

explosion (see Ref. 8).

In conclusion, we note that the results obtained in this paper, in particular, Eq. (16), are valid for the analysis of multipassage interferometers, i.e., interferometers with two interfering rays but with multiple reflection in a system of two or more mirrors used to increase the optical length of the interferometer.

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## Relativistic corrections and corrections for the electromagnetic structure of the nuclei to the energy levels of $\mu$ -mesic molecules of hydrogen isotopes

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An effective Hamiltonian is constructed for a three-body system with allowance for the electromagnetic structure of the particles and relativistic effects of order  $\alpha^2$  that do not depend on the spin orientation of the particles. This Hamiltonian and the nonrelativistic wave functions of a system of three particles with Coulomb interaction found in the adiabatic representation are used in a perturbation-theory calculation to accuracy  $\sim 5 \times 10^{-3}$  eV of the relativistic corrections and the corrections for the electromagnetic structure of the nuclei to the energy levels of the  $\mu$ -mesic molecules of hydrogen isotopes.

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### §1. INTRODUCTION

The recent interest in the physical characteristics of  $\mu$ -mesic molecules of hydrogen isotopes such as the energy levels and their hyperfine structure arises from a number of new high-precision experiments on  $\mu^-$  capture by light nuclei<sup>1</sup> and, above all, investigation of muon catalysis of the synthesis of the nuclei of the heavy isotopes of hydrogen.<sup>2</sup> The coupling in the  $\mu$ -mesic molecules is due entirely to the electromagnetic interaction; this makes it possible to describe their stationary states with high accuracy,<sup>3,4</sup> which, in its turn, increases the value of the experimental results and the reliability of their interpretation. At the same time, because the masses of the  $\mu^-$  meson and the nuclei are comparable, the relative contribution of the corrections to the energy levels of the mesic molecules due to the relativistic dynamics is about two orders of magnitude greater than in ordinary molecules. To describe many processes with spin dependence<sup>1,3,4</sup> (such as  $\mu^-$  capture) and especially the resonance formation of mesic molecules, the nonrelativistic approximation is inadequate, and relativistic effects make a contribution at the level of the ac-

curacy required in these cases in the calculation of the energy levels of the  $\mu$ -mesic molecules, namely,  $\sim 10^{-3}$  eV.

In the present paper, mesic molecules are treated as systems of three spin particles with electromagnetic interaction, and their dynamics is described by the Schrödinger equation with the approximate (accurate to terms of order  $\alpha^2$ ) relativistic Hamiltonian obtained in the framework of the formalism of Foldy and Krajcik.<sup>5</sup> The operators of the two-particle relativistic interaction are constructed in the framework of Todorov's quasipotential approach.<sup>6</sup> The relativistic effects in the Hamiltonian correspond to additive terms of two types: diagonal and nondiagonal with respect to the spin variables.

The interactions associated with the latter generate a hyperfine splitting of the energy levels; they have been considered earlier.<sup>7,8</sup> The present paper is devoted to a study of the relativistic effects that do not depend on the spin orientation of the particles and lead only to shifts of the nonrelativistic energy levels. We consider in general form systems of three particles with spins not exceeding 1, and we take into account their electro-

magnetic structure (§2). To calculate the shifts of the energy levels due to the relativistic effects and those associated with the finite sizes of the particles, we propose a perturbation theory which uses the solutions of the nonrelativistic three-particle problem with Coulomb potential constructed in the adiabatic approach<sup>3</sup> (§3). We calculate to accuracy  $\sim 10^{-3}$  eV the corrections to the energy levels of all the known stationary states of the  $\mu$ -mesic molecules of the hydrogen isotopes, and we discuss the relative contributions of the investigated effects (§4). Finally, we note some as yet unsolved problems.

## §2. APPROXIMATE (ACCURATE TO TERMS OF ORDER $\alpha^2$ ) RELATIVISTIC HAMILTONIAN OF A SYSTEM OF THREE SPIN PARTICLES WITH ELECTROMAGNETIC INTERACTION

In accordance with the work of Foldy and Krajcik,<sup>5</sup> the approximate (accurate to terms  $\sim 1/c^2 \sim \alpha^2$ ) relativistic Hamiltonian  $H$  of a three-particle system has the form

$$H = H^{(0)} + \alpha^2 H^{(1)}, \quad H^{(0)} = \sum_{i=1}^3 \frac{\mathbf{P}_i^2}{2m_i} + U^{(0)}, \quad H^{(1)} = - \sum_{i=1}^3 \frac{\mathbf{P}_i^4}{8m_i^3} + U^{(1)}. \quad (1)$$

Here and in what follows, the symbols  $\mathbf{R}_i$ ,  $\mathbf{P}_i$ ,  $m_i$ ,  $s_i$ ,  $Z_i$ , and  $\mu_i$  will denote, respectively, the coordinate and momentum three-vectors, the mass, spin, charge, and magnetic dipole moment of particle  $i$ . The units are fixed by the condition  $e = \hbar = m_1 m_3 / (m_1 + m_3) = 1$ , where  $e$  is the proton charge, and it is assumed that  $m_1 \geq m_2 \geq m_3$ .

