Theory of bound states in the Coulomb three-body system with unit charges

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The existence of bound states and the discrete-spectrum classification in the three-body Coulomb nonrelativistic system with unit charges is considered. It is shown that in such systems the bound states exist not at arbitrary, but instead only at definite values of the mass ratios, which must lie in a "stable region." The position of this "stable region" is studied for the bound ground S states.

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I. INTRODUCTION

Three-body Coulomb systems are of increasing interest: they play an important role in the diagnostics of high-temperature and laboratory plasmas, solar physics, and muon-catalyzed nuclear reactions. In some recent publications a number of highly accurate calculations have been reported and it is now possible to discuss the theory of the spectra of such systems. However, the problem is complicated since it involves six physical parameters: three masses and three charges. In this article we will consider those systems which have unit charges and for which the Hamiltonian (in atomic units) is

$$H(m_X,m_Y,m_Z;r_X,r_Y,r_Z) = -\tfrac{1}{2}(m_X^{-1}\Delta_X+m_Y^{-1}\Delta_Y+m_Z^{-1}\Delta_Z) + q_Xq_Y/r_{XY}+q_Xq_Z/r_{XZ}+q_Yq_Z/r_{YZ}\ , \quad (1)$$

where q_i $(i=X,Y,Z)$ are charges and m_i are masses. We shall study only the bound-state spectra in such systems; hence one of three charges has a different sign. Without loss of generality we choose $q_X=q_Y=1$ and $q_Z=-1$. We can apply the charge-conjugation operator Q $(Qq_i=-q_i)$ which commutes with the Hamiltonian, from which it follows that the initial Coulomb three-body system and its charge-conjugated system have the same total and binding energies. Because of this there is no difference between two such systems and we shall use the notation $X^+Y^+Z^-$ for the general type of three-particle system. Here X^+, Y^+, and Z^- are the point particles which have unit charges and masses m_X, m_Y, and m_Z.

The choice of the Coulomb three-body systems with unit charges is governed not only by their importance in applications (e.g., so-called exotic systems Ps^-, Mu^-, $^\infty H^-$, mesomolecules), but also by the desirability of analyzing various types of discrete energy spectra as a function of the three particle masses $E(m_X,m_Y,m_Z)$. It should be noted that the type of discrete spectrum is determined by the asymptotic form of the potential $V(r)$ as $r\to\infty$ in the lowest-energy two-body channel of the system, e.g., for $m_X\geq m_Y$ the lowest channel will be

$$X^+Y^+Z^- = XZ+Y\ . \quad (2)$$

In the general case, systems with arbitrary charges, the asymptote of the pair potential $V(r)$ at $r\to\infty$ between the cluster XZ, and the ion Y can be either Coulombic attractive, Coulombic repulsive, or non-Coulombic. If the pair potential of the interaction $V(r)$ between X^+Z^- and Y^+ is the Coulombic attractive potential then the discrete energy spectrum contains an infinitely large number of levels, which converge to the three-body dissociation threshold. If $V(r)$ is the Coulombic repulsive potential then the energy spectrum of bound states is empty. These statements are true for arbitrary masses of particles in such systems. Therefore, in these cases the dependence of the total energy of the system on the particle masses $E(m_X,m_Y,m_Z)$ has a very simple form. The more interesting dependence of the type of discrete spectrum and its structure as a function of particle masses can be observed only in the case of a system with a non-Coulombic asymptotic form of the pair potential $V(r)$ in the channel in Eq. (2). For definite mass ratios the inequality

$$E(X^+Y^+Z^-)<E(X^+Z^-)=-0.5m_Xm_Z/(m_X+m_Z) \quad (3a)$$

will be obeyed for some state. Then this state is bound. The case of the equality

$$E(X^+Y^+Z^-)=E(X^+Z^-)=-0.5m_Xm_Z/(m_X+m_Z) \quad (3b)$$

is of special interest and we shall use it as the definition of the threshold. Here we want to study the case of the stability of bound ground states in the three-body Coulomb systems with unit charges with respect to mass variation. In other words, we will consider the function $E(m_X,m_Y,m_Z)$ for the ground state in such systems. It is shown that in such systems the bound ground states exist only for definite mass ratios, which must lie in a "stable region." The position of the "stable region" is studied for the ground S states in detail.

