Formation of *dt*μ mesic molecules via subthreshold resonances

Yu. V. Petrov and V. Yu. Petrov

B. P. Konstantinov Leningrad Institute of Nuclear Physics, Academy of Sciences of the USSR

(Submitted 14 November 1990)
Zh. Eksp. Teor. Fiz. **100**, 56–74 (July 1991)

A mechanism for the formation of mesic molecules via negative subthreshold resonances is described. At low temperatures and densities, the formation of the $dt\mu$ mesic molecule results primarily from a transition of the D_2 molecule into a mesic-molecule complex with rotational and vibrational quantum numbers $K = 0 \to 1$, $v = 0 \to 2$. The transition matrix elements are calculated without recourse to the standard dipole approximation. The theoretical value of the reduced probability for the formation of the molecule, $\lambda_{dt\mu-d}$, agrees within the errors with the measured values.

1. RESONANCE MECHANISM FOR THE FORMATION OF MESIC MOLECULES

1. The early history of research on nonresonant processes involving mesic molecules has been reviewed by Zel'dovich and Gershteĭn.[1] The resonance mechanism for the formation of $dd\mu$ mesic molecules was proposed in 1967 by Vesman in an effort to find a qualitative explanation for the strong temperature dependence of the rate of this process, which had been observed previously by Dzhelepov *et al.*[2] That mechanism can be outlined as follows:[3] If a mesic molecule (more precisely, a mesic-molecule ion, MMI) has a weakly bound excited state with a negative energy ε_{Jv} (J and v are the rotational and vibrational quantum numbers of the mesic molecule), the mesic atom $(d\mu^-)$ can form a mesic-molecule complex (MMC) in a collision with a D_2 molecule, in the reaction

$$(\mathrm{D}\mu)_F+(\mathrm{D}_2)_{\nu_i\ \ i}\to[(dd\mu)_S{}^{Jv}dee]_{\nu_f\ \ f}, \tag{1.1}$$

in which the MMI $(dd\mu^-)^+$ replaces one of the d nuclei. The excess energy of the negative level of the MMI is expended on exciting vibrational (ν_f) and rotational (K_f) levels of the complex.

The cross section for the resonant formation of a complex can be written in terms of the entrance width[4,5] $\Gamma_e(F,\ \nu_i,\ K_i\to S,\ \nu_f,\ K_f;\ E)$ as follows ($\hbar = e = m_e = 1$):

$$\sigma_{F,\nu_i,K_i\to S,\nu_f,K_f}(E)=\frac{2\pi^2}{p^2}\Gamma_e(F,\nu_i,K_i\to S,\nu_f,K_f;E)\,\delta(E_i-E_f),$$

$$E_i=E+E_{\nu_iK_i}(\mathrm{D}_2)+\Delta E_F,\qquad E_F=-|\varepsilon_{Jv}|+E_{\nu_fK_f}(C)+\Delta E_S, \tag{1.2}$$

where p is the momentum of the mesic atom in the c.m. frame, $E_{\nu_iK_i}(\mathrm{D}_2)$ and $E_{\nu_fK_f}(\mathrm{C})$ are the energies of the levels of the D_2 molecule and of the complex, and ΔE_F and ΔE_S are the energies of the relativistic splitting of the mesic atom, with spin F, and of the mesic molecule, with spin S. The resonance occurs when the energy E of the incoming mesic atom is exactly equal to the energy of the resonance ($E_i = E_f$):

$$E=E_r(n)=-|\varepsilon_{Jv}|+E_{\nu_f,K_f}(\mathrm{C})-E_{\nu_i,K_i}(\mathrm{D}_2)+\Delta E_{FS}, \tag{1.3}$$

$$\Delta E_{FS}=\Delta E_S-\Delta E_F.$$

The probability for the formation of an MMC in a gas with a density $N = \Phi N_0$ ($N_0 = 4.25\cdot 10^{22}$ cm^{-3} is the density of liquid hydrogen) is found by integrating the product $N\sigma(E)v_{CM}f_m(E)$ over the energy, where v_{CM} is the velocity in the c.m. frame, and $f_m(E)$ is the Maxwellian distribution of the colliding particles. This probability, referred to a density $\Phi = 1$, is

$$\lambda^r_{dd\mu}(T)=\frac{2\pi^2}{\mu p_r}\Gamma_e(E_r)N_0\left(\frac{4E_r}{\pi T^3}\right)^{1/2}e^{-E_r/T}, \tag{1.4}$$

where μ is the reduced mass of the basic atom: $2\mu E_r = p_r^2$. Expression (1.4) leads to a characteristic temperature dependence: a sharp exponential decay of $\lambda^r_{dd\mu}$ as $T/E_r \to 0$. Some careful recent measurements of the temperature dependence by various experimental teams[6–8] have yielded results which agree well with the existing theoretical predictions[9] (except at low T).

2. The resonance formation of a $dt\mu$ mesic molecule in the reaction

$$(t\mu)_F+(\mathrm{D}_2)_{\nu_iK_i}\to[(dt\mu)_S{}^{11}dee]_{\nu_fK_f} \tag{1.5}$$

was first predicted theoretically in some pioneering calculations by Ponomarev's group, who found a weakly bound state of a mesic molecule with the same quantum numbers as those of the $dd\mu$ molecule (i.e., $J = v = 1$), but with an energy $|\varepsilon_{11}|$ several times smaller.[10] The time scale of the formation of the MMC was only $\tau_{dt\mu} = \lambda^{-1}_{dt\mu} \approx 10^{-8}$ s—much shorter than the lifetime of the muon itself ($\tau_0 = 2.2\cdot 10^{-6}$ s). Immediately after the formation of the excited mesic molecule, an Auger transition occurs to lower-lying states with $J = 0$, and then nuclear fusion occurs:

$$(\mu dt)\to{}^4\mathrm{He}+n+\mu^-. \tag{1.6}$$

In the process, the muon is liberated, and an energy $E_c = 17.6$ MeV is released. The muon is then recaptured by d and t nuclei, and the cycle in which the muon serves as catalyst occurs again. Although there is a possibility (< 1%) that a muon will stick to the helium which forms, it has time to induce $X_c \sim 100$ fusion events and to release an energy $X_cE_c \approx 2$ GeV over its lifetime τ_0 (Ref. 11). In a hybrid fusion-fission reactor, this energy could be increased by another factor of 100 (Ref. 12), so we might take another look at the question of the practical use of muon catalysis (see the review by Gershteĭn *et al.*[13]).

3. The entrance width in (1.2) can be expressed in first-order perturbation theory in terms of the transition matrix element

$$\Gamma_e(F,\nu_i,K_i\to S,\nu_f,K_f;E)=\frac{\mu p}{\pi}\,|V(E)|^2_{F,\nu_i,K_i\to S,\nu_f,K_f}. \qquad (1.7)$$

As an initial approximation, we adopt a state with a Hamiltonian H_f which describes a D_2 molecule in which one of the deuterons is replaced by an MMI.[1)] The total Hamiltonian is $H = H_f + \hat{V}$, where

$$\hat{V}=U(r_{St})+U(r_{Sd})-U(r_{S\mu})-U(r_{SC}). \qquad (1.8)$$

Here $U(r_{Si})$ is the energy of the interaction between the spectator deuteron S and the corresponding particle (Fig. 1; C is the center of mass of the MMI).

In most papers on calculations of the entrance width in (1.7), the operator $\hat{V}$ has been treated in the dipole approximation. Here we assume that the mesic molecule is much smaller than the D_2 molecule, and we expand (1.8) in the ratio of the distance between the mesic molecule and the distance to the spectator. In first order we then find $\hat{V} = \mathbf{d}\partial U/\partial\rho$, where ρ is the distance from the MMI to the spectator, and **d** is the dipole moment of the MMI. In the limit $E\to 0$, the matrix elements for the s wave in the entrance channel cease to depend on the energy of the colliding particles, and the matrix elements for the higher moments vanish. At low temperatures, the D_2 molecule is in the ground state: $\nu_i = K_i = 0$. As $T\to 0$, there is thus only one nonzero matrix element, that for the transition[10] $\nu_i = K_i = 0\to \nu_f, K_f = 1$:

$$|V(0)|^2_{F,00\to S,\nu_f1}={}^4/_3\pi d_{fi}^2 I_\nu^2, \qquad (1.9)$$

where d_{fi} is the transition dipole moment for the mesic molecule, and $I_\nu = \langle 0, 0|E|\nu_f, 1\rangle$ is the matrix element of the electric field which is acting in the complex on the MMI.

The most important values for the $dt\mu$ mesic molecule are $\nu_f = 2$ and 3, although the original estimates yielded[10] $\nu_f = 4$ and $|V|^2_{00\to 41} = 0.32\cdot 10^{-9}$ a.u. (for the time being, we will omit the subscripts S and F). After the binding energy ε_{11} was calculated more accurately,[14] the value $\nu_f = 3$ (and, possibly, $\nu_f = 2$) was found, as was the following value, according to Ref. 10: $|V|^2_{00\to 31} = 1.1\cdot 10^{-9}$ a.u. The field of the external spectator nucleus causing the transition, $\mathbf{E}_S = \boldsymbol{\rho}/\rho^3$, is screened in the MMC by the electrons. When this screening is taken into account,[16] the effect is to replace the field by $\mathbf{E} = \partial U(\rho)/\partial\rho$, where $U(\rho)$ is the molecular potential of the ${}^1\Sigma_g$ term (the Morse potential or the more accurate Kolos-Wolniewicz potential[16]). The electron

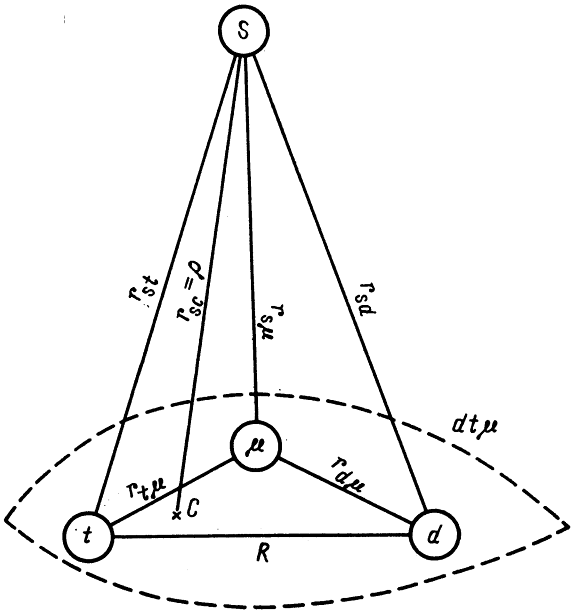

FIG. 1. System of coordinates. S—Spectator deuteron; C—center of mass of the $dt\mu$ mesic molecule.