In the case of the electromagnetic interaction of three particles that possess electromagnetic structure, the nonrelativistic potential  $U^{(0)}$  is a sum of terms describing the modified two-body Coulomb interaction<sup>6</sup>:

$$U^{(0)} = \frac{1}{2} \sum_{i \neq j} U_{ij}^{(0)}, \quad U_{ij}^{(0)} = Z_i Z_j \frac{f_{11}^{(ij)}(|\mathbf{R}_i - \mathbf{R}_j|)}{|\mathbf{R}_i - \mathbf{R}_j|}, \quad (2)$$

where the functions  $f_{kl}^{(ij)}(x)$  are related to the  $k$ -th electromagnetic form factor of particle  $i$  and the  $l$ -th form factor of particle  $j$  by

$$f_{kl}^{(ij)}(x) = x \int \frac{d^3 q}{(2\pi)^3} F_k^{(i)}(-\mathbf{q}) F_l^{(j)}(\mathbf{q}) \frac{4\pi}{q^2} e^{i\mathbf{q}x};$$

we shall also encounter the functions

$$\tilde{f}_{kl}^{(ij)}(x) = \frac{1}{x^3} \left( f_{kl}^{(ij)}(x) - x \frac{d}{dx} f_{kl}^{(ij)}(x) \right);$$

$$\hat{f}_{kl}^{(ij)}(x) = - \frac{1}{x} \frac{d^2}{dx^2} f_{kl}^{(ij)}(x) + 4\pi \delta(x) f_{kl}^{(ij)}(0).$$

The relativistic potential  $U^{(1)}$ , which consists in the general case of two- and three-particle terms,

$$U_2^{(1)} = \frac{1}{2} \sum_{i \neq j} U_{ij}^{(1)}, \quad U_3^{(1)},$$

is constructed as the solution of the system of differential equations obtained from the commutation relations of the Lie algebra of the Poincaré group. Foldy and Krajcik<sup>5</sup> constructed explicitly the particular solution

$$U^{(1)FK} = U_2^{(1)FK} + U_3^{(1)FK}.$$

For  $U^{(0)}$  given by Eq. (2), it takes the form

$$U_2^{(1)FK} = 0, \quad U_3^{(1)FK} = \frac{1}{2} \sum_{i \neq j} U_{ij}^{(1)FK},$$

$$U_{ij}^{(1)FK} = \left\{ - \frac{Z_i Z_j}{2(m_i + m_j)^2} \frac{f_{11}^{(ij)}(r_{ij})}{r_{ij}} \mathbf{P}_{ij}^2 + i \frac{(m_i - m_j) Z_i Z_j}{2(m_i + m_j) m_i m_j} \times f_{11}^{(ij)}(r_{ij}) (\mathbf{r}_{ij} \mathbf{P}_{ij}) - \frac{Z_i Z_j}{2(m_i + m_j)^2} f_{11}^{(ij)}(r_{ij}) (\mathbf{r}_{ij} \mathbf{P}_{ij})^2 \right\} \hat{1}^{spin} + (\text{terms nondiagonal to the spin}),$$

where  $\hat{1}^{spin}$  is the identity operator in the space of the spin variables,  $\mathbf{r}_{ij} = \mathbf{R}_j - \mathbf{R}_i$ ,  $r_{ij} = |\mathbf{r}_{ij}|$  and  $\mathbf{P}_{ij} = \mathbf{P}_i + \mathbf{P}_j$ .

The general solution  $U^{(1)}$  contains the arbitrary scalar functions

$$\Delta U_2^{(1)} = \frac{1}{2} \sum_{i \neq j} \Delta U_{ij}^{(1)}, \quad \Delta U_3^{(1)},$$

which do not depend on the coordinates and momentum of the center-of-mass of the three-particle system and satisfy the separability condition. The uncertainty in  $\Delta U_3^{(1)}$  remains an open question, but in the case of the electromagnetic interaction it is natural to set  $\Delta U_3^{(1)} = 0$ . The separability condition for the Hamiltonian  $H$  fixes in  $\Delta U_{ij}^{(1)}$  the terms that do not depend on  $\mathbf{P}_{ij}$ : When the third particle is removed to infinity, the operator  $U_{ij}^{(1)}(\mathbf{P}_{ij} = 0)$  in the center-of-mass system of particles  $i$  and  $j$  must become identical to the operator which describes the  $\sim \alpha^2$  relativistic effects in the relative motion of the two-particle system ( $ij$ ).

Assuming that the entire dependence of  $U_{ij}^{(1)}$  on the center-of-mass motion of the pair ( $ij$ ) is contained in  $U_{ij}^{(1)FK}$ , and using the expression for the operator of the two-particle interaction obtained in Ref. 6 in Todorov's quasipotential approach,<sup>9</sup> we can represent  $\Delta U_{ij}^{(1)}$  in the form

$$\Delta U_{ij}^{(1)} = U_{ij}^{(1)}(\mathbf{P}_{ij} = 0) = - \frac{(m_i + m_j)}{2m_i m_j} \left( \frac{Z_i Z_j f_{11}^{(ij)}(r_{ij})}{r_{ij}} \right)^2 - \frac{Z_i Z_j}{4m_i m_j} \left[ \tilde{f}_{11}^{(ij)}(r_{ij}) + \frac{2s_i}{2s_i + 1} \frac{m_j}{m_i} \left( \varepsilon_i \tilde{f}_{11}^{(ij)}(r_{ij}) + \frac{\mu_i - \delta_i}{s_i} \tilde{f}_{21}^{(ij)}(r_{ij}) \right) + \frac{2s_j}{2s_j + 1} \frac{m_i}{m_j} \left( \varepsilon_j \tilde{f}_{11}^{(ij)}(r_{ij}) + \frac{\mu_j - \delta_j}{s_j} \tilde{f}_{12}^{(ij)}(r_{ij}) \right) \right],$$

