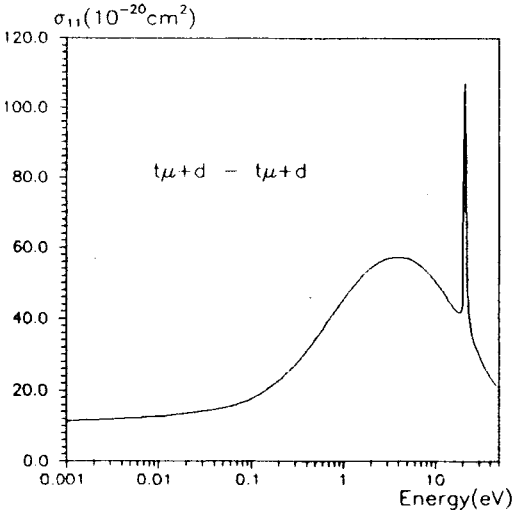


Fig. 6. Total eleastic scattering cross sections of $t\mu$-atoms on deuterium nuclei

Fig. 7. The radial wave functions 1 — $\psi_1^{(1)}$ and 2 — $\psi_2^{(1)}$ for the $l = 0$ corresponding to the scattering process $(t\mu) + d$ with two open channels at the collision energy $E = 0.3$ eV (above the second threshold)

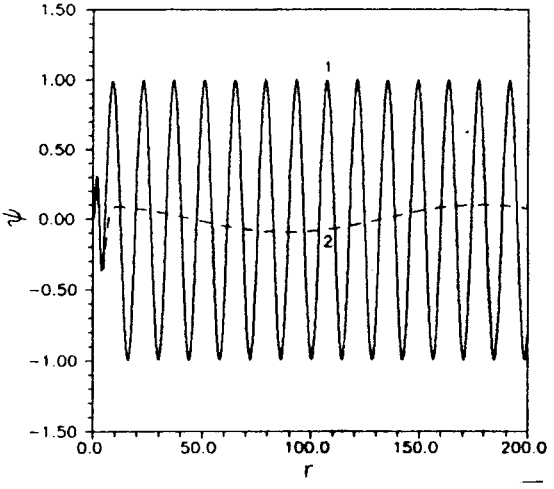
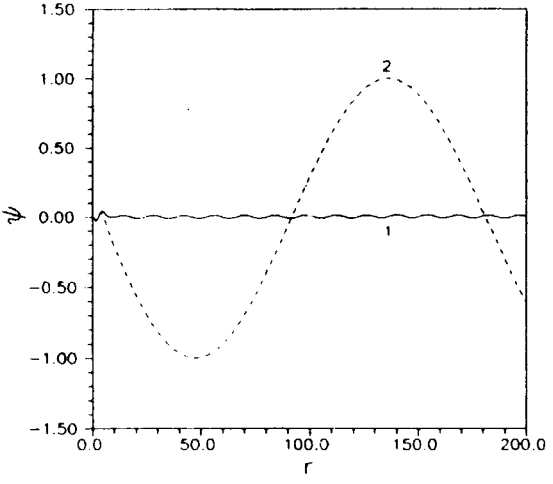


Fig. 8. The radial wave functions 1 — $\psi_1^{(2)}$ and 2 — $\psi_2^{(2)}$ for the $l = 0$ corresponding to the scattering process $(d\mu) + t$ with two open channels at the same collision energy $E = 0.3$ eV



is the generalization of the known Best Adiabatic Approximation [7]. Finally we have obtained the new system of equations

$$\{\delta M\mu^{-1}(R)\frac{d^2}{dR^2} - \delta M[2\tilde{Q}(R, M)\frac{d}{dR} + \tilde{V}(R, M)] + \tilde{p}^2\}\chi(R, \tilde{p}) = 0. \quad (3)$$

