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Weakly bound ground states in three-body Coulomb systems with unit charges

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The stability of weakly bound ground states, with zero total angular momentum, in three-body Coulomb systems with unit charges, is studied by means of highly accurate variational calculations. Weakly bound ground states are predicted for a number of systems, including $d^+t^+p^-$, $t^+K^+\pi^-$, $\pi^+\mu^+\mu^-$, and $\pi^+\mu^+\pi^-$.

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I. INTRODUCTION

Three-body Coulomb systems have a unique role in nonrelativistic quantum mechanics. They are the simplest nontrivial systems which can be treated to extremely high accuracy by approximate quantum-mechanical methods even though they cannot be solved in closed form.

Consider the bound states of three point particles X, Y, and Z with unit charges interacting via Coulomb forces. Without loss of generality, the particles can be chosen to be X^+, Y^+, and Z^- because charges of both signs are needed to obtain bound states, and because charge-conjugation symmetry implies that $X^+Y^+Z^-$ is equivalent to $X^-Y^-Z^+$. The total and binding energies of $X^+Y^+Z^-$ depend only on the particle masses m_X, m_Y, and m_Z, respectively, or, more conveniently, the dimensionless coordinates $v_i = m_i/\sum_j m_j$ $(i=X,Y,Z)$. Only two of the v_i are independent since they sum to unity; we choose v_X and v_Z. Thus an arbitrary three-body system with unit charges can be represented by a point inside the v triangle with unit altitude [1]. The systems with stable states are drawn as points inside the so-called "region of stability." The boundary of this stability region is characterized by the vanishing of the binding energy and therefore by the equation

$$\varepsilon_{L\nu}(v_X, v_Z) = 0 ,$$

where L denotes the total angular momentum, and ν is the "vibrational excitation" or "principal" quantum number.

A partial understanding of the criteria for stable bound states in three-body Coulomb systems with unit charges has emerged from previous studies, primarily numerical calculations [1–6]. Stable ground states with $L=0$ and $\nu=0$ exist for three-body Coulomb systems only if the masses of the positive particles are comparable, i.e., $m_X \approx m_Y$ so that a neutral cluster formed from Z^- and the heavier positively charged particle can be polarized sufficiently by the third particle. Moreover, stable excited states $(L \geq 0, \nu \geq 1)$ exist only when the mass of the negative particle is relatively small in comparison with the masses of the positive ions. The ground state of symmetrical systems such as $X^+X^+Z^-$ is always bound.

However, the location of the boundary of stability needs further refinement especially in the form of new numerical results on prethreshold or weakly bound states which lie near the perimeter of the stability region. Moreover, weakly bound states are of experimental interest as well. Such systems have a sharp cluster structure; that is, when $m_X \geq m_Y$ they can be modeled with very good accuracy by two-body systems where the ion Y^+ moves in the field of the neutral cluster $[X^+Z^-]$. Weakly bound states, and even resonances, can be used to conserve a number of exotic species [7,8]. We do not wish to discuss here such well-known examples as μ catalysis of nuclear reactions where the weakly bound (1,1) state of system $d^+t^+\mu^-$ plays a remarkable role [9]. As a final motivation, we note that the presence of a weakly bound state in $X^+Y^+Z^-$ can significantly distort the cross section for the scattering of Y^+ from the unstable neutral moiety N which decays into X^+ and Z^- (as in the K^0 meson) with a characteristic decay time comparable to the total collision time [10].

The purpose of this paper is to report numerical results on some novel weakly bound ground states $(L=0, \nu=0)$ of three-body Coulomb systems $X^+Y^+Z^-$ to learn more about the border of stability. All three-body Coulomb systems with unit charges are relatively weakly bound; the binding energy is typically 5–10% of the total energy. We shall call a state weakly bound only if the binding energy ε is less than 1% of the total energy E of the system, that is, when $\varepsilon/E = \varepsilon/(\varepsilon + E_{\rm th}) \leq 0.01$ where $E_{\rm th}$ is the threshold or dissociation energy for the $X^+Y^+Z^- \longrightarrow X^+Z^- + Y^+$ process.