where  $\delta_i = 1$  for  $s_i = \frac{1}{2}$ ,  $\delta_i = 0$  for  $s_i \neq \frac{1}{2}$ , and  $\varepsilon_i = (-1)^{2s_i + 1}$ . Finally, the approximate relativistic Hamiltonian  $H$  of the system of three particles with electromagnetic interaction takes the form

$$H = \sum_i \frac{\mathbf{P}_i^2}{2m_i} + \frac{1}{2} \sum_{i \neq j} U_{ij}^{(0)} + \alpha^2 H^{(1)}, \quad (3)$$

$$H^{(1)} = - \sum_i \frac{\mathbf{P}_i^4}{8m_i^3} + \frac{1}{2} \sum_{i \neq j} (\Delta U_{ij}^{(1)} + U_{ij}^{(1)FK}).$$

## §3. METHOD OF CALCULATION

The stationary states  $|\mathcal{F} N \mathcal{F}_3 v n \lambda\rangle$  of the system of three particles with spins  $s_i$  are characterized by the set of quantum numbers  $(\mathcal{F}, \mathcal{F}_3, N, v, n, \lambda)$ :  $\mathcal{F}$  and  $\mathcal{F}_3$  are the quantum numbers of the square and the projection of the total angular momentum  $\mathcal{Y} = s_1 + s_2 + s_3 + \mathbf{J}$  onto the  $Z$  axis of the fixed coordinate system,  $\mathbf{J}$  is the orbital angular momentum of the system of three particles,  $N$  labels the states of the multiplet of the hyperfine structure for given  $\mathcal{F}$ , the vibrational quantum number  $v$  characterizes the relative motion of particles 1 and 2 (the nuclei), and the set of three quantum num-

bers  $n$  characterizes the motion of particle 3 with respect to particles 1 and 2;  $\lambda$  is the parity of the wave function under reflection of the coordinate axes.

The wave functions  $\psi_{\mathcal{N}3}^{\mathcal{N}v n \lambda}$  and energy levels  $E^{\mathcal{N}v n \lambda}$  can be found from the Schrödinger equation with Hamiltonian  $H$  from (3):

$$(H - E^{\mathcal{N}v n \lambda}) \psi_{\mathcal{N}3}^{\mathcal{N}v n \lambda} = 0. \quad (4)$$

In the expression (3) for  $H^{(1)}$ , we separate the parts  $H_{\text{diag}}^{(1)}$  and  $H_{\text{spin}}^{(1)}$  diagonal and nondiagonal with respect to the spin variables,

$$H^{(1)} = H_{\text{diag}}^{(1)} + H_{\text{spin}}^{(1)},$$

and in the expression for  $H^{(0)}$  we separate the nonrelativistic three-particle Hamiltonian with Coulomb interaction  $H_{NR}$  and the term

$$\Delta H^{(0)} = \sum_{i \neq j} Z_i Z_j \frac{f_{ij}^{(0)}(r_{ij}) - 1}{r_{ij}} = \sum_{i \neq j} \Delta H_{ij}^{(0)},$$

which describes the corrections to  $H_{NR}$  due to the effects of the electromagnetic structure of the particles; then  $H$  can be written in the form

$$H = H^{(0)} + \alpha^2 H^{(1)} = \{H_{NR} + (\Delta H^{(0)} + \alpha^2 H_{\text{diag}}^{(1)})\} \hat{1}^{spin} + \alpha^2 H_{\text{spin}}^{(1)}. \quad (3')$$

The operator  $H^{(1)}$  is proportional to  $\alpha^2 \sim 10^{-4}$ , and  $\Delta H^{(0)}$  contains implicitly as small parameters the electromagnetic radii of the particles; it is therefore natural to solve Eq. (4) perturbatively.<sup>1</sup> To achieve accuracy  $\sim 10^{-3}$  eV in the description of the energy spectra of the  $\mu$ -mesic molecules and in a number of other cases, it is sufficient to consider only the first order; in this case, the corrections from the terms  $\Delta H^{(0)}$ ,  $H_{\text{diag}}^{(1)}$ , and  $H_{\text{spin}}^{(1)}$  to the nonrelativistic energy levels  $E^{\mathcal{N}v n \lambda}$  determined from the nonrelativistic Schrödinger equation

$$(H_{NR} - E^{\mathcal{N}v n \lambda}) |J m_J v n \lambda\rangle = 0 \quad (5)$$

are additive.

The hyperfine splitting of the levels generated by the operator  $H_{\text{spin}}^{(1)}$  was considered earlier in Refs. 7 and 8; the aim of the present paper is to study the effects of the operator  $V^{\mathcal{N}v n \lambda}$  diagonal in the spin variables; here

$$V = \Delta H^{(0)} + \alpha^2 H_{\text{diag}}^{(1)}. \quad (6)$$

If we eliminate the term  $H_{\text{spin}}^{(1)}$  in the expression (3') for the Hamiltonian  $H$  of the system, the dependence on the spin variables in the Schrödinger equation (4) factorizes, and the eigenvalues  $J$  and  $m_J$  of the square of the total orbital angular momentum  $\mathbf{J}$  and its projection  $J_z$  onto the  $z$  axis become good quantum numbers of the stationary states of the three-particle system. This means that in every state  $|\mathcal{N} \mathcal{F}_3 v n \lambda\rangle$  the orbital angular momentum has a definite value  $\mathbf{J} = \mathbf{J}_{\mathcal{N}}$ :

$$(J^2 - J_{\mathcal{N}}(J_{\mathcal{N}} + 1)) |\mathcal{N} \mathcal{F}_3 v n \lambda\rangle = (J_z - m_J) |\mathcal{N} \mathcal{F}_3 v n \lambda\rangle = 0.$$