TABLE I. Values of the matrix elements $|V|^2_{00\to\nu_f1}$ for $\nu_i = 0$, $K_i = 0\to\nu_f$, $K_f = 1$ transitions accompanied by the formation of an MMC with $E = 0$.

	ε_{11}, eV$^{(a)}$	ν_f	d_{fi}, 10^{-3} a.u. (10^3 ma.u.)	$I_{0\nu}$, 10^{-2} a.u.	$\|V\|^2_{00\to\nu_f1}$, 10^{-8} a.u.	
1	0,82	4		1,33	0,032	Vinitskiĭ *et al.*,[10] 1978
		3	0,653$^{(b)}$	2,44	0,107	
		2	(0,40)	5,21	0,485	
2	0,82 [10]	3	0,653 [10]	1,10	0,023	Cohen and Martin,[15] 1984
		2	(0,40)	1,73	0,054	
3	—	2	—	0	0	Men'skihov,[17a] 1985
4	0,601	2	3,37 (2,07)	1,77	1,49	Petrov *et al.*,[18] 1987
5	0,64	2	—	—	1,1	Men'shikov and Ponomarev,[19] 1987
6	0,64	2	—	—	1,3	Faifman *et al.*,[20] 1988
7	0,628	2	3,14 (1,93)	—	0,4—0,6	Lane,[21] 1988
8	0,660	2	—	—	0,53	Scrinzi,[22] 1989
9	0,597	2	4,21 (2,59)	1,03	0,789$^{(c)}$	Present study

Note. $^{(a)}\varepsilon_{11}$ is the binding energy of the mesic molecule for which the matrix elements were calculated. $^{(b)}$The matrix element includes a factor $(1 + \eta l_\mu/m_t)^{3/2}$, which is part of Eq. (1.8) in Ref. 10. $^{(c)}$The value $C_1 = 1.006$ (Table II) was used in the calculation of d_{fi} in place of the value $C_2 = 2^{1/2}C_a = 0.812$ which was used on lines 4–8. When C_1 is replaced by C_2, the result is $|V^2_{|00\to 21} = 0.51\times 10^{-8}$ a.u., i.e., a value close to that found by Scrinzi.[22]

TABLE II. Constants used in the calculations.

Quantity	Expression	Value (a.u.) for the $dt\mu$ mesic molecule	Value (a.u.) for the $dd\mu$ mesic molecule
μ_i	$M_d/2$	1835	1835
μ_f	$M_d(M_d+M_t+M_\mu)/(2M_d+M_t+M_\mu)$	2638	2470
μ_a	$M_d(M_t+M_\mu)/(M_d+M_t+M_\mu)$	2233	1886
μ	$2M_d(M_t+M_\mu)/(2M_d+M_t+M_\mu)$	3210	2537
β_1	μ_i/M_d	0,5	0,5
β_2	μ_a/M_d	0,6084	0,5137
β_3	μ_i/μ_f	0,6956	0,7432
$\varkappa$	$(2\mu_a\|\varepsilon_{11}\|)^{1/2}$	9,900	16,63
Ω_i	—	$1,362\cdot10^{-2}$	$1,362\cdot10^{-2}$
Ω_f	—	$1,136\cdot10^{-2}$	$1,174\cdot10^{-2}$
C_1	$2^{1/2}C_a$	1,006	0,959

screening reduces the value of I_v several fold, and it reduces the matrix element by an order of magnitude (Table I).

The $J = v = 1$ level of the mesic molecule is bound only exceedingly weakly, so the size of the mesic molecule in the state is anomalously large. Men'shikov pointed out that at large distances the $dt\mu$ mesic molecule decays into $d + (t\mu)_{1S}$, and the mesic-molecule potential can be ignored in comparison with the centrifugal potential and the binding energy in the Schrödinger equation.[17] The solution of the equation for the motion of a neutral mesic atom in the 1s ground state, with an angular momentum $J = 1$ and a negative energy ε_{11}, in the absence of a field, is

$$\Psi_{1M}(\mathbf{R})=C_1\frac{1+\varkappa R}{(2\varkappa)^{1/2}R^2}e^{-\varkappa R}Y_{1M}(\hat{R}),\qquad(1.10)$$

$$\varkappa=(2\mu_a|\varepsilon_{11}|)^{1/2},\quad \hat{R}=\mathbf{R}/R.$$

Here μ_a is the reduced mass of the MMI (Table II), and the constant C_1 is found by matching with the exact wave function. The large value $\varkappa^{-1}\approx 20$ ma.u. $= 0.1$ a.u. demonstrates that the mesic molecule is large. The exact wave function differs from the asymptotic wave function in (1.10) only at relatively small distances, $R \leqslant 5$ ma.u. It thus becomes possible to calculate d_{fi} analytically.[18] In the limit $E\to 0$, the initial wave function is $\Psi_i = 1$. A mesic atom can be assumed to be a neutral point particle, so the dipole moment is determined only by the distance from the charged deuteron to the center of mass of the MMI: $\mathbf{d} = -\beta_2\mathbf{R}$ (β_2 is given in Table II). As a result we find the following expression for d_{fi}:

$$d_{fi}=\frac{3C_1\beta_2}{\varkappa^{5/2}}=\frac{3C_1\beta_2}{(2\mu_a|\varepsilon_{11}|)^{5/4}}.\qquad(1.11)$$

The matrix element is seen to exhibit the behavior $|V|^2_{00\to21}\propto d^2_{fi}\propto|\varepsilon_{11}|^{-5/2}$.

Men'shikov[17a] showed that all the even matrix elements are zero ($I_{2n} = 0$) in the simple-harmonic-oscillator approximation for the transition $K_i = 0\to K_f = 1$ with $E = 0$. It is thus important to take the anharmonic nature of the potential in the MMC into account in I_v (Ref. 18). In calculations with a realistic Kolos-Wolniewicz potential, the anharmonicity leads to a nonzero value $\bar{I}_2 = 1.77\cdot 10^{-2}$ a.u. (the finite dimensions of the mesic molecule are being taken into account) and to the value $|V|^2_{00\to21} = 1.49\cdot 10^{-8}$ a.u. Independent calculations carried out by other authors[19,20] have yielded approximately the same values (Table I).

All the results reported above were derived in the dipole approximation. However, the size of a mesic molecule in the weakly bound state ($J = v = 1$) is $\chi^{-1} = 0.1$ a.u., i.e., not particularly small in comparison with the size of the D_2 molecule. [The vanishing of the matrix element I_2 for a dipole transition in the harmonic approximation would make the relative contribution of higher multipoles even more important (see also Sec. 3).] We would expect that the corrections to the dipole approximation would be large. Further evidence for this conclusion comes from the results found by Lane,[21] who used the $t\mu + D_2$ initial state rather than the final state as the zeroth approximation of the initial Hamiltonian (Lane also used a perturbation operator in the dipole approximation). For the entrance width Lane found a value smaller by a factor of 3, and he argued that the dipole approximation was not valid for the operator $\hat{V}$ in (1.8). Some numerical results on the matrix element $|V|^2_{00\to21}$ with $E = 0$ were recently found by Scrinzi[22] without the use of the dipole approximation. The results turned out to be close to the results of Ref. 21 (Table I). Below we use the wave function (1.10) to calculate the matrix elements $|V|^2_{0K_i\to2K_f}$ as a function of the energy, and we too will refrain from using the dipole approximation. In particular, the results found for $E\to 0$ reproduce the results of Scrinzi.[22]

Knowing the matrix element and the energy of the resonance, we can predict the probability for the formation of a $dt\mu$ mesic molecule and the temperature dependence of this probability, working from (1.4). The first experiments carried out at Los Alamos[23] showed that the value of $\lambda_{dt\mu-d}$ is indeed large (an order of magnitude larger than was predicted by the theory at the time), but it was nearly independent of the temperature (Fig. 2). On the other hand, a dependence on the gas density Φ was found,[7] although no such dependence is described by expression (1.4) (Fig. 3). It was

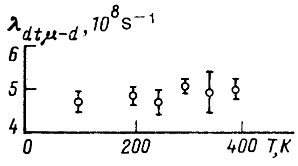

FIG. 2. Experimental temperature (T) dependence[23] of the probability for the formation of the mesic molecule, $\lambda_{dd\mu-d}$, referred to a density $\Phi = 1$. Experimental conditions: $\Phi = 0.45$–0.6 and tritium concentrations $c_t = 0.2$, 0.5, and 0.8.

