

Calculation of ground-state energies of muonic molecules of hydrogen isotopes confined to a two-dimensional region

I. C. da Cunha Lima and M. Fabbri

Instituto de Pesquisas Espaciais—INPE, Avenida dos Astronautas, 1758, 12200 São José dos Campos, São Paulo, Brazil

A. Ferreira da Silva

Instituto de Física da Universidade Federal da Bahia, Campus Universitário da Federação, 40210 Salvador, Bahia, Brazil

A. Troper

Centro Brasileiro de Pesquisas Físicas—CBPF, Rua Dr. Xavier Sigaud, 150, 22290 Rio de Janeiro, Rio de Janeiro, Brazil

(Received 16 October 1989)

We calculate the ground-state energies of muonic molecules formed by deuterium-deuterium, tritium-tritium, and deuterium-tritium nuclei plus a negative muon confined in a two-dimensional (2D) region. We show that the equilibrium distance between nuclei is a factor of 4 smaller and the vibrational energies are about a factor of 5 higher than the corresponding three-dimensional (3D) muonic molecules, thus favoring fusion reactions. In fact, the estimated $d+t$ fusion rate is found to be three orders of magnitude higher in 2D than in 3D.

In recent years, muonic catalysis has attracted much attention, since it can, in principle, provide cold nuclear fusion, circumventing entirely the need for high temperatures.^{1,2} Muon-catalyzed fusion can be described as a series of reactions induced by negative muons in cold "hydrogen," leading to energy-releasing nuclear fusion. In order to get a muon-catalyzed fusion, one must bring a deuterium nucleus and a tritium nucleus into a very close proximity. It occurs that the tritium and deuterium nuclei combined with a negative muon can form a "muonic

molecular ion," in which the muon plays essentially the same role as an electron in an ordinary hydrogen molecule, i.e., the muon holds the nuclei together. However, due to the muon's high mass, the distance between the nuclei in a muonic molecule is of the order of 200 times less than the distance between the nuclei in an ordinary molecule. An important question which arises is the following: is it possible to obtain a situation where the two nuclei in the muonic molecule can be pulled together even closer, thus favoring the occurrence of a faster fusion reaction? In this Brief Report we show that muonic molecules like (i) deuterium, tritium, and muon, (ii) tritium, tritium, and muon, and (iii) deuterium, deuterium, and muon confined in a two-dimensional (2D) region may yield a faster reaction than the corresponding ones in a

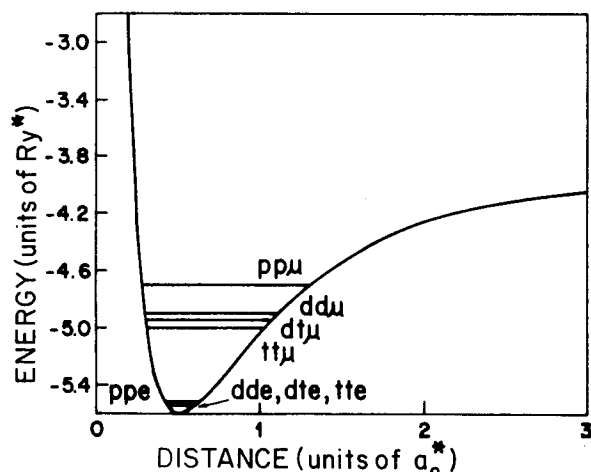


FIG. 1. The curves show the energy of a normal molecule (ion) or an ionic muonic molecule in 2D as a function of distance in units of effective Rydbergs and effective Bohr radius, respectively. The curve is universal for all the cases quoted in Table I. The horizontal bars represent the vibrational ground states.

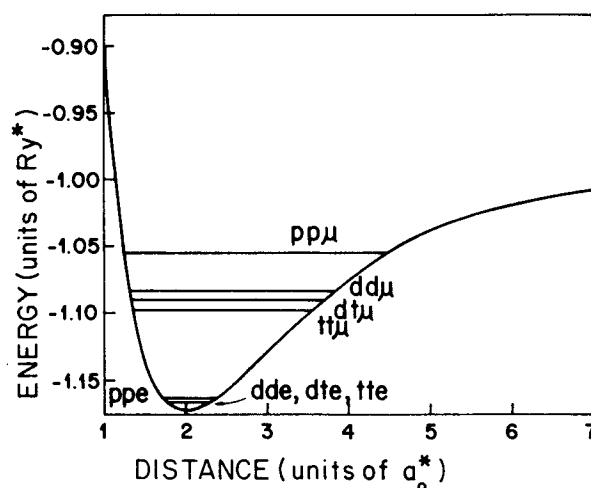


FIG. 2. Same as Fig. 1 for the 3D case.

TABLE I. Binding energies of muonic molecules and electronic molecules in two dimensions (2D) and in three dimensions (3D). The values for the equilibrium distance and minimum energy are calculated in effective units (see text) and depend uniquely on the dimensionality of the system.