Inclusion of the potential  $V$  (6) leads to a shift of the nonrelativistic energy levels by the amount

$$\Delta E^{\mathcal{N}v n \lambda} = \Delta E_{NR}^{(\mathcal{N}v n \lambda)} = \langle J_{\mathcal{N}} v n \lambda, m_J | V | J_{\mathcal{N}} v n \lambda, m_J \rangle, \quad (7)$$

which is the same for all states  $|\mathcal{N} \mathcal{F}_3 v n \lambda\rangle$  belonging to a given multiplet of the hyperfine structure.

We represent the operator of the perturbation  $V$  (6) as a sum of operators:

$$V = \sum_{t=1}^5 V^{(t)}. \quad (8)$$

In terms of the Jacobi coordinates and momenta

$$\mathbf{R}_c = (m_1 + m_2 + m_3)^{-1} (m_1 \mathbf{R}_1 + m_2 \mathbf{R}_2 + m_3 \mathbf{R}_3), \quad \mathbf{R} = \mathbf{R}_2 - \mathbf{R}_1,$$

$$\mathbf{r} = \mathbf{R}_3 - \frac{1}{2}(\mathbf{R}_1 + \mathbf{R}_2), \quad \mathbf{P}_c = -i \nabla_{\mathbf{R}_c}, \quad \mathbf{P} = -i \nabla_{\mathbf{R}}, \quad \mathbf{p} = -i \nabla_{\mathbf{r}},$$

and the vectors  $\mathbf{r}_{1,2} = \mathbf{R}_3 - \mathbf{R}_{1,2}$ , the expression for the operators  $V^{(t)}$  have the following form (for  $\mathbf{R}_c = \mathbf{P}_c = 0$ ):

1)  $t=1$  (corrections to the Coulomb interaction at short distances because of the electromagnetic structure of the particles):

$$V^{(1)} = Z_1 Z_2 \frac{f_{12}^{(1)}(R) - 1}{R} + \sum_{i=1,2} Z_i Z_3 \frac{f_{i3}^{(1)}(r_i) - 1}{r_i}; \quad (9)$$

2)  $t=2$  (contact interaction):

$$V^{(2)} = -\frac{Z_1 Z_2 \alpha^2}{4m_1 m_2} \left\{ \hat{f}_{11}^{(12)}(R) + \frac{2s_1}{2s_1 + 1} \frac{m_2}{m_1} (e_i \hat{f}_{11}^{(12)}(R)) + \frac{\mu_1 - \delta_1}{s_1} \hat{f}_{21}^{(12)}(R) + \frac{2s_2}{2s_2 + 1} \frac{m_1}{m_2} (\hat{f}_{11}^{(12)}(R) \varepsilon_2 + \frac{\mu_2 - \delta_2}{s_2} \hat{f}_{12}^{(12)}(R)) \right\} - \sum_{i=1,2} \frac{Z_i Z_3 \alpha^2}{4m_i m_3} \left\{ \hat{f}_{i1}^{(13)}(r_i) + \frac{2s_i m_3}{(2s_i + 1) m_i} (e_i \hat{f}_{i1}^{(13)}(r_i) + \frac{\mu_i - \delta_i}{s_i} \hat{f}_{i2}^{(13)}(r_i)) \right\}; \quad (10)$$

3)  $t=3$  (squared Coulomb potential):

$$V^{(3)} = -\frac{m_1 + m_2}{2m_1 m_2} \left( \frac{Z_1 Z_2 \alpha f_{11}^{(12)}(R)}{R} \right)^2 - \sum_{i=1,2} \frac{m_i + m_3}{2m_i m_3} \left( \frac{Z_i Z_3 \alpha f_{i1}^{(13)}(r_i)}{r_i} \right)^2; \quad (11)$$

4)  $t=4$  (relativistic recoil):

$$V^{(4)} = -\frac{\alpha^2}{8m_3^3} \left\{ \left( 1 + \left( \frac{m_3}{m_1} \right)^2 + \left( \frac{m_3}{m_2} \right)^2 \right) \mathbf{p}^4 + \left[ \left( \frac{m_3}{m_1} \right)^3 - \left( \frac{m_3}{m_2} \right)^3 \right] (\frac{1}{2} \mathbf{p}^2 (\mathbf{P} \mathbf{p}) + 2(\mathbf{P} \mathbf{p}) \mathbf{P}^2) + \left[ \left( \frac{m_3}{m_1} \right)^3 + \left( \frac{m_3}{m_2} \right)^3 \right] (\frac{1}{2} \mathbf{P}^2 \mathbf{p}^2 + (\mathbf{P} \mathbf{p})^2 + \mathbf{P}^4) \right\}; \quad (12)$$