The problems related to studying $E(m_X,m_Y,m_Z)$ for the Coulomb three-body problem with unit charges have been formulated in Ref. [1]. In earlier papers [2–4] the threshold problem has also been investigated and the interesting examples of three-body Coulomb systems with

unbound ground states or empty spectra have been presented. In Ref. [5] the stability of the ground and some excited states in the three-body Coulomb symmetric systems (Ps^-, Mu^-, $^\infty H^-$) was considered (see also Ref. [6]). In a previous paper [7] the binding energies of a number of symmetric systems such as $X^+X^+Z^-$ with $m_X \leq m_Z$ were considered. Finally, we note that the systematic study of the three-body systems with unit charges was started more than thirty years ago [8–13] and a number of methods have been used: variational expansions in relative coordinates [8–10], the adiabatic representation [11], the three-particle Faddeev-equation method [12], and the hyperspherical-harmonic method [13].

II. CALCULATIONS

Here we use the exponential variational expansion in relative coordinates to compute the bound states. In the case of the ground S state, this expansion takes the form

$$\Psi_{L=0}(r_{31},r_{32},r_{21}) = (1+\delta P_{12}) \sum_i C_i \exp(-\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21}) , \quad (4)$$

where δ equals 1 in the case of a symmetric system (two particles having the same charges and mass) and 0 in all other cases. P_{12} is the permutation operator and r_{ij} are interparticle distances. The nonlinear parameters α_i, β_i, and γ_i are selected quasirandomly from three intervals. The ranges of the parameters α_i, β_i, and γ_i are $0 \leq \alpha_i \leq 1.45$, $0 \leq \beta_i \leq 1.334$, and -0.3 min $\{\alpha_i,\beta_i\} \leq \gamma_i \leq 1.098$, respectively. Note that the rapid convergence of Eq. (4) enables us to use the same fixed values of the nonlinear parameters for different systems. Equation (4) with a quasirandom choice of α_i, β_i, and γ_i was first used by Thakkar and Smith [14] and details of our application of this method are given in Ref. [15]. In all calculations we used 600 basis functions, except for Ps^- where we used 900. To calculate the binding energies we used the conversion factor of $E_H = 27.211\,396\,1$ eV.

Our numerical results are given in Tables I–VIII. In order to discuss them we introduce three dimensionless

TABLE I. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X = m_Y = \lambda m_e$, $m_Z = m_e$. $E_H = 4.359\,748\,2 \times 10^{-18}$ J and 1 eV $= 1.602\,177\,3 \times 10^{-19}$ J. In the case of these systems the threshold energy equals $E_t(\lambda) = -0.5/(1+\lambda^{-1})$. Negative binding energies correspond to bound states.

λ	Total energy (E_H)	Binding energy (eV)
1.0[a]	−0.262 005 070 232	−0.326 674 72
2.0	−0.352 687 35	−0.526 649 9
3.0	−0.400 267 04	−0.687 551 4
4.0	−0.430 962 39	−0.842 529 8
5.0	−0.450 780 24	−0.928 278 0
6.0	−0.466 088 87	−1.020 901 9
7.0	−0.477 943 60	−1.100 527 0
8.0	−0.487 441 06	−1.169 997 9
9.0	−0.495 248 64	−1.231 278 7
10.0	−0.501 800 15	−1.285 866 8
15.0	−0.523 534 60	−1.490 765 6
20.0	−0.536 021 01	−1.628 072 3
25.0	−0.544 290 28	−1.728 496 5
30.0	−0.550 246 20	−1.806 162 7
50.0	−0.563 748 89	−2.001 474 7
100.0	−0.576 414 52	−2.214 055 7
$\mu^+\mu^+e^-$	−0.584 928 65	−2.376 512 0[b]

[a] Ps^-.