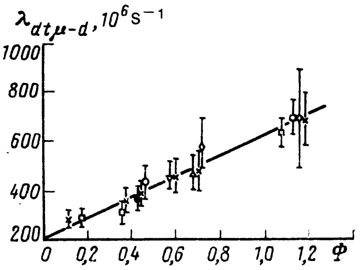

FIG. 3. Experimental density (Φ) dependence[7] of the reduced probability $\lambda_{dt\mu-d}$ for the formation of a mesic molecule in reaction (1.5) at $T < 130$ K at various tritium concentrations. ◇—$c_t = 0.3$; △—0.4; ×—0.5; ●—0.6; □—0.7; ○—0.8; ▽—0.9. The solid line is a fit of the experimental data.

thus found that the Vesman mechanism does not operate in its classical version in the case of the $dt\mu$ mesic molecule.

2. MECHANISM FOR THE FORMATION OF MESIC MOLECULES VIA SUBTHRESHOLD RESONANCES

1. Vesman's mechanism presupposes that the complex survives an infinitely long time (Fig. 4a). Actually, there are several processes which would limit this lifetime and give rise to a nonzero decay width $\Gamma_r/2$ in its wave function (Fig. 4, b–d). For this reason, the δ-function in (1.2) should be replaced by a Breit-Wigner profile.[5] Summing over the resonances, we find the total cross section for the formation of mesic molecules:

$$\sigma_{dt\mu-d}(E)=\frac{\pi}{p^2}\sum_r\frac{\Gamma_{er}\Gamma_{cr}}{(E-E_r)^2+{}^1\!/_4\Gamma_r^2}\qquad(2.1)$$

(this expression incorporates the ratio of the width Γ_{cr}, for the absorption of $t\mu$ atoms, to the total width Γ_r).

If the absorption does not seriously distort the spectrum of the $t\mu$ atoms, the contribution to the integral from the vicinity of the resonance in the course of the integration of the cross section over the spectrum will be essentially the same as Vesman's zero-width approximation, (1.4) (here $\Gamma_r \ll E_r$ is assumed). Along with $\lambda^r_{dt\mu}$, however, we find an additional contribution from low energies. At $E \ll E_r$, the denominator in (2.1) becomes independent of the energy, and for an s wave in the entrance channel [we are taking (1.7) into account] we find Bethe's $1/v_{CM}$ law for the cross section. With Γ_r, $T \ll E_r$, we thus find

$$\lambda_{dt\mu-d}=\overset{r}{\lambda}_{dt\mu-d}+\overset{0}{\lambda}_{dt\mu-d},$$
$$\overset{0}{\lambda}_{dt\mu-d}=N_0\sum|V|^2_{00\to21}\frac{\Gamma_{cr}}{E_r^2}.\qquad(2.2)$$

The term $\lambda^0_{dt\mu-d}$ is predominant at small T. It does not depend on T, while it is proportional to the decay width Γ_{cr}.

A new circumstance here is the appearance in the sum of a contribution from negative subthreshold resonances (there is no such contribution in Vesman's zero-width approximation. These resonances contribute only to $\lambda^0_{dt\mu-d}$. To explain the absence of a T dependence of λ, it is thus sufficient to assume that the reaction in which the mesic molecules are formed occurs primarily through a very small negative resonance with a decay width Γ_{cr} which is not small. This is precisely the situation which prevails in the case of the formation of $dt\mu$ mesic molecules (in contrast with $dd\mu$ molecules), and the predominant transition is $v_i = 0, K_i = 0 \to v_f = 2, K_f = 1$.

2. Let us calculate the energy of this resonance. The energy of the MMI level, ε_{11}, is the sum of the nonrelativistic value for point nuclei, $\varepsilon_{11}^{\mathrm{NR}}$, and a shift $\Delta\varepsilon_{11}^R$, which incorporates the relativistic corrections, the corrections to the Coulomb potential for the finite dimensions of the nuclei, the corrections for the polarization of vacuum and the polarizability of the deuteron, etc. A value $\varepsilon_{11}^{\mathrm{NR}} = -660.3$ meV was recently calculated by a variational method to within 0.1 meV (Refs. 24–26). The shift $\Delta\varepsilon_{11}^R$ is known only within a far greater error. This shift has changed by several millielectron volts over the past few years:[27–32]

Ref.	27	28	29	30	31	32
	32.2	18.9	29.7	29.2	28.9	26.2 meV.

The most reliable value at the moment is $\Delta\varepsilon_{11}^R = 26.2$ meV (Ref. 32).

The fine and hyperfine splitting of the levels of the mesic atom and of the MMI for the transition $F = 0 \to S = 1$ give us

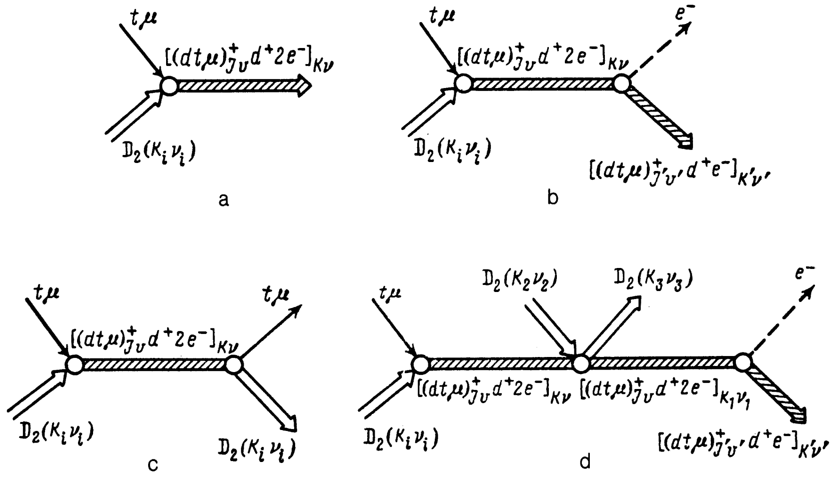

FIG. 4. Feynman diagrams of the formation and decay of a mesic-molecule complex (MMC).[5] a—Vertex corresponding to reaction (1.5); b—Auger transition of the mesic molecule; c—decay of the complex, i.e., the inverse of reaction (1.5); d—transition of the complex to a state with other quantum numbers (and also with the same quantum numbers[36,37]), as a result of collisions with surrounding molecules.

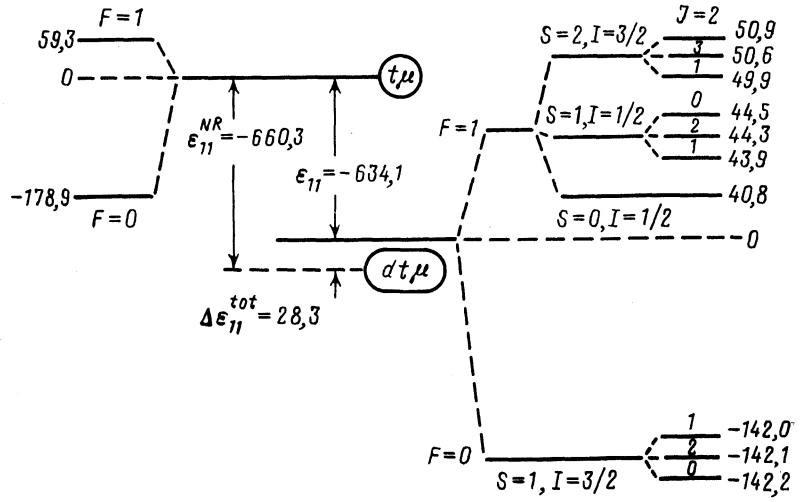

FIG. 5. Relativistic splitting of the levels of a $(t\mu)_F$ mesic atom and a $(dt\mu)_s$ mesic molecule (in millielectron volts).[13]

$\Delta\varepsilon_{FS} = 36.8$ meV (Fig. 5; Ref. 13). The mesic molecule formed in the reaction $(t\mu)_F + d \to (dt\mu)_S$ thus has a binding energy

$$\varepsilon_{11}{}^{th}=\varepsilon_{11}{}^{NR}+\Delta\varepsilon_{11}{}^{R}+\Delta\varepsilon_{01}=-597{,}3\ \text{MeV}. \qquad (2.3)$$

The energy of the excited levels of the MMC was found within 0.1 meV in Ref. 33. Taking account of the energy shift of the ground states in the MMC with respect to D_2, we find, for the transition $v = 0 \to 2$, $K = 0 \to 1$,

$$E_{2,1}(\text{C}) - E_{00}(\text{D}_2) = 584{,}2\ \text{MeV}.$$

According to (1.3), we have $\varepsilon_r^{th}(000 \to 121) = -13.1$ meV. The energy of the resonance with $v_f = 2$ and $K_f = 1$ is thus indeed very small, and it is negative.

3. The decay width Γ_r is the sum of several components: Γ_{sr}, which is the width of the inverse decay to $t\mu + D_2$ (Ref. 4); Γ_{em}, which is the width of electromagnetic transitions of the excited MMI to lower-lying states (primarily through Auger transitions);[34] Γ_f, which is the width for fusion directly from the $J = v = 1$ state;[35] and the collisional width $\Gamma_{\text{coll.}r}(\Phi)$, which reflects both inelastic collisions[5] and elastic collisions (ternary[36] and multiple[37]) of the MMC with surrounding molecules. We thus have

$$\Gamma_r=\Gamma_{sr}+\Gamma_{cr}, \quad \Gamma_{cr}=\Gamma_{em}+\Gamma_f+\Gamma_{\text{coll.}r}(\Phi). \qquad (2.4)$$

At a moderate density we have $\Gamma_{\text{coll.}r}(\Phi) \propto \Phi$. Since we have $\lambda^0_{dt\mu - d} \propto \Gamma_r / E_r^2$ according to (2.2), the reduced probability for the formation of an MMI becomes a linear function of Φ [for the actual probability—not the reduced probability—it is a nonlinear function: $\Lambda_{dt\mu - d} = \Phi\lambda_{dt\mu - d}(\Phi)$]. It thus becomes possible to find a natural explanation for the experimental density dependence.