5)  $t=5$  (the Foldy-Krajcik interaction, which describes the effects of the motion of the centers of mass of the two-particle subsystems):

$$V^{(5)} = -\frac{\alpha^2 Z_1 Z_2}{2(m_1 + m_2)^2} \frac{f_{11}^{(12)}(R)}{R} \mathbf{p}^2 - \frac{\alpha^2 Z_1 Z_3}{2(m_1 + m_3)^2} \frac{f_{i1}^{(13)}(r_i)}{r_i} (\mathbf{P} - \frac{1}{2} \mathbf{p})^2 - \frac{\alpha^2 Z_2 Z_3}{2(m_2 + m_3)^2} \frac{f_{i2}^{(13)}(r_2)}{r_2} (\mathbf{P} + \frac{1}{2} \mathbf{p})^2 + i \frac{\alpha^2 Z_1 Z_2 (m_2 - m_1)}{2m_1 m_2 (m_2 + m_1)} \hat{f}_{11}^{(12)}(R) (\mathbf{R} \mathbf{p}) + i \frac{\alpha^2 Z_1 Z_3 (m_1 - m_3)}{2m_1 m_3 (m_1 + m_3)} \hat{f}_{i1}^{(13)}(r_i) (\mathbf{r} + \frac{1}{2} \mathbf{R}) (\frac{1}{2} \mathbf{p} - \mathbf{P}) + i \frac{\alpha^2 Z_2 Z_3 (m_2 - m_3)}{2m_2 m_3 (m_2 + m_3)} \hat{f}_{i2}^{(13)}(r_2) (\mathbf{r} - \frac{1}{2} \mathbf{R}) (\frac{1}{2} \mathbf{p} + \mathbf{P}) - \frac{\alpha^2 Z_1 Z_2}{2(m_1 + m_2)^2} \hat{f}_{11}^{(12)}(R) (\mathbf{R} \mathbf{p})^2 - \frac{\alpha^2 Z_1 Z_3}{2(m_1 + m_3)^2} \hat{f}_{i1}^{(13)}(r_i) [(\mathbf{r} + \frac{1}{2} \mathbf{R}) (\frac{1}{2} \mathbf{p} - \mathbf{P})]^2 - \frac{\alpha^2 Z_2 Z_3}{2(m_2 + m_3)^2} \hat{f}_{i2}^{(13)}(r_2) [(\mathbf{r} - \frac{1}{2} \mathbf{R}) (\frac{1}{2} \mathbf{p} + \mathbf{P})]^2. \quad (13)$$

In accordance with Eqs. (7) and (8), the determination of the relativistic shifts  $\Delta E^{\mathcal{N}v n \lambda}$  of the energy levels reduces to the calculation of the expectation value of the operators  $V^{(t)}$  between the nonrelativistic wave functions of the stationary states of the system:

$$\Delta E_{NR}^{\mathcal{N}v n \lambda} = \langle J v n \lambda, m_J | V^{(t)} | J v n \lambda, m_J \rangle. \quad (14)$$

For this, we go over from the Cartesian coordinates of the vectors  $\mathbf{R}$  and  $\mathbf{r}$  to the variables  $R, \xi = (r_1 + r_2)/R, \eta = (r_1 - r_2)/R$  and to the angles  $\Phi, \theta,$  and  $\varphi$ , where  $\Phi$  and  $\theta$  are the polar angles of the vector  $\mathbf{R}$  in the fixed coordinate system, and  $\varphi$  is the azimuthal angle of the vector  $\mathbf{r}$  in the rotating coordinate system whose  $z$  axis is along the vector  $\mathbf{R}$  with  $y$  axis in the plane  $OXY$ .<sup>10</sup>

In the adiabatic approach<sup>3,10</sup> one uses the expansion

$$\psi_{m_j}^{j\text{en}\lambda}(\mathbf{R}, \mathbf{r}) = \langle \mathbf{Rr} | J m_j \nu n \lambda \rangle \quad (15)$$

of the nonrelativistic wave function of the three-particle system and a series in the Coulomb spheroidal functions  $\Pi_{n_1 m_1 p}(\xi; R)$ , and  $\Xi_{n_2 m_2 p}(\eta; R)$ :

$$\begin{aligned} \psi_{m_j}^{j\text{en}\lambda}(R, r) = & \sum_{m=0}^J \mathcal{D}_{m m_j}^{j\lambda}(\Phi, \theta, \varphi) \sum_{n_1=0}^J \sum_{p=\xi, \eta} \left\{ \sum_{n_1=0}^J R^{-1} \right. \\ & \times \chi_{n_1 n_2 m_1 p}^{j\text{en}\lambda}(R) N_{n_1 m_1 p}(R) \Pi_{n_1 m_1 p}(\xi; R) \Xi_{n_2 m_2 p}(\eta; R) \\ & \left. + \int_0^{10} dk R^{-1} \chi_{n_1 n_2 m_1 p}^{j\text{en}\lambda}(k, R) N_{n_1 m_1 p}(k, R) \Pi_{m_1 p}(\xi; k, R) \Xi_{n_2 m_2 p}(\eta; R) \right\}. \end{aligned} \quad (16)$$

Here, the functions  $\mathcal{D}_{m m_j}^{j\lambda}$  are expressed in terms of Wigner's  $D$  functions<sup>11</sup>:

$$\mathcal{D}_{m m_j}^{j\lambda} = [(2J+1)/16\pi^2]^{1/2} [(-1)^m D_{m m_j}^J + \lambda(-1)^J D_{-m m_j}^J], \quad m > 0,$$

$$\mathcal{D}_{0 m_j}^{j\lambda} = [(2J+1)/32\pi^2]^{1/2} (1 + \lambda(-1)^J) D_{0 m_j}^J,$$

$N_{n_1 n_2 m_1 p}(R)$  is a normalization factor,<sup>10</sup> and the prime on the sum over  $p$  means that if particles 1 and 2 are identical  $p$  takes of the two values  $g = +1$  and  $u = -1$  only the values  $p = \lambda(-1)^J$ , where  $I(I+1)$  is an eigenvalue of the operator  $\mathbf{I}^2 = (\mathbf{s}_1 + \mathbf{s}_2)^2$ .

