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An analytic and parameter-free wavefunction for studying the stability of three-body systems

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Abstract An analytic wavefunction is proposed for the ground state of general atomic three-body systems in which two light particles are negatively charged and the third (heavy) is positively charged. By construction the wavefunction (i) has the same analytical form for all systems; (ii) is parameter-free; (iii) is nodeless; (iv) satisfies all two-particle cusp conditions; and (v) yields reasonable ground state energies for several three-body systems, including the prediction of a bound state for H^-, D^-, T^- and Mu^-. Simple polynomial fits are provided for certain important subcases, allowing for a rapid estimate of the ground state energy and of the stability of three-body systems.

Keywords Three-body systems · Stability · Cusp conditions

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1 Introduction

In a previous paper [1], we have proposed a simple and pedagogical wavefunction for the ground *S* state of two-electron atoms with a nuclear mass considered as infinite. Here, we generalize it to more general atomic three-body systems in which one of the particles is positively charged and heavier than the other two which are

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negatively charged. The aim is to have a simple wavefunction for the ground state which has a unique mathematical form for all situations, is nodeless and satisfies all two–body cusp conditions [2]. Moreover, we want this function to be parameter free, so that it is fully determined given a set of three charges and three masses. Outside the fundamental and spectroscopical importance of finding a unique mathematical wavefunction for many (traditional and exotic) three–body systems, the result should be of interest to the collision community. Indeed, simple enough, but sufficiently accurate, wavefunctions are very useful as a starting point for cross sections calculations; besides, the importance of the fulfilment of the Kato cusp conditions by the trial wavefunction has been pointed out for the study of several physical processes, such as photon or electron impact double ionization (see, e.g., [3–5]).

As in paper [1], the simplicity of the proposed wavefunction is such that analytical expressions for the ground state energy can be derived. Hence, the results provide a useful predictive and simple tool to estimate the energy, and therefore to study the stability, of exotic Coulombic three–body systems. To our knowledge, such a tool is not available in the literature.

2 Simple parameter-free ground state wavefunctions

Consider the general case of three charged particles z_i and masses m_i ($i = 1, 2, 3$), and denote $[m_1 m_2 m_3]$ the three-body system. We define the quantities $\nu_{ij} = \mu_{ij} z_i z_j$ with the reduced masses given by $\mu_{ij} = \frac{m_i m_j}{m_i + m_j}$ ($i \neq j = 1, 2, 3$). We will deal, in what follows, with atomic systems where 3 will be the heaviest particle, positively charged ($z_3 > 0$), and the two lighter particles (1 will be the lightest) are negatively charged, $z_1 < 0$ and $z_2 < 0$; the quantities ν_{13} and ν_{23} are negative while ν_{12} is positive. We further choose to place particle 3 at the origin of the coordinates, so that the interparticles coordinates are r_1, r_2 and r_{12}.

The generalization of the Ψ_{ARG} wavefunction, which was suggested for infinite nuclear mass helium–like systems [1], reads

$$\Psi_{ARG}^{\mathrm{GEN}} = N_{ARG}^{\mathrm{GEN}}\, e^{\nu_{13} r_1 + \nu_{23} r_2}\, (1 + \nu_{12} r_{12}) \left[1 + c(r_1^2 + r_2^2)\right], \tag{1}$$

where c has to be determined (atomic units are used throughout: $\hbar = m_e = e = 1$). The wavefunction satisfies exactly Kato's two-body "cusp conditions" [2] which provide the correct linear behavior that $\Psi(r_1, r_2, r_{12})$ must have close to the singularity points. Let H be the non-relativistic Hamiltonian. The mean energy $E_{ARG}^{\mathrm{GEN}} = \langle \Psi | H | \Psi \rangle \,/\, \langle \Psi | \, \Psi \rangle$ and the normalization constant N_{ARG}^{GEN} can be evaluated analytically in terms of c and the three sets (m_i, z_i). The optimization of the energy with respect to c, provides an analytic positive optimal c_{opt} value, and thus the energy E_{ARG}^{GEN} is expressed only in terms of the three charges and three masses.