4. As $\Phi \to 0$, the $\Gamma_{\text{coll.}r}$ component of Γ_{cr} can be ignored. For $dt\mu$, the value[38] $\Gamma_f = 2 \cdot 10^{-4}$ meV is much smaller than $\Gamma_{em} = 0.78$ meV (Ref. 39), and we have $\Gamma_{cr} = \Gamma_{em}$. The expression for $\lambda^0_{dt\mu}$ contains an additional small factor, $(4\pi^{1/2}/e)^{-1}\Gamma_{em}/E_r = 0.02$, which is not present when the resonance with the same value of E_r is at a positive energy, $T = E_r$ [see (1.4)], and Vesman's mechanism operates. Nevertheless, the value $\lambda^0_{dt\mu}$ is large enough to give us the experimental value (Sec. 4). The mechanism for the formation of mesic molecules via subthreshold resonances, when the finite width of the latter is taken into account, thus gives us a complete explanation of all the experimental facts on the $dt\mu$ mesic molecule. For the $dd\mu$ mesic molecule, the width Γ_{cr} is smaller by a factor of several thousand ($3 \cdot 10^{-4}$ meV; Ref. 9), and the resonances $K_i = 0 \to K_f = 1$ lie at a positive energy. Consequently, Vesman's resonance mechanism operates.

Since we have $pR \sim 1$ ($R = \beta_2\rho_0$, $\rho_0 = 1.4$ a.u. is the size of D_2; see Table II regarding β_2) at $E = 11$ meV, even at low values of T not only s waves but also p, d, and f waves can contribute in the entrance channel. As a result, resonances with higher values of K_f and with an energy shifted upward by an amount $B_f K_f (K_f + 1)$ ($B_f = 2.4$ meV) will form.[33] In calculating the reaction cross section we thus need to know several matrix elements for transitions $v_i = 0$, $K_i \to v_f$, K_f and their energy dependence.

3. MATRIX ELEMENTS FOR THE TRANSITION $v=0$, $K_i \to v_f$, K_f

1. As we pointed out back in Sec. 1, the $dt\mu$ mesic molecule consists primarily of a point $t\mu$ atom and a d nucleus, which interact with each other weakly. We take this circumstance into account by setting $\mathbf{r}_t = \mathbf{r}_\mu$ in the perturbation operator (1.8). Introducing coordinates as shown in Fig. 1, we find the perturbation operator[22]

$$V=U(r_{st})-U(r_{sc})=U(|\rho-\beta_2\mathbf{R}|)-U(\rho). \qquad (3.1)$$

Here ρ is the distance from the spectator deuteron to the center of mass of the MMI, $\mathbf{R}$ is the distance between the deuteron and the tritium in the $dt\mu$, and β_2 is given in Table II. In first-order perturbation theory, the transition matrix element is

$$V_{fi}= \int d^3r\, d^3R\, d^3\rho\, \Psi_i{}^*(\mathbf{r},\mathbf{R},\rho) \times[U(\rho)-U(\rho-\beta_2\mathbf{R})]\,\Psi_f(\mathbf{r},\mathbf{R},\rho). \qquad (3.2)$$

Here $\Psi_i(\mathbf{r},\ \mathbf{R}\ \rho,)$ is the initial wave function of the $t\mu$ atom and the D_2 molecule; it is given by

$$\Psi_i = \exp(i\mathbf{pX})\varphi_{1s}(\mathbf{r}_t-\mathbf{r}_\mu)\frac{\chi_0(\mathbf{r}_d-\mathbf{r}_s)}{|\mathbf{r}_d-\mathbf{r}_s|}Y_{K_i m_i}\left(\frac{\mathbf{r}_d-\mathbf{r}_s}{|\mathbf{r}_d-\mathbf{r}_s|}\right). \tag{3.3}$$

The plane wave in (3.3) describes the relative motion of the $t\mu$ atom and the D_2 molecule, with a momentum p; X is the distance between their centers of mass, given by

$$\mathbf{X} = \frac{\mathbf{r}_t M_t + \mathbf{r}_\mu M_\mu}{M_t + M_\mu} - \frac{\mathbf{r}_d + \mathbf{r}_s}{2}; \tag{3.4}$$

φ_{1s} is the wave function of the $1s$ state of the mesic atom; and χ_0 and $Y_{K_i m_i}$ are the radial and angular parts of the wave function of the D_2 molecule.

The wave function Ψ_f describes the MMC in the final state:[17]

$$\Psi_f = \Psi_{1M}(\mathbf{R})\frac{\chi_v(\rho)}{\rho}Y_{K_f m_f}(\hat{\rho})\varphi_{1s}(\mathbf{r}_t-\mathbf{r}_\mu), \quad \hat{\rho} = \boldsymbol{\rho}/\rho. \tag{3.5}$$

Here $\Psi_{1M}(\mathbf{R})$ is the wave function of the $J = v = 1$ state of the mesic molecule, and $\chi_v(\rho)$ and $Y_{K_f m_i}$ are the radial and angular parts, respectively, of the wave function of the mesic-molecule complex. We replace the wave function of the mesic molecule by its asymptotic expression (1.10). In our case, it is more legitimate to use this asymptotic expression than the wave functions which were found by numerical methods in Ref. 40 and which would appear to be more accurate. As we will see below, the matrix elements in (3.2) depend on distances out to 100 ma.u. The effect of such distances on the energy of the level of the $dt\mu$ mesic molecule is very small. The wave functions (designed for calculating the energy of the level very accurately) are thus quite different from the exact asymptotic expression in (1.9) at these distances (see also Refs. 22 and 41). The contribution from $\rho < 5$ ma.u., in contrast, where we cannot use the asymptotic expression, is no greater than 1% in the matrix element. To calculate the matrix element we thus do not need to know the behavior of the wave function at small ρ; it is sufficient to determine the coefficient C_1 in (1.10). Joining the asymptotic expression in (1.10) with the variational wave function in the intermediate region, $\rho = 10$–40 ma.u., we find the values of C_1 shown in Table II (Ref. 41).

2. We substitute the wave functions into the matrix element (3.2). The integral with the wave functions of the mesic atom, φ_{1s}, yields 1. For our purposes, it is convenient to take the remaining integral over $\mathbf{R}$ and $\boldsymbol{\rho}$ in terms of the variables $\mathbf{r}_1$ and $\mathbf{r}_2$, which are the distances from the spectator to the $dt\mu$ center of mass and to the deuteron center of mass, respectively [Fig. 1 ($\mathbf{r}_1 = \boldsymbol{\rho}$, $\mathbf{r}_2 = \boldsymbol{\rho} - \beta_2\mathbf{R}$)]:

$$V_{fi} = \frac{C_1}{2^{1/2}\varkappa\beta_2}\int d^3r_1\, d^3r_2 \exp(-i\beta_1\mathbf{r}_1\mathbf{p})\exp\left[-\frac{i\beta_3}{\beta_2}(\mathbf{r}_1-\mathbf{r}_2)\mathbf{p}\right]$$
$$\times \psi_M[\beta_2^{-1}(\mathbf{r}_1-\mathbf{r}_2)]\frac{\chi_0(r_2)}{r_2}Y^*_{K_i m_i}(\hat{r}_2)\frac{\chi_v(r_1)}{r_1}$$
$$\times Y_{K_f m_f}(\hat{r}_1)[U(r_1)-U(r_2)], \tag{3.6}$$

$[\Psi_{1M}(\mathbf{R}) \equiv C_1\psi_M(\mathbf{R})(2\varkappa)^{-1/2}]$. In (3.6) we evaluate the integrals over the angles of the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$. For this purpose we expand the difference function

$$\Phi_M = \exp\left[-\frac{\beta_3}{\beta_2}(\mathbf{r}_1-\mathbf{r}_2)\mathbf{p}\right]\psi_M[\beta_2^{-1}(\mathbf{r}_1-\mathbf{r}_2)] \tag{3.7}$$

in a series in orbital angular momenta corresponding to the angular coordinates of the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ and also the momentum $\mathbf{p}$. This expansion is (see the Appendix)

$$\Phi_M = -\frac{4\cdot 3^{1/2}\pi}{2}\beta_2^2\sum Y_{Tt}^*(\hat{p})Y^*_{l_1m_1}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2)$$
$$\times \mathscr{R}_{Tj}^{l_1l_2}(r_1,r_2)\,i^T(-1)^{m_2+m_l}$$
$$\times(2j+1)[(2l_1+1)(2l_2+1)(2T+1)]^{1/2}$$
$$\times\begin{pmatrix} l_1 & T & j \\ m_1 & t & -m_j\end{pmatrix}\begin{pmatrix} 1 & l_2 & j \\ M & -m_2 & m_j\end{pmatrix} \tag{3.8}$$

The summation is to be understood here over all possible angular momenta l_1, l_2, T, and j and their projections m_1, m_2, t, and m_j. The function $\mathscr{R}$, introduced in the Appendix, depends on the magnitudes of the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ (and also on the magnitude of the momentum, p), but it does not depend on the orientations of these vectors. It is also independent of the angular-momentum projections m_1, m_2, t, and m_j, depending on only the values of these angular momenta themselves. The function $\mathscr{R}$ can be expressed in terms of modified spherical Bessel functions.