The functions  $\chi(R)$  are found as solutions to the Sturm-Liouville problem for the system of integro-differential equations obtained by substituting the expansion (16) in the Schrödinger equation (5) and subsequent averaging over all the variables except  $R$ .<sup>10</sup> The expressions for the operators  $V^{(t)}$ ,  $t = 1, \dots, 5$ , in the variables  $R, \xi, \eta, \Phi, \theta, \varphi$  are given in the previous paper Ref. 6.

#### §4. CORRECTIONS TO THE ENERGY LEVELS OF THE STATIONARY STATES OF THE MESIC MOLECULES OF HYDROGEN ISOTOPES

The formalism presented in §§2 and 3 was used to calculate the relativistic corrections and the corrections for the electromagnetic structure of the nuclei to the energy levels of the  $\mu$ -mesic molecules of the hydrogen isotopes.

The electromagnetic form factors of the proton, deuteron, triton were approximated by functions of the type

$$F^{op}(-q^2) = \sum_n \frac{c_n}{(1+q^2/\Lambda_n^2)^{l_n}}$$

with the parameters obtained earlier in Ref. 6; the  $\mu^-$  meson was treated as a structureless particle. The employed masses and magnetic dipole moments<sup>12</sup> are given in Table I; the fine structure constant was taken from Ref. 13,  $\alpha = 1/137.0360$ , and for the transition to atomic units we used the value  $Ry = 13.6058$  eV.

TABLE I. Masses and magnetic dipole moments of  $\mu^-$  mesons and the nuclei  $p, d,$  and  $t$  used in the paper.

Particle	$\mu^-$	$p$	$d$	$t$
Mass $m_i$ (MeV/c <sup>2</sup> )	105.65646	938.2796	1875.628	2806.9438
Magnetic dipole moment $\mu_i \left( \frac{e\hbar}{2m_i c} \right)$	1.0012	2.7928	1.7139	8.9180

All the calculations were made so as to ensure an absolute accuracy of  $\delta E \approx 10^{-3}$  eV in the values of the energy levels of the mesic molecules. Such an accuracy is sufficient to describe the processes of resonance formation of mesic molecules and corresponds to an error  $\delta T \approx 10^\circ \text{K}$  in the determination of the resonance temperature.<sup>2</sup> This made it possible to simplify somewhat the calculations by ignoring terms whose contribution is smaller than the chosen limit. Because  $m_3/m_{1,2} \leq 10^{-1}$  for all mesic molecules, in the expression (12) for  $V^{(4)}$  we retained only the first term:

$$V^{(4)} = -\frac{\alpha^2}{8} \left\{ \left( \frac{1}{m_3^2} + \frac{1}{m_1^2} + \frac{1}{m_2^2} \right) p^4 + O\left( \left( \frac{m_3}{m_2} \right)^3 \right) \right\}.$$

The corrections for the electromagnetic structure to the internuclear Coulomb potential (9) and for the contact interaction between the nuclei (10) are negligibly small. The effect from the Foldy-Krajcik interaction  $V^{(5)}$  is less than  $10^{-3}$  eV, as is shown by calculations of the hyperfine structure of mesic molecules<sup>8</sup> and an estimate of the order of the quantities in  $V^{(5)}$ , and it was therefore also ignored.

In calculating the matrix elements (14) of the operators  $V^{(t)}$ ,  $t = 1, \dots, 4$ , we did not take into account the contribution to the adiabatic expansion (16) from the terms corresponding to the continuous spectrum of the two-center problem<sup>14</sup>; the results of analogous calculations of the previous paper Ref. 7 indicate that the error thus introduced does not exceed the allowed limits. For the Coulomb spheroidal functions  $\Pi_{n_1 m_1 p}(\xi; R)$  and  $\Xi_{n_2 m_2 p}(\eta; R)$  we used, respectively, expansions in a Jaffe series and in a series in powers of  $(1 \pm \eta)^{14}$ ; in the calculations, these series were truncated so as to guarantee a relative accuracy of them of  $\sim 10^{-5}$ . The integration over  $\eta$  was performed analytically and that over  $\xi$  numerically, with relative error  $\sim 10^{-5}$  for  $\nu_{000p,000p}^{j\text{en}\lambda,t}$  and  $\sim 10^{-3}$  in the remaining cases.<sup>6</sup> For  $\chi_{n_1 n_2 m_1 p}^{j\text{en}\lambda}(R)$ , we used the solutions obtained in Ref. 15; the integration over  $R$  was over the interval (0, 20.0) with step 0.1, and over the interval (20.0, 60.0) with step 1.0; comparison with the results obtained with twice this step indicates that the relative error of the integration does not exceed  $10^{-4}$ .