II. NUMERICAL RESULTS

All our calculations are variational. The ansatz is

$$\Psi = (1+\delta P_{12}) \sum_{k=1}^{M} C_k \exp(-\alpha_k r_{32} - \beta_k r_{31} - \gamma_k r_{12}) , \tag{1}$$

where P_{12} is a permutation operator, and $\delta=0$ for the nonsymmetrical systems considered in this work. The nonlinear parameters are chosen by a pseudorandom algorithm first used by Thakkar and Smith [11]. Further details can be found elsewhere [1,11]. The masses of the proton (p), deuteron (d), triton (t), muon (μ), and the K and π mesons, relative to the electron mass m_e, were taken from CODATA 1986 to be [16]

$$m_p/m_e=1836.152\,701\ ,\quad m_d/m_e=3670.483\,014\ ,$$
$$m_t/m_e=5496.921\,58\ ,\quad m_\mu/m_e=206.768\,262\ ,$$
$$m_K/m_e=966.1521\ ,\quad m_\pi/m_e=273.126\,95\ .$$

The conversion factor 2 Ry = 27.211 396 1 eV was used to obtain binding energies from total energies.

Table I shows that the deuteron-triton-antiproton system $d^+t^+p^-$ has a bound ground state, although it obviously does not have any other bound states. The table also includes results for the model (231) system with $m_X=2m_Z$ and $m_Y=3m_Z$ for comparison. Since particle masses are subject to experimental revision, we determined the constants $\alpha\approx0.224$ and $\beta\approx0.068$ (in "proton atomic units" where $m_p=1$) for the conversion formula

$$E'(d^+t^+p^-)=E(d^+t^+p^-)+\alpha(m_p'/m_t'-m_p/m_t)+\beta(m_p'/m_d'-m_p/m_d)\ ,$$

where the unprimed quantities are current values and primed quantities are revised ones. $\alpha\gg\beta$ lends further support to the cluster structure $[t^+p^-]+d^+$. The physical properties of $d^+t^+p^-$ are obviously of great interest since it is an anomalously weakly bound system with relatively heavy particles; the binding energy ≈-319 eV, while the value of the potential hole is $\approx-40\,000$ eV. Moreover, it has two competing decay channels: annihilation with width Γ_γ,

$$d^+t^+p^-=d^++n+n+1876.56\ \text{MeV}\ ,$$

and nuclear fusion with width Γ_f,

$$d^+t^+p^-=\alpha^{2+}+n+p^-+17.559\ \text{MeV}\ .$$

The ratio of these widths is approximately

$$\Gamma_f/\Gamma_\gamma\approx(l_{\rm tot}/l_{\rm CL})^3\approx10^3\ ,$$

where $l_{\rm CL}$ is a characteristic length of the $[t^+p^-]$ cluster (t^+-p^- distance), while $l_{\rm tot}$ is a characteristic length of $d^+t^+p^-$ (d^+-t^+ distance). Analysis of the neutron spectra, produced when this system decays, could lead to direct information about the geometry of the system and vice versa. Note that the binding energies of the bound states in the analogous symmetrical systems $d^+d^+p^-$ and $t^+t^+p^-$ which are not weakly bound can easily be determined with good accuracy from the data of Table I in Frolov and Bishop [1].

Results for the mesonic systems $p^+K^+\pi^-$, $t^+K^+\pi^-$, and $d^+K^+\pi^-$ are presented in Table II, and for $p^+K^+\mu^-$, $d^+K^+\mu^-$, and $t^+K^+\mu^-$ in Table III. These states turn out not to be weakly bound in the sense that the binding energies are greater than 1% of the total energies. However, it is interesting to note the decrease in the ε/E ratio as p^+ is replaced by d^+ and then t^+.

Table IV lists results for three-body Coulomb systems containing both muons and π mesons. Both systems are remarkably weakly bound. It is very interesting that there are no other known bound states in nonsymmetrical systems with muons and π and K mesons, although the corresponding symmetrical systems must have a bound ground state. We do not consider the latter here, since they are not weakly bound. Some results for such symmetrical systems can be found elsewhere [12]. Moreover, energies for Ps$^-$-like systems, such as $\mu^+\mu^-\mu^-$, can be obtained by simple rescaling of the Ps$^-$ energies, for example, $\varepsilon(\mu^+\mu^-\mu^-)=m_\mu\varepsilon(\text{Ps}^-)$. The results presented in Tables II–IV may be useful in meson physics because a number of such systems have been observed in nuclear experiments; see, for example, Refs. [13,14].

TABLE I. Total energies in p.a.u. ("proton" atomic units with $m_p=1$, and 1 p.a.u. of energy $\approx8.005\,163\,45$ fJ) and binding energies in eV (1 eV$\approx0.160\,217\,73$ aJ) for the ground S state of $d^+t^+p^-$. The threshold energy $\approx0.374\,803\,347\,77$ p.a.u. Total energies for the model (231) system defined by $m_X=2m_Z$ and $m_Y=3m_Z$ are also given in quasiatomic units ($m_Z=1$); the thresold energy is 0.375. M is the number of basis functions.