We now substitute expansion (3.8) into expression (3.6) for the matrix element V, and we evaluate the integrals over the orientations of $\mathbf{r}_1$ and $\mathbf{r}_2$. We can do this by expanding the plane wave in a series in angular momenta:

$$\exp(-i\beta_1\mathbf{pr}_1) = 4\pi\sum Y_{Lm}(\hat{p})i^{-L}Y^*_{Lm}(\hat{r}_1)j_L(\beta_1 pr_1), \tag{3.9}$$

where j_L is the spherical Bessel function. The integral over the angles $\hat{r}_2$ equates l_2 to the initial angular momentum K_i, while the integral over $\hat{r}_1$ reduces to an integral of three spherical harmonics. Also adding the angular momenta $\mathbf{L}$ and $\mathbf{T}$ to the total angular momentum Λ, we finally find

$$V_{fi} = \frac{4\pi}{3^{1/2}}d_{fi}\sum Y_{\Lambda m_\Lambda}(\hat{p})\begin{pmatrix} 1 & K_i & j \\ M & -m_i & m_j\end{pmatrix}$$
$$\times\begin{pmatrix} \Lambda & T & L \\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} K_f & j & \Lambda \\ -m_f & m_j & m_\Lambda\end{pmatrix}$$
$$\times\begin{pmatrix} K_f & L & l \\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix} K_f & j & \Lambda \\ T & L & l\end{Bmatrix} i^{K_f+L-l-\Lambda}\cdot(-1)^{j+m_f+m_i+1}$$
$$\times(2j+1)(2l+1)(2T+1)$$
$$\times(2L+1)[(2K_i+1)(2K_f+1)(2\Lambda+1)]^{1/2}B_{jT,L}^{lK_i}, \tag{3.10}$$

$$B_{jT,L}^{l_1l_2} = \int_0^\infty dr_1\, r_1\int_0^\infty dr_2\, r_2\chi_v(r_1)\chi_0(r_2)[U(r_1)-U(r_2)]$$
$$\times\mathscr{R}_{jT}^{l_1l_2}(r_1,r_2)j_L(\beta_1 pr_1) \tag{3.11}$$

($l_1 \equiv l$). Here d_{fi} is the transition dipole moment calculated with the wave function (3.5) [see (1.11)].

We are interested in the square of the matrix element, summed over all the final projections of the angular momenta (m_f, M, m_j) and averaged over the initial projections:

$$|V|^2_{K_i\to K_f}=\frac{1}{2K_i+1}\sum_m |V_{fi}|^2. \tag{3.12}$$

Substituting (3.10) in here, we finally find

$$|V|^2_{K_i\to K_f}=\frac{4\pi}{3}d^2_{fi}\sum_{\Lambda,j}(2K_f+1)(2j+1)(2\Lambda+1)|A^{\Lambda j}_{K_iK_f}|^2,$$

$$A^{\Lambda j}_{K_iK_f}=\sum_{T,L,l}(2T+1)(2L+1)(2l+1)i^{L-l}.$$

$$\times\begin{pmatrix}\Lambda & T & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}K_f & L & l\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}K_f & j & \Lambda\\ T & L & l\end{Bmatrix}B^{lK_i}_{jT,L}. \tag{3.13}$$

As shown in the Appendix, series (3.13) is a power series in the quantity

$$\delta=\beta_2 p/\varkappa=1,1(E[\mathrm{eV}])^{1/2}. \tag{3.14}$$

At small values of δ we have $B^{lK_i}_{jT,L}\propto\delta^T$. The quantity δ plays the role of the parameter kR for a mesic molecule (its size is $\sim\varkappa^{-1}$). In contrast with kR for the D_2 molecule (Sec. 1), this parameter reaches a value on the order of unity only at $E = 1$ eV. For $\delta\ll 1$, we can restrict the series in T in (3.14) to a few terms (in actuality, the calculations were carried out with terms $\sim\delta^2$; at an energy $E\leqslant 10$ meV, for example, this approach corresponds to an error of order 1%). With these values of K_i and K_f, the summation over the other angular momenta in (3.14) is then restricted to a few terms.

Expression (3.13) for the matrix element simplifies dramatically in the case $E = 0$. In this case, K_i may differ from K_f only by unity. For the matrix element for the transition $K_i = 0\to K_f = 1$ we find (1.9):

$$|V|^2_{0\to1}={}^4/_3\pi d_{fi}{}^2\bar I^2_{0,\nu_f},$$

where

$$\bar I_{0,\nu_f}=\gamma^4\int_0^\infty dr_1\int_0^\infty dr_2[U(r_1)-U(r_2)]\chi_\nu(r_1)\chi_0(r_2)$$

$$\times[\theta(r_1-r_2)k_1(\gamma r_1)i_0(\gamma r_2)$$

$$+\theta(r_2-r_1)i_1(\gamma r_1)k_0(\gamma r_2)], \tag{3.15}$$

k_l and i_l are spherical Bessel functions, introduced in the Appendix, and $\gamma = \varkappa/\beta_2$. Distances $r\sim 1$ a.u. are important in the integral, so we have $\gamma r\gg 1$. Ignoring the exponentially small terms in (3.15), and introducing the variables $\rho = r_1$, $x = (r_1 - r_2)/\beta_2$, we finally find

$$\bar I_{0,\nu_f}=\frac{1}{2\beta\varkappa^2}\int_{-\infty}^{\infty}dx\int_0^\infty d\rho\exp(-\varkappa|x|)[U(\rho)-U(\rho-\beta_2x)]$$

$$\times\chi_{\nu_f}(\rho)\chi_0(\rho-\beta_2x)\left(\operatorname{sign}x+\frac{\beta_2}{\varkappa\rho}\right). \tag{3.16}$$

3. Expression (3.16) can be used to find an accurate result, which can then be compared with the dipole approximation in Refs. 17 and 20. In the estimates for χ_ν we can use the harmonic approximation (since the mass of the μ_f nuclei is large). Relatively large distances $z = \rho - \rho_0$ contribute to the matrix element $\bar I_{0\nu}$ during the formation of both $dt\mu$ and $dd\mu$ (although they contribute for different reasons in these two cases). For the even transition $\nu = 0\to 2$ ($dt\mu$), the region in which the potential differs from a harmonic potential is important in $\bar I_{0\nu}$. This region is at large z. For the case of odd but large ν_f ($\nu_f = 7$ in the case of the formation of $dd\mu$), the final wave function oscillates markedly, "cutting up" the integral in the region $z<\nu_f(M_f\Omega_f)^{1/2}$ (Ω_f is the oscillation frequency). In both cases, the correction coming after the dipole correction in the expansion of the potential should be important.

The potential in (3.16) falls off exponentially at distances $\alpha_M^{-1}\approx 1$ a.u., and the product $\chi_0\chi_\nu$ falls off exponentially at distances $\sim(M_f\Omega_f)^{-1/2}\approx 0.2$ a.u. The integrand is thus truncated by $\chi_0\chi_\nu$. The correction in the argument of $\chi_0(z-\beta_2x)$ for the circumstance that the mesic molecule is not of point size is $\xi\approx\beta_2(M_f\Omega_f)^{1/2}\varkappa^{-1}\approx 0.34<1$ in order of magnitude, and the expansion in ξ converges. One should bear in mind here that the factor $\overline{x^n} = n!$ slows down the conversions. The first nonvanishing term in the expansion of I_{02} in $\beta_2/\varkappa$ (this is the dipole approximation) gives us $I^{(1)}_{02} = -1.73$ a.u. (Ref. 18). The next correction is, after an integration over x,

$$\Delta I^{(2)}_{02}=\frac{\beta_2{}^2}{\varkappa^2}\left\langle\nu_f\left|\frac{\partial^3U}{\partial\rho^3}+3\frac{\partial^2U}{\partial\rho^2}\frac{\partial}{\partial\rho}-\frac{2}{\rho_0}\frac{\partial U}{\partial\rho}\frac{\partial}{\partial\rho}\right.\right.$$

$$\left.\left.-\frac{1}{\rho_0}\frac{\partial^2U}{\partial\rho^2}\right|0\right\rangle. \tag{3.17}$$

In the anharmonic approximation, (3.17) is dominated by the second term:

$$\Delta I^{(2)}_{02}\approx\frac{3\beta_2{}^2}{\varkappa^2}\left\langle\nu_f\left|\frac{\partial^2U}{\partial\rho^2}\frac{\partial}{\partial\rho}\right|0\right\rangle\approx\frac{9}{2^{1/2}}\xi^2\Omega_f=0{,}88\cdot10^{-2}\ \text{a.u.} \tag{3.18}$$

Since $I^{(1)}_{02}$ and $\Delta I^{(2)}_{02}$ have opposite signs, the correction is significant. When the wave functions of the more accurate Kolos-Wolniewicz potential are used [without an expansion of $\chi_0(\rho-\beta_2x)$], we find $\bar I^{(1)}_{02}+\Delta\bar I^{(2)}_{02} = -0.85\cdot10^{-2}$ a.u. This value is closer to the exact value, $\bar I_{02} = -1.03$ a.u.

For the formation of $dd\mu$, expression (3.16) with the

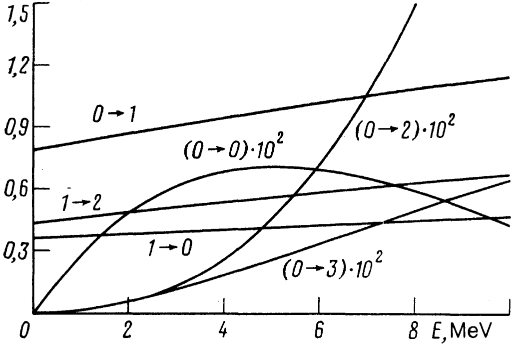

FIG. 6. The matrix elements $|V|^2_{K_i\to K_f}$ for the transition $\nu = 0\to2$ versus the energy E (c.m.) for reaction (1.5).