Here $\tilde{p} = 2M\varepsilon$ is the matrix of channel momenta,

$$\tilde{Q}(R, M) = Q(R) + (2M)^{-1}\Delta Q(R),$$

$$\tilde{V}(R, M) = V(R, M) + (2M)^{-1}\Delta V(R)$$

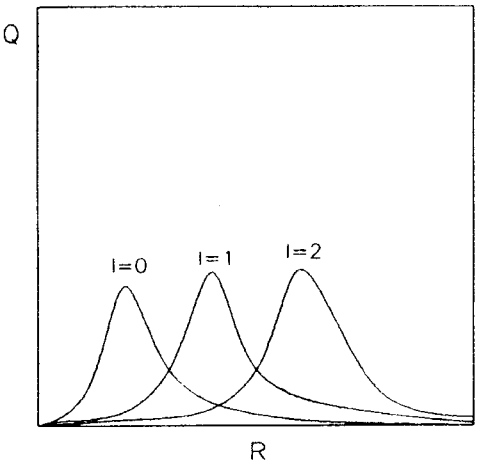


Fig. 9. The behaviour of the matrix elements $Q(R)$ relating to continuous spectrum

are the new potentials;

$$\mu^{-1}(R) = 1 + (2M)^{-1}\Delta\mu^{-1}(R)$$

is the new effective mass depending on R and satisfying the asymptotic condition

$$\delta M\mu^{-1}(R) \to 1 \tag{4}$$

if $R \to \infty$. Note, that $\delta M = \mathbf{M}/M$ is the matrix of corrections between the Jacobi $\mathbf{M}$ and the adiabatic M masses;

$$-\Delta\mu_{ii}^{-1}(R) = 4\sum_{j\neq i}^{\infty} Q_{ij}(R)Q_{ji}(R)(E_i(R) - E_j(R))^{-1} \tag{5}$$

are diagonal corrections to unit. The relation (5) is valid only if the sum is complete. Since in the calculations this sum has a finite number of terms, the relation (4) is not valid exactly.

On the other hand we have the approximate relation

$$\mu^{-1}(\infty) = 1 - (2M)^{-1}\frac{1}{2} \approx 0.973 \tag{6}$$

$$(2M)^{-1} \approx 0.05339 \text{ (exactly for } dd\mu).$$

If we use only the finite number of states of the continuous spectrum, then we have the following value

$$\tilde{\mu}^{-1}(\infty) = 1 - (2M)^{-1}0.28 = 0.985. \tag{7}$$

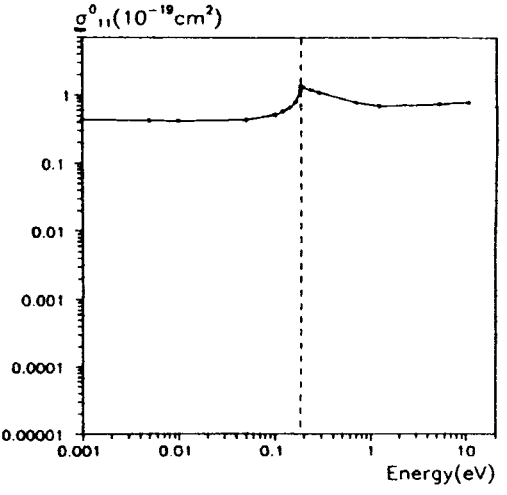
We explain this fact by the specific behaviour of the matrix elements relating to the continuous spectrum. This behaviour is schematically shown in fig.9.

Therefore if l is fixed and $R \to \infty$, the contribution of the continuous spectrum is lost in formula (6) since it is a locally incomplete set.

As a result we have

$$|(\mu^{-1}(\infty) - \tilde{\mu}^{-1}(\infty))/\mu^{-1}(\infty)| \approx 1\%.$$

Fig. 10. The cross section σ^0_{11} $(10^{-19}$ cm$^2)$ for reaction $p\mu\ (F = 0) + p \to p\mu\ (F' = 0) + p, s = 1/2$



The relative difference between variational and adiabatic results is also about 1% for both $dd\mu$ and $dt\mu$ weakly bound states.