	Vibrational energy	
	2D	3D
Muonic molecule		
<i>ppμ</i>	-4.669	-1.055
<i>ddμ</i>	-4.897	-1.084
<i>dtμ</i>	-4.944	-1.090
<i>ttμ</i>	-5.000	-1.098
Normal molecule		
<i>ppe</i>	-5.513	-1.163
<i>dde</i>	-5.539	-1.166
<i>dte</i>	-5.544	-1.166
<i>tte</i>	-5.550	-1.167

three-dimensional (3D) region. Indeed, we show that in 2D the equilibrium distance $X^{(0)}$ between the two nuclei is much smaller than the corresponding one in 3D

$$\frac{X^{(0)}(2D)}{X^{(0)}(3D)} \cong \frac{1}{4}. \quad (1)$$

This favors quantum-mechanical tunneling, increasing the probability that the nuclei pass through the barrier of their mutual repulsion and become so close that the strong nuclear force can propel them to fuse.

Although it is beyond the scope of this work to propose an experiment where the 2D confinement is realized, we point out that in many solid-state applications [e.g., heterostructures, inversion layers in metal-oxide semiconductors (MOS), etc.³], this kind of low-dimensional behavior is commonplace.

The muonic molecular system is described by the Hamiltonian

$$H_{\mu} = -\nabla^2 - \frac{2}{X_a} - \frac{2}{X_b}, \quad (2)$$

which corresponds to a muon in the 3D field of two positive charges (nuclei) fixed at positions a and b . In the

Born-Oppenheimer approximation (which is adequate for our purposes here^{4,5}), the ground-state energy of the muonic molecule is given by the lower eigenstate of H_{μ} plus the Coulomb interaction between nuclei, i.e.,

$$E(X_{ab}) = E_{\mu}(X_{ab}) + 2/X_{ab}. \quad (3)$$

In the above equations, energies and distances are expressed, respectively, in effective Rydbergs and effective Bohr radii:

$$R^* = m_{\mu} e^4 / 2h^2, \quad (4)$$

$$a_0^* = \hbar^2 / m_{\mu} e^2, \quad (5)$$

where m_{μ} refers to the muon's mass.

If we let small oscillations occur around the equilibrium distance $X_{ab}^{(0)}$, i.e., if we include vibrational modes, the ground-state energy becomes

$$E^{(0)} = E_{\mu}(X_{ab}^{(0)}) + (k/2fm^*)^{1/2}, \quad (6)$$

where

$$k = \left. \frac{\partial^2 E_{\mu}}{\partial X_{ab}^2} \right|_0, \quad (7)$$

$$m^* = \frac{m_a m_b}{m_a + m_b}. \quad (8)$$

f is the ratio of the mass of the proton and that of the muon, $f = \frac{1863}{207}$, and m_a and m_b are the masses in atomic units.

We obtained $E_{\mu}(X_{ab}^{(0)})$ by minimizing the following trial function:

$$\psi(X) = \phi^{1s}(X_a) + \phi^{1s}(X_b), \quad (9)$$

where the 2D 1s function is given by⁶

$$\phi^{1s}(X) = \left[\frac{8}{\pi} \right]^{1/2} \alpha e^{-2\alpha x}. \quad (10)$$

Equation (6) is a very good approximation for the first vibrational level, as long as it is located near the minimum of E_{μ} ; this is true for the *dde*, *dte*, and *tte* molecules. For the *ppe* and the muonic molecules, we obtained the level $E^{(0)}$ by solving numerically the vibrational Schrödinger equation in the Born-Oppenheimer ap-

TABLE II. The values near the origin of the wave function for the lowest vibrational level in 3D and 2D.

	$ \Psi^{2D}(0) ^2$	$ \Psi^{3D}(0) ^2$	$ \Psi^{2D}(0.04) ^2$	$ \Psi^{3D}(0.04) ^2$	$ \Psi^{2D}(0.04) ^2/ \Psi^{3D}(0.04) ^2$
Muonic molecule					
<i>ppμ</i>	1.46×10^{-2}	5.11×10^{-5}	2.37×10^{-2}	6.74×10^{-5}	350
<i>ddμ</i>	3.41×10^{-3}	3.31×10^{-6}	8.67×10^{-3}	5.66×10^{-6}	1530
<i>dtμ</i>	2.03×10^{-3}	1.23×10^{-6}	6.08×10^{-3}	2.31×10^{-6}	2630
<i>ttμ</i>	9.86×10^{-4}	3.05×10^{-7}	3.75×10^{-3}	6.67×10^{-7}	5620
Normal molecule					
<i>ppe</i>	7.57×10^{-29}	$< 10^{-40}$	6.08×10^{-19}	$< 10^{-40}$	$> 10^{20}$