[b] In this case the muonic mass was $m_\mu = 206.768\,64 m_e$.

TABLE II. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X = 1.5 m_Y = 1.5\lambda m_e$, $m_Z = m_e$. In the case of these systems the threshold energy equals $E_t(\lambda) = -0.5/[1+1/(1.5\lambda)]$, if $\lambda > 1$ and $E(\lambda) = -0.5/\{[1+1/(1.5\lambda)]\lambda\}$, if $\lambda < 1$ and $\lambda_t = 0.985$.

λ	Total energy (E_H)	Binding energy (eV)
5.0	−0.467 615 14	−0.719 433 1
4.0	−0.449 405 26	−0.566 917 8
3.0	−0.423 183 95	−0.383 491 2
2.0	−0.381 365 12	−0.173 203 8
1.6	−0.356 303 55	−0.091 494 8
1.4	−0.340 752 24	−0.055 580 9
1.2	−0.322 363 30	−0.025 435 3
1.1	−0.311 794 03	−0.012 878 4
1.06	−0.307 255 21	−0.008 310 4
1.0	−0.300 070 06	−0.001 906 3
0.99	−0.298 825 41	−0.000 897 6
0.95	−0.293 702 63	+0.003 202 5
0.9	−0.286 956 23	+0.008 399 6

TABLE III. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X = 2m_Y = 2\lambda m_e$, $m_Z = m_e$. In the case of these systems the threshold energy equals $E_t(\lambda) = -0.5/(1+0.5/\lambda)$ and $\lambda_t = 1.456$.

λ	Total energy (E_H)	Binding energy (eV)
10.0	−0.518 734 48	−1.157 681 8
9.0	−0.513 420 01	−1.081 266 7
8.0	−0.507 107 42	−0.993 737 9
7.0	−0.499 461 14	−0.892 383 4
6.0	−0.489 969 15	−0.773 638 8
5.0	−0.477 807 59	−0.632 995 2
4.0	−0.461 553 67	−0.465 565 9
3.0	−0.438 496 30	−0.270 069 5
2.5	−0.422 788 90	−0.166 594 6
2.0	−0.402 590 32	−0.070 486 1
1.8	−0.392 726 86	−0.038 708 5
1.6	−0.381 449 49	−0.013 527 1
1.55	−0.378 356 72	−0.008 379 6
1.5	−0.375 134 93	−0.003 671 6
1.45	−0.371 771 82	+0.000 627 3
1.4	−0.368 253 66	+0.004 554 9

TABLE IV. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X=3m_Y=3\lambda m_e$, $m_Z=m_e$. In the case of these systems the threshold energy equals $E_t(\lambda)=-0.5/[1+1/(3\lambda)]$ and $\lambda_t=1.925$.

λ	Total energy (E_H)	Binding energy (eV)
9.0	−0.520 535 26	−1.044 711 0
8.0	−0.514 908 89	−0.949 919 7
7.0	−0.508 141 95	−0.839 994 8
6.0	−0.499 822 37	−0.711 256 0
5.0	−0.489 309 51	−0.559 452 9
4.0	−0.475 552 97	−0.381 354 2
3.0	−0.456 710 45	−0.182 600 8
2.5	−0.444 381 32	−0.087 208 4
2.0	−0.429 127 32	−0.015 127 0
1.8	−0.421 800 99	+0.002 013 8
1.5	−0.408 433 98	+0.017 877 6

parameters v_X, v_Y, and v_Z where $v_i=m_i/\sum_i m_i$ $(i=X,Y,Z)$. It is obvious that $v_X+v_Y+v_Z=1$ and $0\le v_i\le 1$, i.e., only two v coordinates are independent. We choose these as v_X and v_Z. In general, the total energy of the three-body Coulomb system can be written as