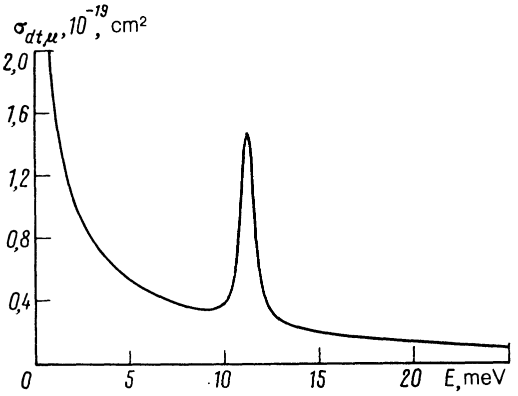

FIG. 7. The cross section $\sigma_{dt\mu-d}$ for the formation of an MMC versus the energy E [$\varepsilon_r(K=0\to 1) = -13.1$ meV].

parameter values in Table II yields $\bar{I}_{07} = -2.77\cdot 10^{-3}$ a.u. The dipole approximation leads to $I_{07}^{(1)} = -3.45\cdot 10^{-3}$ a.u., i.e., to a value 1.55 times $|V|^2_{00\to 71}$.

4. At low energies, only the $\nu = 0\to 2$, $K_i = 0\to K_f = 0$, 1, 2, 3 and $K_i = 1\to K_f = 0.2$ transitions are important. Figure 6 shows the energy dependence of the matrix elements for these transitions as calculated from (3.16). As expected, the matrix element of the $K = 0\to 1$ transition dominates for $E \ll 10$ meV. This matrix element is larger than the others by a factor of hundreds.[18,42]

4. CROSS SECTION AND PROBABILITY FOR THE REACTION AT SMALL *T* AND Φ

1. Using the calculated matrix elements, we can determine the energy dependence of the cross section for reaction (1.5) for $\nu = 0\to 2$ transitions (Fig. 7):

$$\sigma_{dt\mu}(E) = \frac{1}{v_{CM}} \times \sum_{K_i K_f} W(K_i)|V|^2_{0K_i\to 2K_f}\cdot \frac{\Gamma_{cr}}{(E-\varepsilon_{r,K_i,K_f})^2 + \Gamma^2_{r,K_f}/4}. \tag{4.1}$$

Here $W(K_i)$ is the population of the levels of the D_2 molecule at the given temperature. For the equilibrium populations of ortho- and para-deuterium we have[43]

$$W(K_i) = \frac{1}{Z_{rot}}\eta(K_i)(2K_i+1)\exp(-\varepsilon_i/T), \tag{4.2}$$

where

$$Z_{rot} = \sum \eta(K_i)(2K_i+1)\exp(-\varepsilon_i/T), \quad \varepsilon_i \approx B_i K_i(K_i+1),$$

$$\eta(K_i) = \begin{cases} 2/3, & K_i = 0, 2, \ldots \\ 1/3, & K_i = 1, 3, \ldots \end{cases}.$$

The total width of the inverse decay to various initial states k enters the total width Γ_r, K_f in (4.1) (Refs. 17, 18, and 20):

$$\Gamma_{s,K_f} = \sum_k \frac{2\mu p_k}{\pi}\eta(K_k)|V|^2_{K_f\to K_k} = 0{,}854\cdot 10^6\left[\frac{\text{eV}}{\text{a.u.}}\right]\cdot \times \sum_k \eta(K_k)|V|^2_{K_f\to K_k}(E[\text{eV}])^{1/2}. \tag{4.3}$$

The following relation holds between the matrix elements for the forward and inverse transitions:

$$|V|^2_{K_f\to K_k} = \frac{2K_k+1}{(2K_f+1)(2J+1)}|V|^2_{K_k\to K_f}. \tag{4.4}$$

The simplest case in which to make a comparison with experiment is at low densities ($\Gamma_{\text{coll},K_f} \ll \Gamma_{\text{em}}$) and low temperatures ($T \ll 11$ meV). At $T = 23$ K (2 meV), for example, only 3.6% of the levels of the D_2 molecule with $K_i = 1$ are populated. At such temperatures, we can also ignore the inverse decay ($\Gamma_{s,K_f} \ll \Gamma_{\text{em}}$). The total cross section for the formation of mesic molecules is shown in Fig. 7 for the theoretical value $\varepsilon_{r01} = -13.1$ meV of the energy of the principal subthreshold resonance, for the transition $K = 0\to 1$ (Sec. 2). This cross section has a resonance peak for the $0\to 3$ transition at $\varepsilon_{r03} = 11$ meV. However, this cross section is determined primarily by the subthreshold resonance of the $K = 0\to 1$ transition.

The transition probability with cross section (4.1), referred to a density $\Phi = 1$, is

$$\lambda_{dt\mu-d} = N_0 \int f(E)\sigma_{dt\mu-d}(E)v_{CM}dE, \tag{4.5}$$

where $f(E)$ is the spectrum of the $t\mu$ atoms. This spectrum may differ from an equilibrium Maxwellian spectrum because of the strong absorption at low velocities and also because of the contribution of slowing $t\mu$ atoms. If $\sigma_{dt\mu-d} \propto v_{CM}^{-1}$, however, the product $\sigma_{dt\mu-d}v_{CM}$ will be independent of the energy and can be taken through the integral sign. We then have $\int f(E)dE = 1$ by virtue of the normalization (if we ignore the formation of $dt\mu$ during the slowing of the $t\mu$). Incorporating the decay of the muon changes only the normalization. At $T = 2$ meV, and with a Maxwellian spectrum, we have $\lambda_{dt\mu-d} = 2.2\cdot 10^8$ s^{-1}. As expected, the transition $K = 0\to 1$ dominates (Table III). Its matrix ele-

TABLE III. The energies $\varepsilon_{K_iK_f}$ and the contribution to $\lambda_{dt\mu-d}$ of the various transitions $K_i\to K_f(\nu = 0\to 2)$ at $T = 2$ meV.

K_f	$K_i = 0$, $W = 0{,}964$		$K_i = 1$, $W = 0{,}036$	
	$\varepsilon_{K_iK_f}$, MeV	$\lambda_{dt\mu-d}(K_i\to K_f)$, s^{-1}	$\varepsilon_{K_iK_f}$, MeV	$\lambda_{dt\mu-d}(K_i\to K_f)$, s^{-1}
0	—17,9	$5{,}85\cdot 10^5$	—25,3	$2{,}75\cdot 10^7$
1	—13,1	$1{,}99\cdot 10^8$	—20,5	—
2	—3,4	$1{,}93\cdot 10^6$	—10,8	$1{,}54\cdot 10^8$
3	11,2	$1{,}70\cdot 10^7$	3,2	—
4	30,5	—	23,1	—
$\sum_{K_f}\lambda^{0\to K_f}_{dt\mu-d}$		$2{,}19\cdot 10^8$	$\sum_{K_f}\lambda^{1\to K_f}_{dt\mu-d}$	$1{,}82\cdot 10^8$

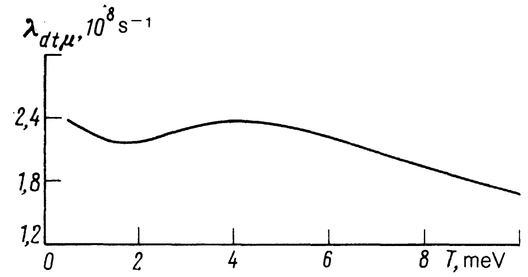

FIG. 8. Theoretical temperature (T) dependence of the probability $\lambda_{dt\mu-d}$, for the formation of an MMC [$\varepsilon_r(K=0\rightarrow 1) = -13.1$ meV, $\Phi < 0.1$].

ment increases slightly with the energy (Fig. 6). The effect of the spectrum of the $t\mu$ atoms thus cannot be important. The small contribution (8%) from the positive resonance for the $K = 0\rightarrow 3$ transition decreases when we allow for the erosion of the spectrum of $t\mu$ atoms.

2. At small values of T, the calculated value of $\lambda_{dt\mu-d}$ is nearly independent of the temperature (Fig. 8), in total agreement with the experimental results (Fig. 2). For a quantitative comparison, we need to know the experimental value of $\lambda^{\text{exp}}_{dt\mu-d}$ at low densities. A linear extrapolation of the data of the Los Alamos group to $\Phi\rightarrow 0$ (Fig. 3) yields $\lambda^{\text{exp}}_{dt\mu-d} = 2.1\cdot 10^8$ s^{-1}, which is close to the theoretical value. However, measurements by another experimental group, at Villingen (Switzerland; see the review in Ref. 44) show that at $\Phi < 0.1$ the cycle time decreases nonlinearly, and at $\Phi = 0.03$ the value of $\lambda^{\text{exp}}_{dt\mu-d}$ is $1.3\cdot 10^8$ s^{-1} (Ref. 45). In order to reach this value, we would have to shift the energies of all the resonances several millielectron volts downward. A final refinement of the positions of the resonances would require more-detailed measurements at small values of T and Φ.

5. CONCLUSION

The theory predicts (and the experiments confirm) that the $dt\mu$ mesic molecule in reaction (1.5) form at low temperatures primarily by virtue of the subthreshold resonance with the transition $v = 0\rightarrow 2$, $K = 0\rightarrow 1$. Although the individual features of Vesman's mechanism are preserved here (the energy expenditure of the excitation of vibrational and rotational levels of the complex), this mechanism cannot be regarded as a resonance mechanism, since with a positive energy the $t\mu$ atom could not reach a resonance with a negative energy. The formation cross section is probably of a near-resonant nature, since it is due to the Breit-Wigner limb of the negative resonance which arises from the finite lifetime of the MMC.[5] The mechanism of subthreshold resonances makes the temperature and density dependence of the $dt\mu$ formation probability totally different from that for $dd\mu$, in which case the classic Vesman resonance mechanism operates.

In this paper we have calculated the probability for the formation of the $dt\mu$ mesic molecule without making use of any adjustable parameters. The calculations have been greatly simplified by the circumstance that we do not need to know the exact wave function of the mesic molecule. It is sufficient to know simply two numbers: the constant C_1 in the asymptotic behavior and the exact energy ε_{11} of the weakly bound state. The transition matrix elements were determined without invoking the dipole approximation for the interaction of the mesic molecule with the field of surrounding particles. It turns out that the dipole approximation increases the probability for the formation of the $dt\mu$ mesic molecule by a factor of nearly 3, and that for the $dd\mu$ molecule by a factor of 1.6.