M	Total energy $d^+t^+p^-$	Binding energy $d^+t^+p^-$	Total energy (231) system
100	−0.381 188 995 6	−319.054 289	−0.381 363 214
200	−0.381 190 860 6	−319.147 471	−0.381 365 111
300	−0.381 190 898 2	−319.149 348	−0.381 365 149
400	−0.381 190 900 7	−319.149 473	−0.381 365 152
500	−0.381 190 901 2	−319.149 500	−0.381 365 153
600	−0.381 190 901 4	−319.149 509	−0.381 365 153
700	−0.381 190 901 5	−319.149 514	−0.381 365 153

TABLE II. Binding energies (in eV) for the ground states of $p^+K^+\pi^-$, $d^+K^+\pi^-$, and $t^+K^+\pi^-$ which have threshold energies $\approx$3234.893 7513 eV, 3458.714 003 0 eV, and 3540.180 973 1 eV, respectively.

M	$p^+K^+\pi^-$	$d^+K^+\pi^-$	$t^+K^+\pi^-$
100	−106.898 755	−69.712 353	−60.284 505
200	−107.566 339	−70.978 879	−61.803 549
300	−107.572 215	−70.999 516	−61.839 138
400	−107.572 704	−71.002 585	−61.844 488
500	−107.572 748	−71.002 799	−61.844 862
600	−107.572 766	−71.002 900	−61.845 036
700	−107.572 768	−71.002 933	−61.845 101

TABLE III. Binding energies (in eV) of the ground states of $p^+K^+\mu^-$, $d^+K^+\mu^-$, and $t^+K^+\mu^-$ which have threshold energies $\approx$2528.494 086 0, 3458.714 0030, and 3540.180 973 1 eV, respectively.

M	$p^+K^+\mu^-$	$d^+K^+\mu^-$	$t^+K^+\mu^-$
100	−122.889 382	−98.305 775	−91.796 119
200	−122.978 323	−98.406 403	−91.913 322
300	−122.979 448	−98.408 099	−91.915 649
400	−122.979 520	−98.408 176	−91.915 731
500	−122.979 526	−98.408 185	−91.915 741
600	−122.979 528	−98.408 187	−91.915 743
700	−122.979 528	−98.408 188	−91.915 744

TABLE IV. Binding energies (in eV) of the ground states of $\pi^+\mu^+\mu^-$ and $\pi^+\mu^+\pi^-$ which have threshold energies $\approx$1601.116 1709 eV and 1858.041 4268 eV, respectively.

M	$\pi^+\mu^+\mu^-$	$\pi^+\mu^+\pi^-$
200	−8.970 36	−2.264 72
300	−9.683 52	−4.070 82
400	−9.719 67	−4.222 03
500	−9.746 14	−4.359 05
600	−9.747 22	−4.368 96
700	−9.748 00	−4.376 02
800	−9.748 52	−4.382 34

III. DISCUSSION

As mentioned above, a three-body Coulomb system with unit charges such as $X^+Y^+Z^-$ has a bound state if the lightest positive ion Y^+ can polarize the neutral cluster $[X^+Z^-]$ sufficiently. The ground state of an arbitrary $X^+Y^+Z^-$ can be considered [1] a weakly bound state of the two-body system consisting of the neutral cluster $[X^+Z^-]$ and the ion Y^+. This simplification allows us to introduce a model two-body potential that, at least initially, can be chosen as a central potential $V(r)$ that does not depend on the angular momentum l. This reduces the three-body problem to the two-body radial Schrödinger equation

$$\{(2\mu_{XZ,Y})^{-1}[-\partial^2/\partial r^2+l(l+1)/r^2]+V(r)\}\psi_l(r) = E\psi_l(r) , \quad (2)$$

where $\mu_{XZ,Y}=(m_X+m_Z)m_Y/(m_X+m_Y+m_Z)$ is the reduced mass of the cluster $[X^+Z^-]$ and the ion Y^+, and E and l are the binding energy and total angular momentum of the underlying three-body system. Then the number of bound S states (N) in the initial three-body problem is the number of bound S states for the effective two-body system which can be obtained via the Bargman theorem [15]:

$$N=2\mu_{XZ,Y}\int_0^\infty r|V(r)|dr . \quad (3)$$

It is possible, in principle, to construct a model potential $V(r)$ by using Eqs. (2) and (3) with the results of many binding energy calculations for bound states of three-body Coulomb systems with unit charges, including prethreshold states. Then the potential can be used in the correlation of scattering data. Such an investigation would be worth undertaking.

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