It is useful to define the following dimensionless ratios

$$r = \frac{m_2}{m_3}, \qquad u = \frac{z_2}{z_3}, \qquad t = \frac{m_2}{m_1}. \tag{2}$$

The value $r = 0$ corresponds to the virtual case of an infinitely heavy particle 3. While the analytical expression in the general case are quite large, when $z_1 = z_2 < 0, z_3 > 0$ and in important subcases, relatively simple analytical expression for the optimized energy—and the coefficient c_{opt}—can be obtained in terms of the ratios (2).

3 Illustration: stability in the cases $m_1 = m_2$ and $m_3 \to \infty$

In [6] we have considered several examples of traditional and exotic three-body systems with unit charges $z_1 = z_2 = -1$ and arbitrary masses, including cases with $z_3 = 1$ and $z_3 = 2$. It turned out that the optimized values c_{opt}/ν_{13}^2 are always positive and smaller than one. In view of the simplicity of $\Psi_{ARG}^{\mathrm{GEN}}$, the ground state energies obtained can be considered as rather good [6]. Of course they cannot compete with advanced variational wavefunctions which involve large number of basis functions (see, e.g., [7, 8] and references therein). The latter, however (i) generally do not satisfy Kato cusp conditions exactly; and (ii) do not have a predictive character since they have to be optimized each time for a given three–body system.

To study the stability of a three-body system $[m_1 m_2 m_3]$, one should compare its ground state energy $E[m_1 m_2 m_3]$ with that of the separate two-body sub-systems $E[m_i m_j]$ $(i \neq j)$. If m_1 is the lightest particle, the stability condition reads [9]

$$E[m_1 m_2 m_3] < -\frac{1}{2}(z_2 z_3)^2 \mu_{23} = E[m_2 m_3]. \tag{3}$$

Consider the case where the two particles 1 and 2 are equal $m_1 = m_2$, $z_1 = z_2 < 0$. The optimized c_{opt}/ν_{13}^2 and the energy predicted $E_{ARG}^{\mathrm{GEN}}/E[m_2 m_3]$ depend only on the ratios $r = m_2/m_3$ and $u = z_2/z_3$. By fixing the charge ratio u to a given value, we may then plot these quantities as a function of r. From Fig. 1 we observe that for $u = -1/2$, the ratio $E_{ARG}^{\mathrm{GEN}}/E[m_2 m_3]$ is always greater than 1 so that the wavefunction $\Psi_{ARG}^{\mathrm{GEN}}$ predicts a stable system for any value of $r \in [0, 1]$. For $u = -1$, on the other hand, for $r > 0.47$ the three-body system is predicted not to be stable. Since the quantities c_{opt}/ν_{13}^2 and $E_{ARG}^{\mathrm{GEN}}/E[m_2 m_3]$ vary smoothly with the ratio r, in order to provide a useful predictive tool, we may also give a simple polynomial fit of these curves. For example, for $u = -1$, we find

$$\begin{aligned} c_{opt}/\nu_{13}^2 &= 0.01[9.4724 + 4.7368r - 0.69674r^2 - 0.43207r^3 + 0.56766r^4 \\ &\quad -0.44010r^5 + 0.29281r^6 - 0.18598r^7 + 0.11993r^8 - 0.081364r^9] \end{aligned} \tag{4}$$

$$\begin{aligned} E_{ARG}^{\mathrm{GEN}}/E[m_2^- m_3^+] &= 0.01[103.96 - 11.649r + 9.3050r^2 - 6.7775r^3 + 4.5571r^4 \\ &\quad -2.8469r^5 + 1.6592r^6 - 0.90620r^7 + 0.46847r^8 - 0.23475r^9] \end{aligned} \tag{5}$$

For given masses $m_1 = m_2$ and m_3, and the ratio $u = z_2/z_3$, one may directly find the optimal c_{opt} value and the corresponding energy.

The stability condition (3) gives, for a given ratio $r = m_1/m_3$, a critical value of the charges ratio $u = z_2/z_3$. The three-body system is stable if the condition

$$-\frac{1}{u} = -\frac{z_3}{z_2} > 0.94537 + 0.1465r - 0.08221r^2 + 0.04499r^3 - 0.0196r^4 + 0.00443r^5 \tag{6}$$

is satisfied. As a particular case, we may consider an infinitely heavy m_3 particle ($r = 0$), so that the critical charge ratio is $-z_3/z_2 > 0.94537$. This value has to be compared to 0.91102 given in the literature [10].