The simplest variant of the proposed approach consists in using the relation (4) on whole interval $0 \le R < \infty$.

Then we obtain a two level approximation

$$\{\frac{d^2}{dR^2} - \delta M\ [2Q(R)\frac{d}{dR} + V(R, M)] + \tilde{p}^2\}\ \chi(R, \tilde{p}) + 0, \tag{8}$$

where δM is a variable parameter.

Note that we can find this parameter with a fit of the discrete spectrum and then use the equation (8) for the calculation of the cross sections of mesic atoms.

We have considered the more complicated case for using the new effective mass. We have calculated the cross section of the scattering process

$$p\mu\ (\uparrow\downarrow) + p \to p\mu\ \ (\uparrow\downarrow) + p$$

and obtained the true treshold behaviour as on fig.10. For this example in fig.11, 12 we demonstrate also the corresponding behaviour of the new effective mass and the potential from the eq.(3).

We intend now to solve the inverse spectral problem in two-level adiabatic approximation

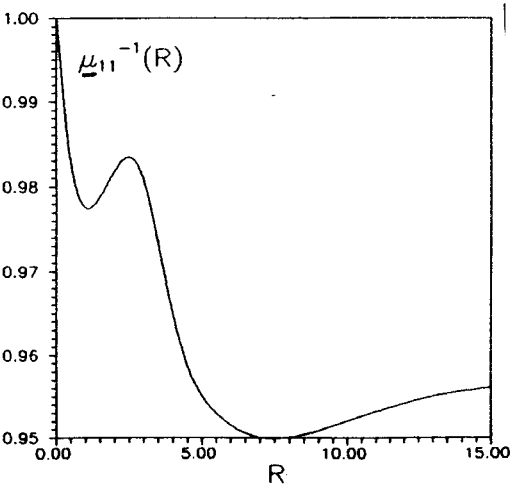


Fig. 11. The effective mass μ^{-1} (R) of the mesic molecul $pp\mu$ for $J = 0$

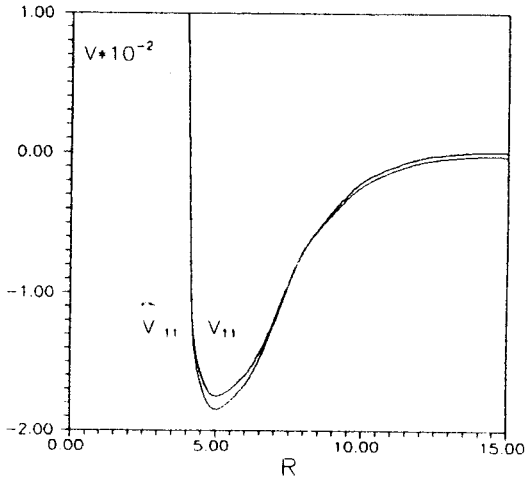


Fig. 12. The effective $\tilde{V}$ and adiabatic V potentials of the mesic molecule $pp\mu$, $J = 0$

for the investigation of the new effective masses of muonic systems.

References

1. Ponomarev L.I., Fiorentini G. — Muon Catalysed Fusion, 1987, 1, p.3.
2. Puzynin I.V., Vinitsky S.I. — Muon Catalysed Fusion, 1988, 3, p.307.
3. Korobov V.I., Puzynin I.V., Vinitsky S.I. — Muon Catalysed Fusion, 1992, 7, p.63.
4. Vinitsky S.I., Ponomarev L.I. — Sov. J. Part. Nucl., 1982, 13, p.557.
5. Ponomarev L.I., Puzynin I.V., Puzynina T.P. — JINR Report P4-8884, Dubna, 1975; J. Comp. Phys., 1976, 22, p.25.
6. Chiccoli C. et al. — IFNFN/BE-91/09 Bologna, 1991.
7. CVohen J.S., Struensee M.S. — Phys. Rev., 1991, A 41(7), p.3460.

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