The theoretical binding energy of the $dt\mu$ mesic molecule in the $S=J=v=1$ state is $\varepsilon^{th}_{11} + \Delta\varepsilon_{01} = -597.3$ meV [see (2.3)] and is presently known to within a few millielectron volts. This error is determined primarily by the error in the calculation of the various relativistic and other corrections (see Subsection 2.2). The experimental value of $\varepsilon^{\text{exp}}_{11}$ agrees with the theoretical value and is known to within approximately the same error, because there are no reliable data on $\lambda_{dt\mu-d}$ at low densities and temperatures. Consequently, the progress which has been achieved toward an understanding of the process by which mesic molecules form and progress in computational methods since the pioneering work by Vesman, back in 1967, has made it possible to improve the accuracy in the determination of ε_{11} by a factor of thousands.

We wish to thank S. S. Gershteĭn, I. I. Gurevich, and especially L. I. Ponomarev for interest in this work and for useful comments. We are also indebted to E. A. G. Armor, D. D. Bakalov, J. S. Cohen, L. I. Men'shikov, M. Leon, M. Rafelski, A. Scrinzi, M. P. Faĭfman, D. Harley, and A. I. Shlyakhter for a useful discussion of individual questions.

APPENDIX. EXPANSION OF THE WAVE FUNCTION OF THE MESIC MOLECULE IN ANGULAR MOMENTA

Let us expand the wave function of a mesic molecule in orbital angular momenta. Doing so brings out the angular dependence of this wave function. For this purpose we will use a Fourier representation of this wave function. This representation is ($\beta_2\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2$)

$$\psi_M(\beta_2^{-1}(\mathbf{r}_1-\mathbf{r}_2))$$
$$=\frac{1+\varkappa R}{r^2}e^{-\varkappa R}Y_{1,M}(\hat{R})$$
$$=\int\frac{d^3k}{(2\pi)^3}\frac{4\pi ik}{k^2+\gamma^2}Y_{1M}(\hat{k})\exp[-i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)] \qquad \text{(A1)}$$

(for brevity, we will use $\gamma = \varkappa/\beta_2$). This is a convenient expression in that it allows us to use an expansion of the plane wave in spherical waves (3.9). We then find

$$\psi_M(\beta_2^{-1}(\mathbf{r}_1-\mathbf{r}_2))=8i\sum i^{l_1-l_2}Y^{\bullet}_{l_1m_1}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2)\Omega_{l_1l_2}D_{l_1l_2}. \qquad \text{(A2)}$$

Here the summation is to be understood over the angular momenta l_1 and l_2 and their projections m_1 and m_2, and $\Omega_{l_1l_2}$ is the angular integral

$$\Omega_{l_1l_2}=\int do_k\,Y^{\bullet}_{l_2m_2}(\hat{k})Y_{l_1m_1}(\hat{k})Y_{1M}(\hat{k})=(-1)^{m_2}i^{l_1-l_2+1}$$
$$\times\begin{pmatrix} l_2 & l_1 & 1\\ -m_2 & m_1 & M\end{pmatrix}\begin{pmatrix} l_2 & l_1 & 1\\ 0 & 0 & 0\end{pmatrix}\left[\frac{3(2l_1+1)(2l_2+1)}{4\pi}\right]^{1/2}. \qquad \text{(A3)}$$

The radial part of the integral over k is

$$D_{l_1l_2}=(-1)^{l_1+l_2}\int\limits_0^{\infty}dk\,\frac{k^3}{\gamma^2+k^2}\,\frac{r^{l_1+l_2}}{k^{l_1+l_2}}\left(\frac{1}{r_1}\,\frac{d}{dr_1}\right)^{l_1}\left(\frac{1}{r_2}\,\frac{d}{dr_2}\right)^{l_2}$$

$$\times\frac{\sin kr_1}{kr_1}\,\frac{\sin kr_2}{kr_2}. \qquad \text{(A4)}$$

We extend the integral to minus infinity (making use of the even parity of the integrand) and evaluate it in terms of its poles. As a result we find

$$D_{l_1l_2}={}^1/_2\pi\gamma^2P_{l_1l_2}(\gamma r_1,\ \gamma r_2),$$

where

$$P_{l_1l_2}(x_1,\ x_2)=[i_{l_1}(x_1)k_{l_2}(x_2)\theta(x_2-x_1)+k_{l_1}(x_1)i_{l_2}(x_2)\theta(x_1-x_2)], \qquad \text{(A5)}$$

and $i_l(r)$ and $k_l(r)$ are modified spherical Bessel functions, given by

$$k_l(x)=(-x)^l\left(\frac{1}{x}\,\frac{d}{dx}\right)^l\frac{e^{-x}}{x},$$

$$i_l(x)=(-x)^l\left(\frac{1}{x}\,\frac{d}{dx}\right)^l\frac{\operatorname{sh}x}{x}. \qquad \text{(A6)}$$

Substituting (A3) and (A5) into (A2), we finally find

$$\psi_M(\beta_2^{-1}(\mathbf{r}_1-\mathbf{r}_2))=\sum\frac{2[3\pi(2l_1+1)(2l_2+1)]^{1/2}}{\gamma^2 i^{1+l_1+l_2}}(-1)^{m_2}$$

$$\times\begin{pmatrix} l_2 & l_1 & 1\\ -m_2 & m_1 & M\end{pmatrix}\begin{pmatrix} l_2 & l_1 & 1\\ 0 & 0 & 0\end{pmatrix}\ Y^{*}_{l_1m_1}(\hat{r}_1)\gamma^4P_{l_1l_2}(\gamma r_1,\gamma r_2)Y_{l_2m_2}(\hat{r}_2). \qquad \text{(A7)}$$

Similarly, we can expand the function $\Phi_M(\mathbf{r}_1-\mathbf{r}_2)$ in a series in angular momenta. To do this, we go back to (A1) and shift the integration variable: $\mathbf{k}=\mathbf{k}-\mathbf{q}$, where $\mathbf{q}=\beta_3\mathbf{p}/\beta_2$. Also using the known formula[46]

$$[(\mathbf{k}-\mathbf{q})^2+\gamma^2]^{-1}=\frac{2\pi}{kq}\sum_{Tt}Q_T\left(\frac{k^2+s^2}{2kq}\right)Y_{Tt}^{*}(\hat{q})Y_{Tt}(\hat{k}),$$

$$s^2=\gamma^2+q^2=\frac{\varkappa^2+\beta_3^2p^2}{\beta_2^2} \qquad \text{(A8)}$$

(Q_T are the Legendre polynomials of the second kind), we find the following representation of the function Φ_M:

$$\Phi_M=16\pi\sum i^{-l_1+l_2+1}Y^{*}_{l_1m_1}(\hat{r}_1)Y_{l_2m_2}(\hat{r}_2)Y_{Tt}^{*}(\hat{q})$$

$$\times\int\limits_0^{\infty}\frac{dk\,k}{q}Q_T\left(\frac{k^2+s^2}{2kq}\right)j_{l_1}(kr_1)j_{l_2}(kr_2)$$

$$\times\int do_k\,Y_{Tt}(\hat{k})Y_{l_1m_1}(\hat{k})Y^{*}_{l_2m_2}(\hat{k})$$

$$\times[kY_{1M}(\hat{k})-qY_{1M}(\hat{q})] \qquad \text{(A9)}$$

[Here we have made use of the circumstance that $kY_{1M}(\hat{k})$ is a linear function of the Cartesian coordinates of the momentum]. We now evaluate the integrals over the angles specifying the orientation of the vector **k**, and we obtain Eq. (3.8) in Sec. 3 of the test proper. In that equation, the role of the function $\mathscr{R}$ is played by the quantity

$$\mathscr{R}_{Tj}^{l_1l_2}(r_1,r_2)$$

$$=\int\limits_0^{\infty}\frac{dp\,k}{q}Q_T\left(\frac{k^2+s^2}{2kq}\right)j_{l_1}(kr_1)j_{l_2}(kr_2)\left[\begin{pmatrix} l_1 & T & j\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} 1 & l_2 & j\\ 0 & 0 & 0\end{pmatrix}\right.$$

$$\left.-q\sum(-1)^{j+j'}(2j'+1)\begin{Bmatrix} l_1 & T & j\\ 1 & l_2 & j'\end{Bmatrix}\begin{pmatrix} j' & 1 & T\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l_2 & j' & l_1\\ 0 & 0 & 0\end{pmatrix}\right]. \qquad \text{(A10)}$$

The integral over the magnitude k of the momentum, is dominated by $k=\gamma$. Consequently, if the condition $\delta\ll 1$ holds [δ is defined in (3.14)], the argument of the Legendre polynomial is large. We know[45] that at large values of x the quantity $Q_T(x)$ has an x^{-T} behavior, so it is sufficient to restrict the discussion to functions $\mathscr{R}$ with small values of T. Also of assistance in evaluating the integrals in (A10) are the formulas

$$\int\limits_0^{\infty}\frac{dkk^2}{\pi iq}j_{l_1}(kr_1)j_{l_2}(kr_2)\left(\frac{2kq}{k^2+s^2}\right)^{n+1}$$

$$=\frac{2^nq^n}{n!\,i^{n+l_1+l_2}}\left(\frac{d}{ds^2}\right)^n(s^{n+2}P_{l_1l_2}(sr_1,sr_2)),$$

$$\int\limits_0^{\infty}\frac{dp\,k}{\pi q}j_{l_1}(kr_1)j_{l_2}(kr_2)\left(\frac{2kq}{k^2+s^2}\right)^{n+1} \qquad \text{(A11)}$$

$$=\frac{2^nq^n}{n!\,i^{n+l_1+l_2}}\left(\frac{d}{ds^2}\right)^n(s^{n+1}P_{l_1l_2}(sr_1,sr_2))$$

[in the first of these formulas, it is assumed that $n+l_1+l_2$ is odd, while in the second it is assumed that this quantity is even; the function $P(r_1,\ r_2)$ is defined in (A5)]. These formulas are derived by extending the integral to minus infinity and evaluating it by means of its poles.