A similar study can be done for three-body systems $[m_1 m_2 \infty]$ for which particle 3 has a virtual infinite mass [6]. The optimized c_{opt}/ν_{13}^2 and the predicted energy $E_{ARG}^{\mathrm{GEN}}/E[m_2 m_3]$ depend only on the ratios $t = m_2/m_1$ and $u = z_2/z_3$. By fixing the mass ratio t to a given value, we may then plot these quantities as a function of u (see

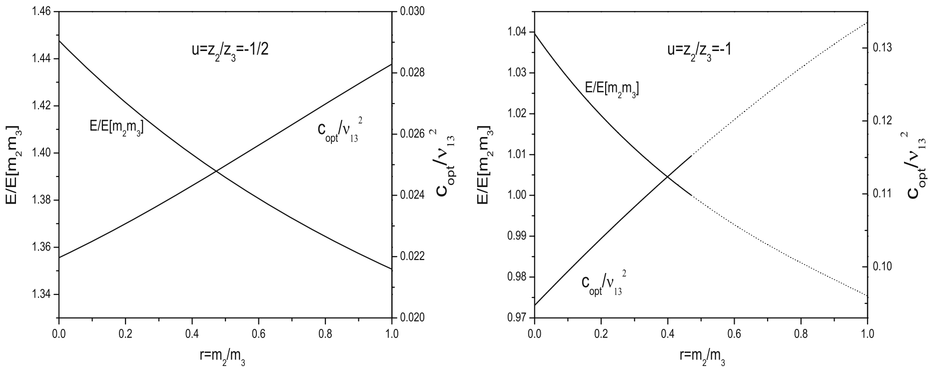

Fig. 1 Energy ratio $E_{ARG}^{\mathrm{GEN}}/E[m_2 m_3]$ and optimal value c_{opt}/ν_{13}^2 as a function of $r = m_2/m_3$ for $u = z_2/z_3 = -1/2$ (*left*) and $u = z_2/z_3 = -1$ (*right*). The three-body system is predicted to be stable (*solid lines*) or unstable (*dotted lines*)

Fig. 3 of [6] for $t = 1$), and again deduce a polynomial fit in u. With these fits one may easily find the energies for the $^\infty$He (or other helium-like ions) infinite nuclear mass systems, with arbitrary light particles m_1 and m_2. For example, take a nucleus such as $^\infty Li^{3+}$, $u = -1/3$; the fits yield $c_{opt}/\nu_{13}^2 = 0.0103777$ and $E_{ARG}^{\mathrm{GEN}}/E[m_2 m_3] = 1.614808$. Hence $E_{ARG}^{\mathrm{GEN}} = -7.26664$ for the $[e^- e^- \, ^\infty Li^{3+}]$ system (in agreement with the value already given in [1], and in fair agreement with the numerically "*exact*" value -7.2799 [8]) and $E_{ARG}^{\mathrm{GEN}} = -1502.51$ for the $[\mu^- \mu^- \, ^\infty Li^{3+}]$ system. For each ratio $t = m_2/m_1$ a critical value of the charges ratio $u = z_2/z_3$ is found. With the wavefunction $\Psi_{ARG}^{\mathrm{GEN}}$, the system $[m_1 m_2 \infty]$ is predicted to be stable if the condition

$$-\frac{1}{u} = -\frac{z_3}{z_2} > 1.25722 + 0.08655t - 0.18297t^2 - 0.48018t^3 + 0.26458t^4 \tag{7}$$

is satisfied. From this, an analytical expressions for the critical charge can be deduced.

4 Concluding remarks

We have proposed a simple wavefunction for the ground state of three-body coulombic systems in which one of the particle (positively charged) is heavier than the other two (negatively charged). The wavefunction $\Psi_{ARG}^{\mathrm{GEN}}$: (i) has the same form for all systems; (ii) is parameter–free; (iii) is nodeless; (iv) satisfies all two-particle cusp conditions; and (v) yields reasonable ground state energies for several systems.

The simplicity of the proposed wavefunction is such that analytical expressions for the ground state energy can be derived. Hence, the results provide a useful predictive and simple tool to estimate the energy, and therefore to study the stability, of exotic three–body systems.

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