

# Energies of three-particle systems with Coulomb interactions

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The nonrelativistic energy of a symmetric Coulomb system with particle charges  $z_1 = z_2 = \pm 1$  and  $z_3 = \mp 1$  and masses  $m_1 = m_2 = m$  and  $m_3$  is expressed in the form  $E = m\beta\epsilon(\beta)$ , where  $\beta = m_3/(2m + m_3)$ . An approximate formula for the function  $\epsilon(\beta)$ , which makes it possible to calculate the energies of the systems for all possible values of the masses  $m$  and  $m_3$ , is derived. The results of such calculations agree well with previous precise calculations of the energies of symmetric mesic molecules and predict the energies of many diverse Coulomb systems whose energies have not previously been calculated.

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Three-particle systems with Coulomb interaction are of considerable interest in various problems of atomic, molecular, and nuclear physics. A number of papers has appeared in the last decade in which nonadiabatic calculations of the energies of such systems with allowance for the motion of all three particles are presented. Reviews of such calculations have been published by Bishop and Cheung<sup>1,2</sup> for isotopic modifications of the molecular hydrogen ion, and by Ponomarev *et al.*<sup>3,4</sup> for mesic-molecular ions; calculations have also been published<sup>5-9</sup> for the  $e^-e^+e^-$  system. Since different authors use different approaches, however, the results of the calculations are frequently quite discrepant (this can be seen by comparing Refs. 3 and 4 with Refs. 10 and 11, and Refs. 5 and 6 with Refs. 7, 8, and 9).

Here we shall show that by employing a scale transformation and expanding the energy in powers of the Born-Oppenheimer parameter we can obtain a formula for the energy of three-particle Coulomb systems for all possible values of the particle masses. That formula encompasses the isotopic modifications of the molecular hydrogen ion, symmetric mesic molecules, atomic systems in which two mesons are bound by a proton, deuteron, or triton, as well as the negative atomic hydrogen ion and its isotopic modifications, including the analog of that ion whose nucleus is a positively charged meson.

We shall use atomic units ( $|e| = m_e = \hbar = 1$ ) throughout except when the contrary is specifically stated.

We shall consider a system of three particles consisting of two particles with equal masses  $m_1 = m_2 = m$  and charges  $z_1$  and  $z_2$ , a third particle of mass  $m_3$  and charge  $z_3$ . After separating the motion of the center of mass, the nonrelativistic energy operator for this system,

$$\hat{H} = -\frac{1}{2m}(\Delta_1 + \Delta_2) - \frac{1}{2m_3}\Delta_3 + \frac{z_1 z_2}{r_{12}} + \frac{z_2 z_3}{r_{23}} + \frac{z_1 z_3}{r_{13}} \quad (1)$$

reduces to the form

$$\hat{H} = m\beta\hat{h}(s, t; \beta). \quad (2)$$

We have introduced scale-transformed relative coordinates, which are related as follows to the initial particle coordinates;

$$s = m\beta(\mathbf{r}_1 - \mathbf{r}_2), \quad t = m\beta(\mathbf{r}_1 + \mathbf{r}_2 - 2\mathbf{r}_3). \quad (3)$$

Here

$$\beta = m_3/(2m + m_3). \quad (4)$$

The quantity  $\hat{h}$  in (2) denotes the operator

$$\hat{h} = -\beta\Delta_s - \Delta_t + z_1 z_2/|s| + 2z_2 z_3/|t-s| + 2z_1 z_3/|t+s|. \quad (5)$$

Let  $\epsilon(\beta)$  be the lowest eigenvalue of the operator (5). It is related as follows to the ground-state energy of the system described by the energy operator (2):

$$E(m, m_3) = m\beta\epsilon(\beta). \quad (6)$$

It is evident from (4) that  $0 < \beta < 1$ . The function  $\epsilon(\beta)$  is defined on this same interval; if this function is known, the energies of all Coulomb systems of the type under discussion (with arbitrary values of  $m$  and  $m_3$  but with fixed values of the particle charges  $z_1, z_2$ , and  $z_3$ ) can be found.

It is evident from the structure (5) of the operator  $\hat{h}$  that the Born-Oppenheimer parameter  $\kappa$  for this operator is proportional to  $\beta^{1/4}$ . Hence the expansion of the eigenvalue  $\epsilon$  in  $\beta$  will contain half-integral and integral powers of  $\beta$ . Since  $\beta$  occurs in the operator  $\hat{h}$  as the coefficient of a positive-definite operator,  $\epsilon$  increases monotonically with increasing  $\beta$ .