An important question is the choice of the origin for the energy of the bound states of the three-particle systems. It is natural to measure the binding energy  $-\varepsilon^{j\text{en}\lambda}$  of the mesic molecule from the ground-state level  $E^0$  of the mesic atom of the heavier of the nuclei<sup>4</sup>:

$$\varepsilon^{j\text{en}\lambda} = E_{NR}^{j\text{en}\lambda} - E^0.$$

Allowance for the spin-independent relativistic corrections and the other corrections mentioned above leads to a shift of the nonrelativistic energy levels of both the

mesic molecule [by the amount  $\Delta E_{NR}^{J\nu\lambda}$  (14)] and the ground state of the mesic atom (by the amount  $\Delta E^0$  obtained earlier<sup>6</sup>). If by analogy with the separation in Eq. (14) we separate in  $\Delta E^0$  the contributions  $\Delta E^{0,t}$  from the different terms in the operator of the two-particle interaction (see Ref. 6), we can represent  $\Delta E^{J\nu\lambda}$  in the form

$$\Delta E^{J\nu\lambda} = \sum_t \Delta E^{J\nu\lambda,t} = \sum_t (\Delta E_{NR}^{J\nu\lambda,t} - \Delta E^{0,t}). \quad (17)$$

The values of all the given quantities for the mesic molecule  $d\mu$  ( $J=1, \nu=1$ ) were given in the previous paper Ref. 6 as a test illustration of the computational procedure. For all the remaining known stationary states of the mesic molecules we give in Table II only the values of the corrections  $\Delta E^{J\nu\lambda,t}$  and  $\Delta E^{J\nu\lambda}$  to the binding energy. All these states are "ground states with respect to the meson motion,"<sup>4</sup> and we therefore omit the quantum numbers  $n=(0,0,0)$  and  $\lambda=(-1)^J$ , which are the same for all of them.

It should be noted that in the calculation of the corrections to the binding energy  $-\varepsilon^{J\nu}$  of the mesic molecules in accordance with Eq. (17) there is appreciable self-cancellation of the contributions of nearly equal magnitude made by  $\Delta E_{NR}^{J\nu\lambda,t}$  and  $\Delta E^{0,t}$  for  $t=1, 2, 3$ , which is not observed in the case  $t=4$  (see Ref. 6). This indicates that the corrections for relativistic recoil are an essentially three-particle effect, whereas the corrections for the electromagnetic structure of the particle effects.

In this paper, we have not considered vacuum polarization effects, since the corresponding terms in the Hamiltonian  $H$  are of higher order in  $\alpha$ ; however, because of the large mass of the  $\mu^-$  meson they are important in a number of cases. The vacuum-polarization corrections to the binding energy of the stationary states of the mesic molecules (denoted by  $\Delta E^{J\nu,VP}$ ),<sup>16</sup> and also

TABLE II. Corrections to the nonrelativistic energy levels of mesic molecules of hydrogen isotopes. The following corrections are given (in eV): for the distortion of the Coulomb potential at short distances due to the electromagnetic structure of the nuclei ( $\Delta E^{J\nu,1}$ ), for the contact interaction ( $\Delta E^{J\nu,2}$ ), for the squared Coulomb interaction ( $\Delta E^{J\nu,3}$ ), for relativistic recoil ( $\Delta E^{J\nu,4}$ ), and for vacuum polarization ( $\Delta E^{J\nu,VP}$ ); the total shift  $\Delta E_{tot}^{J\nu}$  is also given.

Mesic molecule, $J\nu$	Electromagnetic structure, $t=1$	Contact interaction, $t=2$	Squared Coulomb, $t=3$	Recoil, $t=4$	Vacuum polarization (Ref. 16) $\Delta E^{J\nu,VP}$	Total shift, $\Delta E_{tot}^{J\nu}$
$p\mu$	0 0	+0.0032	+0.0199	-0.0684	+0.0383	-0.285
	1 0	+0.0002	+0.0013	-0.0268	+0.0225	-0.067
$p d\mu$	0 0	-0.0660	+0.0282	-0.0740	+0.0699	-0.342
	1 0	-0.0737	+0.0110	-0.0371	+0.0440	-0.152
$p t\mu$	0 0	-0.0390	+0.0289	-0.0758	+0.0688	-0.342
	1 0	-0.0438	+0.0122	-0.0409	+0.0532	-0.143
$d d\mu$	0 0	+0.0386	+0.0251	-0.0828	+0.0681	-0.348
	1 0	-0.0185	+0.0120	-0.0494	+0.0543	-0.196
$d t\mu$	0 0	-0.0037	-0.0024	-0.0189	+0.0395	-0.002
	1 1	+0.0034	+0.0022	-0.0176	+0.0463	+0.004
$t t\mu$	0 0	-0.0624	+0.0147	-0.0884	+0.0777	-0.428
	1 0	+0.0476	+0.0267	-0.0608	+0.0648	-0.267
$t d\mu$	0 0	+0.0293	+0.0002	-0.0273	+0.0496	-0.068
	1 1	+0.0281	+0.0033	-0.0221	+0.0550	+0.056
$t t\mu$	0 0	+0.0022	-0.0006	-0.0069	+0.0524	-0.003
	1 0	+0.0289	+0.0290	-0.0902	+0.0815	-0.479
$t t\mu$	0 0	+0.0185	+0.0186	-0.0683	+0.0701	-0.329
	1 0	+0.0047	+0.0048	-0.0376	+0.0553	-0.130
$t t\mu$	0 0	-0.0063	-0.0063	-0.0095	+0.0440	+0.044
	1 0	+0.0058	+0.0058	-0.0295	+0.0581	-0.097
$t t\mu$	0 1	+0.0010	+0.0011	-0.0177	+0.0533	-0.034
	1 1	+0.0010	+0.0011	-0.0177	+0.0533	+0.004