Expanding the Legendre polynomials in (A10) in inverse powers of the argument, and using (A11), we can calculate the expansion of the functions $\mathscr{R}$ in δ with any desired accuracy. In practice, the calculations were carried out to second order inclusively; the corresponding error is on the order of 1%.

[1)] See Ref. 17 for more details.

---

[1] Ya. B. Zel'dovich and S. S. Gershteĭn, Usp. Fiz. Nauk **71**, 518 (1960). [*sic*].

[2] V. P. Dzhelepov, P. F. Ermolov, V. I. Moskalev, and V. V. Fil'chenkov, Zh. Eksp. Teor. Fiz. **50**, 1235 (1966) [Sov. Phys. JETP **23**, 820 (1966); V. M. Bystritskiĭ, V. P. Dzhelepov, K. O. Oganesyan *et al.*, Zh. Eksp. Teor. Fiz. **66**, 61 (1974) [Sov. Phys. JETP **39**, 27 (1974)].

[3] É. A. Vesman, Pis'ma Zh. Eksp. Teor. Fiz. **5**, 113 (1967) [JETP Lett. **5**, 91 (1967)].

[4] A. M. Lane, Phys. Lett. A **98**, 337 (1983).

[5] Yu. B. Petrov, Preprint 1058, Leningrad Institute of Nuclear Physics, Leningrad, 1985; Ju. V. Petrov, Phys. Lett. B **163**, 28 (1985).

[6] D. V. Balin, A. A. Vorob'ev, An. A. Vorob'ev *et al.*, Pis'ma Zh. Eksp. Teor. Fiz. **40**, 318 (1984) [JETP Lett. **40**, 1112 (1984)]; D. V. Balin, A. A. Vorob'ev, An. A. Vorob'ev *et al.*, Phys. Lett. B **161**, 1 (1984).

[7] S. E. Jones, A. N. Anderson, A. J. Gaffrey *et al.*, Phys. Rev. Lett. **56**, 588 (1986).

[8] J. Zmescal, W. H. Breunlich, M. Cargnelli *et al.*, Muon Catalyzed Fusion **1**, 109 (1987).

[9] L. I. Men'shikov, L. I. Ponomarev, T. A. Strizh, and M. P. Faĭfman, Zh. Eksp. Teor. Fiz. **92**, 1173 (1987) [Sov. Phys. JETP **65**, 656 (1987)].

[10] S. I. Vinitskiĭ, L. I. Ponomarev, I. V. Puzynin *et al.*, Preprint R4-10929, Joint Institute for Nuclear Research, Dubna, 1977; Zh. Eksp. Teor. Fiz. **74**, 849 (1978) [Sov. Phys. JETP **47**, 444 (1978)].

[11] S. S. Gerstein and L. I. Ponomarev, Phys. Lett. B **72**, 80 (1977).

[12] Yu. V. Petrov, *Proceedings of the Fourteenth Winter School of the Leningrad Institute of Nuclear Physics*, Leningrad, 1979, p. 139; Ju. V. Petrov, Nature **285**, 466 (1980).

[13] S. S. Gershteĭn, Yu. V. Petrov, and L. I. Ponomarev, Usp. Fiz. Nauk **160**(8), 3 (1990) [Sov. Phys. Usp. **33**(8), 591 (1990)].

[14] S. I. Vinitskiĭ, V. S. Melezhik, L. I. Ponomarev *et al.*, Fiz. Elem. Chastits At. Yadra **13**, 1336 (1982) [Sov. J. Part. Nucl. **13**, 557 (1982)].

[15] J. S. Cohen and R. L. Martin, Phys. Rev. Lett. **53**, 738 (1984).

[16] W. Kolos and L. J. Wolniewicz, Chem. Phys. **43**, 2429 (1965).

[17] L. I. Men'shikov, Yad. Fiz. **42**, 1184 (1985) [Sov. J. Nucl. Phys. **42**, 750 (1985); Yad. Fiz. **42**, 1449 (1985) [Sov. J. Nucl. Phys. **42**, 918 (1985); L. I. Men'shikov and M. P. Faĭfman, Yad. Fiz. **43**, 650 (1986) [Sov. J. Nucl. Phys. **43**, 414 (1986)].

[18] Yu. V. Petrov, V. Yu. Petrov, and A. I. Shlyakhter, Preprint 1279, LNPI, Leningrad, May 1987; Muon Catalyzed Fusion, **2**, 261 (1988).

[19] L. I. Men'shikov and L. I. Ponomarev, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 471 (1987) [JETP Lett. **45**, 602 (1987)].

[20] M. P. Faifman, L. I. Menshikov, and L. I. Ponomarev, Muon Catalyzed Fusion **2**, 285 (1988); M. P. Faifman, L. I. Menshikov, and T. A. Strizh, Muon Catalyzed Fusion **4**, 1 (1989).

[21] A. M. Lane, J. Phys. B **21**, 2159 (1988).

[22] A. Scrinzi, *Dissertation*, Institut für Mittelenergiephysik, Vienna, 1989.

[23] S. E. Jones, A. N. Anderson, A. J. Gaffrey *et al.*, Phys. Rev. Lett. **51**, 1757 (1983).

[24] I. V. Puzynin and S. I. Vinitsky, Muon Catalyzed Fusion **3**, 307 (1988).

[25] M. Kamimura, Phys. Rev. A **38**, 621 (1988).

[26] S. A. Alexander, H. J. Monkhorst, and K. Szalewicz, in *AIP Conf. Proc.*, Vol. 181, New York, 1989, p. 246.

[27] D. D. Bakalov, S. I. Vinitskiĭ, V. S. Melezhik, and L. I. Men'shikov, Preprint R4-84-693, Joint Institute for Nuclear Research, Dubna, 1984; D. D. Bakalov, S. I. Vinitsky, V. S. Melezhik, and L. I. Menshikov, Phys. Lett. B **161**, 5 (1985); D. D. Bakalov and V. S. Melezhik, Preprint R4-84-693, Joint Institute for Nuclear Research, Dubna, 1985.

[28] D. D. Bacalov, Muon Catalyzed Fusion **3**, 321 (1988).

[29] D. D. Bacalov and V. I. Korobov, Rapid communication of JINR 2-89, 1988; W. H. Breunlich, P. Kammel, J. S. Cohen, and M. Leon, Ann. Rev. Nucl. Part. Sci. **39**, 311 (1989).

[30] M. Kamimura, *Talk Given at International Symposium MCF-88,* Sanibel Island, Florida, May 1988.

[31] H. J. Monkhorst, G. Aissing, and D. D. Bacalov, *Proceedings of the International Symposium MCF-89,* RAL, 1990, p. 88.

[32] D. D. Bacalov, *Talk Given at International Symposium MCF-90,* Vienna, May 1990.

[33] M. P. Faifman, L. I. Menshikov, L. I. Ponomarev *et al.*, Z. Phys. D **2**, 79 (1986).

[34] S. I. Vinitskiĭ, L. I. Ponomarev, and M. P. Faĭfman, Preprint R4-81-572, Joint Institute for Nuclear Research, Dubna, 1981; Zh. Eksp. Teor. Fiz. **82**, 985 (1982) [Sov. Phys. JETP **55**, 578 (1982)].

[35] L. N. Bogdanova, V. E. Markushin, V. S. Melezhik, and L. I. Ponomarev, Preprint R4-82-87, Joint Institute for Nuclear Physics, Dubna, 1982; Zh. Eksp. Teor. Fiz. **83**, 1615 (1982) [Sov. Phys. JETP **56**, 931 (1982)].

[36] L. I. Menshikov and L. I. Ponomarev, Phys. Rev. Lett. **167**, 141 (1986).

[37] V. Yu. Petrov, Yu. V. Petrov, Preprint 1390, LNPI, Leningrad, 1988; *AIP Conf. Proc.*, Vol. 181, New York, 1989, p. 124; Muon Catalyzed Fusion **4**, 73 (1989).

[38] J. G. Larson, S. F. Fink, and Chi-Yu-Hu, Muon Catalyzed Fusion **4**, 49 (1989).

[39] A. Scrinzi and K. Szalewicz, Phys. Rev. A **39**, 2855 (1989).

[40] S. I. Vinitskiĭ and L. I. Ponomarev, Fiz. Elem. Chastits At. Yadra **13**, 1336 (1982) [Sov. J. Part. Nucl. **13**, 557 (1982)].

[41] G. Aissing, H. J. Monkhorst, and Yu. V. Petrov, Phys. Rev. A **42**, 6894 (1990).

[42] M. Leon, Muon Catalyzed Fusion **1**, 163 (1987).

[43] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Nauka, Moscow, 1964 (Addison-Wesley, Reading, Mass, 1969).

[44] W. N. Breunlich, P. Kammel, J. S. Cohen, and M. Leon, Ann. Rev. Nucl. Part. Sci. **39**, 311 (1989).

[45] W. H. Breunlich *et al.*, Muon Catalyzed Fusion **1**, 67 (1987); C. Petitjean *et al.*, Muon Catalyzed Fusion **2**, 37 (1988); (see also M. A. Paciotty *et al.*), *AIP Conf. Proc.*, Vol. 181, New York, 1989, p. 38.

[46] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products*, Academic, New York, 1966.

Translated by D. Parsons