In view of what was said above, we adopted the expression

$$\epsilon(\beta) \approx f(\beta) = \sum_{j=0}^5 C_j \beta^{j/2}, \quad (7)$$

which contains six unknown coefficients  $C_j$ , as an approximation to the function  $\epsilon(\beta)$ . The values of the coefficients  $C_j$  were so chosen as to make formula (7) exact for six "reference" systems. The reference systems were chosen as follows: a) the molecular hydrogen ion  $H_2^+(\infty)$  with infinitely massive nuclei, whose energy is<sup>12</sup>  $E = -0.6026342$ ; b) and c) the molecular ions  $H_2^+$  and  $D_2^+$ , whose energies, calculated for the masses  $M_p = 1836.152$  and  $M_d = 3670.479$ , are<sup>1</sup>  $E = -0.5971391$  and  $E = -0.5987888$ ; d) the negative atomic hydrogen ion, whose energy is  $E = -0.5274458$  for the masses  $m = 1$  and  $m_3 = 1835.92$ ; e) the negative hydrogen ion  $H^-(\infty)$  for an infinitely massive nucleus, whose energy is<sup>13</sup>  $E = -0.5277510$ ; and f) the  $e^-e^+e^-$  system consisting of two electrons and one positron, whose energy,

according to Ref. 5, is  $E = -0.2619956$ . Then the coefficients  $C_j$  in Eq. (7) turn out to have the following numerical values:

$$C_0 = -1.20\ 526\ 843; \quad C_1 = 0.64\ 166\ 462; \quad C_2 = 0.28\ 883\ 986; \\ C_3 = -0.17\ 033\ 848; \quad C_4 = -0.19\ 973\ 985; \quad C_5 = 0.11\ 709\ 127.$$

We chose the reference systems as we did in order to extract the greatest amount of information from precise calculations of the energies of ordinary atomic and molecular systems such as  $H_2^+$  and  $H^-$ , and the  $e^-e^+e^-$  system in order to use that information in calculations of the energies of diverse Coulomb systems, including "exotic" systems containing mesons.

It is important that formula (6) was derived without any assumptions concerning adiabatic separation of the variables. The formula is therefore valid for the exact nonrelativistic energies of three-particle systems. It follows from formula (6) and the values given above for the energies of systems such as  $H_2^+$  and  $H^-$  with infinitely massive nuclei that as  $\beta$  increases from 0 to 1, the function  $\varepsilon(\beta)$  increases from  $\varepsilon(0) = -1.2052684$  to  $\varepsilon(1) = -0.5277510$ ; within these limits are included the values of  $\varepsilon$  for all symmetric three-particle Coulomb systems in which  $z_1 = z_2 = \pm 1$ ,  $z_3 = \mp 1$ , and  $m_1 = m_2 = m$ , the masses  $m_3$  and  $m$  being arbitrary.

In approximating the exact function  $\varepsilon(\beta)$  by the function  $f(\beta)$  [Eq. (7)] the effects of nonadiabaticity have also been taken into account, both by including high powers of the Born-Oppenheimer parameter (up to  $\kappa^{10} = \beta^{5/2}$ , inclusive) and by using accurate energies of the reference systems in evaluating the coefficients  $C_j$ . Hence the function  $f(\beta)$  constructed here yields the energies of symmetric Coulomb systems with very high accuracy.<sup>1)</sup>

The results of the calculations are presented in Table I. The systems are listed in order of increasing  $\beta$ . The "reference" systems are included in the table for completeness;

they are marked by asterisks. The results of our energy calculations are given in the penultimate column. The high accuracy of our results for small values of  $\beta$  (i.e. for isotopic modifications of the molecular hydrogen ion) and for values of  $\beta$  close to unity (for isotopic modifications of the negative atomic hydrogen ion) is guaranteed by the very choice of the reference systems: three of them lie close to the point  $\beta = 0$ , and two of them are close to the point  $\beta = 1$ . It is therefore of great interest to compare our results with precise calculations for intermediate values of  $\beta$  lying between the reference points  $\beta = 0$  and  $\beta = 1/3$ , and between the points  $\beta = 1/3$  and  $\beta = 1$ . The first of these regions include symmetric mesic molecules for which reliable energy calculations have been made.<sup>4</sup> It is evident from the table that our results agree well with those calculations. For the interval from  $\beta = 1/3$  to  $\beta = 1$  (in particular, for mesic analogs of the negative atomic hydrogen ion) there are no accurate energies in the literature. By analogy with the mesic molecules, we may expect our results in this region to have relative errors of the order of  $10^{-5}$ . The important part played by the accurate value of the energy of the electron-positron system  $eee^+$  in constructing the approximating function  $f(\beta)$  should also be noted: if the value of this energy found in Refs. 7, 8, or 9 had been used instead of the more accurate value found in Ref. 5, the errors in approximating the energies of mesic molecules would reach several electron volts.