the total shift

$$\Delta \varepsilon_{tot}^{J\nu} = \Delta \varepsilon^{J\nu} + \Delta \varepsilon^{J\nu,VP}$$

are given in Table II. Comparison shows that for the ground state and the low-lying levels of the mesic molecules it is the contribution from  $\Delta \varepsilon^{J\nu,3}$ ; however, on the transition to the excited states its value, like the corrections for the electromagnetic structure of the nuclei and for the contact interaction, decreases rapidly, and the correction for relativistic recoil is dominant. In the case of the mesic molecule  $d\mu$  ( $J=1, \nu=1$ ), the contribution from the last correction is 80% of the total shift of the energy level, which is approximately 8% of the binding energy of this state.

## §5. CONCLUSIONS

The main result of the present paper is the calculation of the relativistic corrections and the corrections for the electromagnetic structure of the nuclei to the nonrelativistic energy levels of the mesic molecules of the hydrogen isotopes. In conjunction with the vacuum-polarization corrections obtained earlier,<sup>16</sup> the results of the present paper make it possible to calculate the total shifts of the nonrelativistic energy levels with accuracy  $\sim 5 \times 10^{-3}$  eV.

Not yet allowed for are the effects of polarization of the nuclei and screening by the field of the molecular electrons; it can be expected that their contribution to the binding energy of the mesic molecules will not exceed  $10^{-3}$  eV. From the computational point of view, it is still an open question how one should take into account consistently the contribution to  $\Delta E^{J\nu\lambda}$  (14)–(17) from the two-center functions of the continuum. Of fundamental importance is the calculation of the contribution to the binding energy from the two-body interactions which depend on the center-of-mass motion of the pairs of particles [such as the Foldy–Krajcik interaction  $V^{(5)}$  (13)].

In accordance with preliminary estimates for  $\mu^-$  mesic molecules of the hydrogen isotopes, the contributions from these effects are  $< 10^{-3}$  eV, but a further increase in the accuracy of the calculations of the energy spectra of the  $\mu^-$ -mesic molecules, and also the systematic study of other three-particle systems are possible only after the solution of these problems.

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<sup>1</sup>The exact solution of Eq. (4) entails fundamental difficulties because of the presence of fourth-order derivatives in  $U^{(1)FK}$ .

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## Shifts of the nonlinear methane resonance at $3.39 \mu\text{m}$

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Shifts of the nonlinear resonance in methane at the  $F_2^{(2)}$  line due to various physical factors have been investigated, using frequency stabilized He-Ne lasers with methane absorption cells. The measured shifts of the resonance on varying the field intensity in the resonator, the methane pressure in the cell, and the strength of an applied longitudinal magnetic field are in agreement with theoretical calculations. The shifts depend nonlinearly on the uniform width  $2\Gamma$  of the resonance. When  $\Gamma \sim 100$  kHz the observed field shift is large and is due to differences in the field broadening of the magnetic hyperfine structure components and to the effect of crossed resonances. When  $\Gamma \sim 10$ – $20$  kHz the field shift is small and is due mainly to relative changes in the intensities of the principal hyperfine structure components resulting from saturation. The nonlinear pressure dependence of the resonance shift is due to the effect of the magnetic hyperfine structure and to particle collisions. At methane pressures above 1 mTorr the shift is due mainly to collisions and amounts to  $\sim 400$  Hz/mTorr; at pressures below 1 mTorr the impact shift of the resonance is compensated by a shift due to the effect of the magnetic hyperfine structure, and the resultant shift is small.

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### INTRODUCTION

Narrow nonlinear optical resonances have made it possible to make precise measurements of the shifts of spectral lines of gases under the influence of various physical factors.<sup>1</sup> This has proved to be especially important in studying lines due to molecular vibrational-rotational (VR) transitions. The collisional shift of molecular VR lines amounts to  $\sim 100$  kHz at  $\sim 1$  Torr, and this is some  $10^3$  times smaller than the Doppler width of the line. It is virtually impossible to study such small line shifts by the traditional methods of linear spectroscopy. The lines are substantially broader at high pressures and the individual VR components of the molecular transitions overlap; this also makes it difficult to analyze the profile of an isolated spectrum line. We note that for complex molecules the VR lines overlap even within the limits of their Doppler widths. The shifts of such lines can be studied only with the aid

of nonlinear resonances whose widths are  $10^3$ – $10^4$  times smaller than the Doppler width.

In this paper we report detailed studies of the shifts of the methane  $F_2^{(2)}$  line at  $\lambda = 3.39 \mu\text{m}$  under the action of various physical factors. This line was chosen for study for a number of reasons. The narrowest resonances in the optical range have been obtained from this methane transition and have been used to achieve high stability and reproducibility at a level of  $10^{-13}$ – $10^{-14}$  of the frequency of a He-Ne laser working at  $\lambda = 3.39 \mu\text{m}$ .<sup>2,3</sup> The use of lasers whose frequency can be adjusted with high accuracy to the peak of the resonance makes it possible to measure shifts of the methane resonance with an accuracy of the order of 10 Hz. The studies proved to be important for an understanding of the physical nature of the shifts of the  $F_2^{(2)}$  line and shed light on the problem of achieving high frequency reproducibility in a He-Ne/CH<sub>4</sub> laser.