$$E(m_X,m_Y,m_Z)=mE(v_X,v_Z)\ , \tag{5}$$

where m is a dimensional mass parameter, e.g., the minimum of the three masses and without loss of generality can be made equal to unity. v_X and v_Z are two dimensionless parameters and E is a function of these parameters only. Let the minimal mass m be fixed $(=1)$, then the use of the v parameter makes it possible to plot an arbitrary Coulomb system with unit charges as a point inside a triangle with unit height, with triangular coordinates $v_X=ab$, $v_Y=ac$, $v_Z=ad$ (see Fig. 1), and also $ab+ac+ad=1$. The condition $v_X\ge v_Y$ makes it possible to consider only the right side of the triangle. It should be remembered that one point on the v plane

TABLE V. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X=4m_Y=4\lambda m_e$, $m_Z=m_e$. In the case of these systems the threshold energy equals $E_t(\lambda)=-0.5/[1+1/(4\lambda)]$ and $\lambda_t=1.986$.

λ	Total energy (E_H)	Binding energy (eV)
5.0	−0.495 585 20	−0.527 757 4
4.0	−0.483 294 16	−0.345 746 0
3.0	−0.466 983 65	−0.148 171 2
2.5	−0.456 725 31	−0.059 317 0
2.0	−0.444 493 97	−0.001 347 6
1.98	−0.443 943 60	+0.000 070 5
1.9	−0.441 670 89	+0.005 158 5
1.8	−0.438 641 66	+0.010 414 5
1.5	−0.427 766 40	+0.021 906 0
1.0	−0.398 576 22	+0.038 743 1

TABLE VI. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X=m_Z=\lambda m_e$, $m_Y=m_e$. In the case of these systems the threshold energy equals $E_t(\lambda)=-0.25\lambda$ and $\lambda_t=1.3775$.

λ	Total energy (E_H)	Binding energy (eV)
1.0[a]	−0.262 005 07	−0.326 674 7
1.05	−0.271 909 80	−0.256 053 9
1.10	−0.282 104 52	−0.193 323 9
1.15	−0.292 609 84	−0.139 046 0
1.20	−0.303 438 44	−0.093 564 8
1.25	−0.314 593 16	−0.056 957 7
1.30	−0.326 060 87	−0.028 867 7
1.35	−0.337 810 22	−0.008 441 5
1.36	−0.340 188 87	−0.005 139 3
1.37	−0.342 576 02	−0.002 068 5
1.375	−0.343 772 62	−0.000 615 5
1.378	−0.344 491 51	+0.000 230 9
1.38	−0.344 971 16	+0.000 784 9

[a] Ps^-.

represents two Coulomb three-body systems with unit charges $X^+Y^+Z^-$ and its charge conjugate. Some difficulties are related to the existence of singular points on the v plane at the corners of this triangle. Each such point does not correspond to only one (or two) Coulomb systems, but rather to an infinite number of such systems. At a singular point two v coordinates equal zero and the third one equals unity, or in terms of masses two masses have a finite value and the third one has an infinite value. Such systems form a one-parameter series. The parameter is the ratio of the finite masses. For example, at point Z (see Fig. 1) we have $\lambda=m_X/m_Y$, $m_Z=\infty$ and at point X we have $\lambda=m_Y/m_Z\ge 1$, $m_X=\infty$.

Table I presents the numerical results (the total and

TABLE VII. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X=\infty m_e, m_Y=\lambda m_e$, $m_Z=m_e$. In the case of these systems the threshold energy equals $E_t(\lambda)=-0.5$ and $\lambda_t=2.335$.