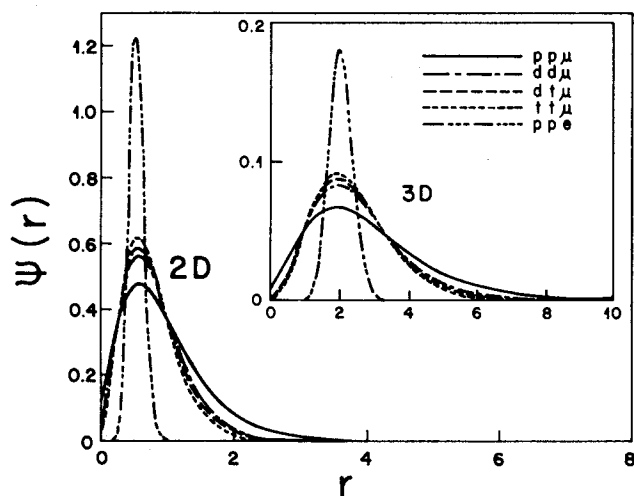


FIG. 3. Normalized eigenfunctions of the first vibrational mode for the 2D muonic molecules; we see a window with the corresponding 3D wave functions, for comparison. Also depicted is the extremely localized *ppe* eigenfunction.

proximation. In 3D we write the vibrational eigenfunction $\Psi^{3D}(r)$ as

$$\Psi^{3D}(r) = \frac{\varphi(r)}{4\pi r}, \quad (11)$$

and $\varphi(r)$ satisfies the radial wave equation (in normalized units):

$$-\frac{m_\mu}{m^*} \frac{d^2\varphi}{dr^2} + E_\mu(r)\varphi = E\varphi, \quad (12)$$

whereas in 2D we write

$$\Psi^{2D}(r) = \frac{\xi(r)}{2\pi r^{1/2}}, \quad (13)$$

and $\xi(r)$ satisfies

$$-\frac{m_\mu}{m^*} \frac{d^2\xi}{dr^2} + \left[E_\mu(r) - \frac{m_\mu}{m^*} \frac{1}{4r^2} \right] \xi = E\xi. \quad (14)$$

The numerical algorithm was built by a combination between a shooting method with minimization of the Rayleigh quotient described by Fox⁷ and integration by the Numerov Royal-road formula. The eigenvalues and eigenfunctions were obtained with an accuracy better than 1%. Initial guesses for $E^{(0)}$ were calculated by Eq.

(6). The results for $E^{(0)}$ are shown in Fig. 1. In Fig. 2 we show the equivalent 3D results, for the sake of comparison. One sees clearly that the muonic situation is in sharp opposition to the case of normal molecules where the vibrational spectrum is much richer. Only one vibrational bound state exists for all combinations quoted in Table I for the 3D case. However, for 2D, two vibrational bound states occur (only the lowest one is shown here). We do not discuss here the rotational states, which can be easily included in our formulation.

It is worthwhile to comment that we have also included in Eq. (2) electronic terms in order to obtain a neutral molecule. In this case one is found with an extra electron-muon Coulomb term, which has been treated with a Heitler-London approximation. One obtains the result, in this case, in both 2D and 3D situations, that the muonic molecule is loosely bound, maintaining quite the same ratio

$$\frac{X^{(0)}(2D)}{X^{(0)}(3D)} \cong \frac{1}{4}. \quad (15)$$

The fusion rate Λ is proportional to the probability that the nuclei are very close together:

$$\Lambda = A|\Psi(\rho)|^2, \quad (16)$$

where Ψ is the normalized wave function describing their relative motion. The internuclear separation ρ is usually taken to be approximately 10 fm ($\sim 0.04a_0^*$).

We make no assertions here about the dependence of the nuclear rate constant A on dimensionality. The s -like wave function associated with the nuclear motion corresponds to the ground state of Eqs. (12) and (14), for the 3D and 2D cases, respectively.

In Table II we show the values obtained for $|\Psi(0)|^2$ and $|\Psi(0.04)|^2$ in the 3D and 2D cases. It is seen that the enhancement of the fusion rate in the d - t system due to the larger tunneling probability in 2D is expected to be around three orders of magnitude.

In Fig. 3 we show the calculated eigenfunctions for the vibrational ground state of the muonic molecules in 2D and 3D; the corresponding eigenfunction for the *ppe* molecule is also shown for comparison. We stress the striking difference obtained in the 2D muonic molecule as compared to the usual 3D situation, favoring a higher rate of muonic fusions in a lower dimensionality.

The authors are grateful to J. Leite Lopes for very fruitful discussions.

¹See, e.g., S. E. Jones, *Nature (London)* **321**, 127 (1986) and references therein.

²L. Bracci and G. Fiorentini, *Phys. Rep.* **86**, 169 (1982).

³T. Ando, A. B. Fowler, and F. Stern, *Rev. Mod. Phys.* **54**, 37 (1982).

⁴A. J. Leggett and G. Baym (unpublished).

⁵A. J. Leggett and G. Baym, *Phys. Rev. Lett.* **63**, 191 (1989).

⁶The $\phi^{1s}(x)$ in Eq. (8) is obtained from S. Flügge and H. Marchall, *Rechenmethoden der Quanten Theorie*, 2nd ed. (Springer-Verlag, Berlin, 1952).

⁷L. Fox, *Numerical Solution of Ordinary and Partial Differential Equations* (Pergamon, Oxford, 1962), pp. 90–93.