We note two more possible applications of our approximating function  $f(\beta)$ . The first concerns aggregates consisting of two electrons and a hole (or of an electron and two holes) in a semiconductor whose current carriers have isotropic masses. The formation of such aggregates is the first stage leading to the appearance of an electron-hole "liquid." The second possible application involves compact charged systems such as mesic-molecular ions  $M^+$  that are much smaller in size than the electron shell of an atom and can play the part of atomic nuclei for electrons. From this point of view, our formula (7) yields an approximate description of

TABLE I. Energies of symmetric three-particle Coulomb systems

System	$\beta$	$f(\beta)$	Energy of the system	
			from Eqs. (6) and (7)	previously published values
$H_2^+(\infty)^*$	0	-1.205268	-0.60263421	-0.60263421 [12]
$T_2^+(tte)$	$0.9095179 \cdot 10^{-4}$	-1.199123	-0.5995068	-
$D_2^+(dde)^*$	$1.362034 \cdot 10^{-4}$	-1.197741	-0.5987888	-0.5987888 [1]
$H_2^+(ppe)^*$	$2.722345 \cdot 10^{-4}$	-1.194603	-0.5971391	-0.5971391 [1]
$\mu^+\mu^+e$	$0.2412324 \cdot 10^{-2}$	-1.173077	-0.5851237	-
$t\mu^-$	$1.846052 \cdot 10^{-2}$	-1.113244	{ -112.9674	-3074.13 eV [4]
			{ (-3074.03 eV)	-3072.6 eV [10, 11]
			{ -139.8090	-2988.19 eV [4]
$d\mu^-$	$2.739486 \cdot 10^{-2}$	-1.092059	{ (-2988.08 eV)	-2987.41 eV [10, 11]
			{ -102.2109	-2781.36 eV [4]
$p\mu^-$	$5.330371 \cdot 10^{-2}$	-1.044314	{ (-2781.32 eV)	-2781.53 eV [10, 11]
$eee^+*$	0.3333333	-0.7859868	-0.2619956	{ -0.2619956 [5]
				{ -0.2620011 [6]
$\mu^-\mu^-\mu^+$	0.3333333	-0.7859868	-162.5177	
$p\mu\mu$	0.8161800	-0.5780158	-97.54635	
$d\mu\mu$	0.8987424	-0.5541721	-102.9829	
$t\mu\mu$	0.9300328	-0.5457009	-104.9393	
$\mu^+ee$	0.9904200	-0.5301327	-0.5250540	
$H^-(pee)^*$	0.9989118	-0.5280204	-0.5274458	-0.5274458 [13]
$D^-(dee)$	0.9994554	-0.5278858	-0.5275983	
$T^-(tee)$	0.9996363	-0.5278410	-0.5276490	
$H^-(\infty)^*$	1	-0.5277510	-0.5277510	-0.5277510 [13]

such systems as  $M^+ee$ , where  $M^+$  is treated as a single particle whose mass is equal to the sum of the masses of two nucleons and a meson.

On the whole, our results show that scaling the Hamiltonian and using a truncated expansion of the Born-Oppenheimer type makes it possible to predict the dependence of the energy of symmetric three-particle Coulomb systems on the mass ratio (on the parameter  $\beta = m_3/(2m + m_3)$ ) with quite satisfactory accuracy. It is significant that in such a case formula (7) is more accurate than moderately accurate purely theoretical calculations of the energies. For asymmetric Coulomb systems in which the masses of all three particles are different, scaling the Hamiltonian results in a Hamiltonian that depends on two parameters. Hence the expansion of the energies of asymmetric systems in parameters of the Born-Oppenheimer type is a more complicated problem; nevertheless, it may have useful applications.

<sup>1</sup>The greatest relative error in the energies of the reference systems amounts to  $10^{-7}$ . We give the coefficients  $C_j$  to one "extra" decimal place to avoid the accumulation of random errors. Accordingly, formula (7) ensures a relative error of the order of  $10^{-7}$  in the calculation of energies near the reference points, i.e., near the values  $\beta = 0$ ,  $\beta = 1/3$ , and  $\beta = 1$ .

On receding from the reference values, the error in formula (7) increases, but it can hardly exceed  $10^{-5}$  anywhere in the range of variation of  $\beta$  (from zero to unity). More accurate values of the energies of the reference systems will make it possible to calculate the coefficients  $C_j$  more accurately; at present, for example, the energies of the  $H_2^+$  and  $H^-$  ions with stationary nuclei have been calculated to 13 and 9 significant figures, respectively.

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