λ	Total energy (E_H)	Binding energy (eV)
10.0	−0.540 099 10	−0.091 152 4
5.0	−0.516 707 61	−0.454 637 3
4.0	−0.509 746 57	−0.265 217 6
3.0	−0.502 872 09	−0.078 153 7
2.7	−0.501 271 41	−0.034 596 9
2.6	−0.500 844 27	−0.022 973 7
2.5	−0.500 483 88	−0.013 167 1
2.4	−0.500 195 15	−0.005 310 3
2.35	−0.500 077 48	−0.000 210 8
2.3	−0.499 976 44	+0.006 411 8
2.25	−0.499 890 45	+0.002 981 0
2.2	−0.499 817 61	+0.004 963 1
2	−0.499 618 85	+0.010 371 6

TABLE VIII. The total energies (in atomic units) and the binding energies (in electron volts) of three-body Coulomb systems $X^+Y^+Z^-$, where $m_X=\lambda m_e$, $m_Y=m_e$, $m_Z=\infty m_e$. In the case of these systems the threshold energy equals $E_t(\lambda)=-0.5\lambda$ and $\lambda_t=1.237$.

λ	Total energy (E_H)	Binding energy (eV)
1.0[a]	−0.527 751 016 507	−0.755 143 90
1.05	−0.542 346 92	−0.472 038 4
1.10	−0.559 600 03	−0.261 230 1
1.15	−0.579 285 77	−0.116 621 9
1.20	−0.601 156 30	−0.031 464 5
1.225	−0.612 786 86	−0.007 806 0
1.235	−0.617 539 89	−0.001 085 7
1.2365	−0.618 256 70	−0.000 182 4
1.2375	−0.618 735 29	+0.000 400 3
1.24	−0.619 933 65	+0.001 805 5
1.25	−0.624 751 85	+0.006 752 4
1.3	−0.649 237 05	+0.020 760 8

[a] $^\infty H^-$.

binding energies) for a number of symmetric systems $X^+X^+Z^-$ with the mass ratio $m_X/m_Z \geq 1$. These results include our previous results [7], where we considered the inverse condition $m_X/m_Z \leq 1$. The results in Table I and in Ref. [7] can be represented in terms of the v plane as the points which lie on the line OZ below and above the point A (Ps^-). An arbitrary system has at least one bound state. Below point A the discrete spectrum of the system $X^+X^+Z^-$ consists in the general case of a number of bound states. From Ref. [7] we know that the ^1P state appears at $m_Z/m_X=0.237\,026$, the $2\,^1S$ state at $m_Z/m_X=0.097\,998$, and the ^1D state at $m_Z/m_X=0.087\,070\,1$. In the limit $m_Z/m_X\to\infty$ the number of the bound states increases to infinity ($^\infty H_2^+$ ion). Note that the equation of the line OZ in the v triangle is $v_Y=v_X$, $v_Z=1-2v_X$. The energy of the positronium ion ($-0.262\,005\,070\,2E_h$), which was calculated using 900 basis functions, is the best value to date.

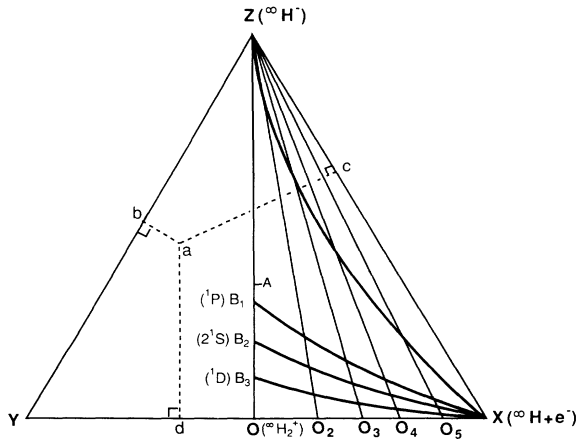

FIG. 1. The equilateral v triangle for the Coulomb three-body system with unit charges.

Tables II–VIII show the typical situation when a threshold point exists. We consider in Tables II–V the systems which, respectively, have the parameters

$$1.5v_Y=v_X,\quad v_Z=1-2.5v_X\ , \tag{6a}$$

$$2v_Y=v_X,\quad v_Z=1-3v_X\ , \tag{6b}$$

$$3v_Y=v_X,\quad v_Z=1-4v_X\ , \tag{6c}$$

$$4v_Y=v_X,\quad v_Z=1-5v_X\ . \tag{6d}$$

The thresholds points and the equations for the threshold energies are listed with each table. The lines generated by Eq. (6) in the v triangle cross the OX axis at the points O_2, O_3, O_4, and O_5 ($O_1\equiv O$) and contain the Z singular point. In Table VI the results for systems which are determined by the equation $v_Y=1-2v_X$, $v_Z=v_X$ are presented. This line contains the Ps^- system and crosses the XZ side of the v triangle at the middle point. It also has a threshold point.

The situation at the singular points X and Z is presented in Tables VII and VIII. These points have the threshold values listed in the tables. Note that at $\lambda=1$ the system at the point Z ($^\infty H^-$) is bound and the system at the point X ($^\infty H+e^+$) is unbound.

All threshold points in Tables II–VIII determine the boundary of the "stable region" for the Coulomb three-body systems with unit charges. The equation of the boundary has the form of Eq. (3b) and can be presented in terms of the binding energy and v coordinates as follows: $\varepsilon(v_X,v_Z)=0$. Note that the vanishing of the binding energy is related to the large difference in particle mass. Above the threshold the third particle (Y^+, say) cannot polarize the neutral "quasiatom" (X^+Z^-) enough (to produce a real bound state) if the mass ratio is less than the threshold value.

III. CONCLUSIONS

We have considered the bound-state spectra in the Coulomb three-body system with unit charges. It has been shown that the bound states in such systems exist not at arbitrary, but only at definite, values of the mass ratios; these lie in the "stable region." We have determined the position of the boundary of this "stable region" for the ground state in the dimensionless v coordinates. The situation is presented in Fig. 1. The use of a triangular description is similar to the one used to depict the composition of a three-component mixture in thermodynamics [16].

In conclusion, let us note a number of problems which should be investigated in the future. First, it will be important to consider in the same manner the excited states, including the states with $L\geq 1$. For the moment we know only that the boundary of the "stable region" for the general excited state crosses the OZ altitude at point B_i which lies below point A (Ps^-) in the v triangle (Fig. 1). The singular point X lies also on an arbitrary boundary. The threshold points can be determined only as a result of numerical calculations. Without these calcula-

tions we can only give a few typical qualitative boundaries for the "stable regions" in the v triangle, as in Fig. 1. However, at present the question of the intersection of different boundaries on the v plane is not fully clear. It can be shown that these threshold energy curves do not intersect in the cases of ground states with different L. In the case of exited states, this is not so clear. Hence, in principle, the order of the appearance of a new bound state in the discrete spectrum may be changed with continuous mass variation. In this last case additional degeneracy will be present at such intersection points. It will be interesting to test the central potential $V(r)$ in Eq. (16) found with the data of the ground-state calculations in the cases of excited states, including states with $L \geq 1$.

Second, for such systems the problem related to the existence of quasistationary states (prethreshold resonances) seems very interesting. These quasistationary states exist in the vicinity of the "stable-region" boundary. Such resonances are well known for a number of exotic and mesomolecular systems.

Third, it will be important to test a condition which follows from the general theory of weakly bound states. This condition can be formulated as the vanishing of the normal derivative of the binding energy on the boundary of the "stable region." If we use the equation of the boundary on the v plane as $\varepsilon(v_X, v_Z)=0$ we can obtain the condition

$$(\nabla\varepsilon\cdot\mathbf{n})|_{\Gamma}=0 ,$$

where $\mathbf{n}$ $[=\mathbf{n}(v_X, v_Z)]$ is the unit normal vector to the boundary of the "stable region" (Γ) on the v plane. This equation follows form the general theory of weakly bound two-body states in the field of an arbitrarily fast decrease in the potential (faster then r^2).

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