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Article (Published Version)

King, Andrew W, Herlihy, Patrick E and Cox, Hazel (2014) Predicting the stability of atom-like and molecule-like unit-charge Coulomb three-particle systems. *Journal of Chemical Physics*, 141 (4). 044120. ISSN 0021-9606

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Citation: *The Journal of Chemical Physics* **141**, 044120 (2014); doi: 10.1063/1.4890658

View online: <http://dx.doi.org/10.1063/1.4890658>

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# Predicting the stability of atom-like and molecule-like unit-charge Coulomb three-particle systems

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(Received 29 May 2014; accepted 9 July 2014; published online 28 July 2014)

Non-relativistic quantum chemical calculations of the particle mass,  $m_2^\pm$ , corresponding to the dissociation threshold in a range of Coulomb three-particle systems of the form  $\{m_1^\pm m_2^\pm m_3^\mp\}$ , are performed variationally using a series solution method with a Laguerre-based wavefunction. These masses are used to calculate an accurate stability boundary, i.e., the line that separates the stability domain from the instability domains, in a reciprocal mass fraction ternary diagram. This result is compared to a lower bound to the stability domain derived from symmetric systems and reveals the importance of the asymmetric (mass-symmetry breaking) terms in the Hamiltonian at dissociation. A functional fit to the stability boundary data provides a simple analytical expression for calculating the minimum mass of a third particle required for stable binding to a two-particle system, i.e., for predicting the bound state stability of any unit-charge three-particle system. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4890658>]

## INTRODUCTION

Helium and the hydrogen molecule and its ions have been the “laboratory” of quantum chemistry for over 80 years, driving attempts to accurately model the correlated motion of electrons and the chemical bond. Yet much of popular modern day quantum chemistry is built on hydrogenic wavefunctions, and electron correlation is dealt with through various increasingly sophisticated schemes. Popelier<sup>1</sup> recently brought together ideas and methods not prevalent in current mainstream quantum chemistry in his inspiring book “Solving The Schrödinger Equation: Has Everything Been Tried?” In this vein, one such method is the series solution method, which obviates the need for integration. This paper is concerned with solving the “the mother equation of chemistry,”<sup>1</sup> namely the time-independent Schrödinger equation, for three-particle Coulomb systems. It is solved here using a series solution method developed by Pekeris for helium<sup>2</sup> and extended by Cox and others to (i) include the finite mass of all particles present,<sup>3,4</sup> and (ii) unify the accuracy of the treatment of atomic and molecular three-particle systems.<sup>5,6</sup> In these high accuracy quantum chemical calculations, all particles are treated equivalently, and a coordinate system is used that includes the “ $r_{12}$ ” term, i.e., the distance between like-charged particles. Thus this methodology not only allows for the possibility of treating electron correlation directly and is without recourse to the Born-Oppenheimer (B-O) approximation, it also allows for a treatment where all the particles are of similar mass (e.g., the positronium or muonium negative ion).<sup>5,7</sup>

In our recent paper,<sup>5</sup> henceforth referred to as I, a lower bound to the stability of unit-charge three-particle systems was presented. It was shown that by treating all particle masses as finite and using a Laguerre-based wavefunction

with two nonlinear parameters, and by taking advantage of charge conjugation invariance, it was possible to move smoothly from electron-correlated atomic systems (such as  $H^-$ ) to non-B-O molecular systems (such as  $H_2^+$ ). Bound state stability is fundamental to a large part of chemistry and physics. It enables, for example, an understanding of the chemical reactivity and spectroscopy of atoms and molecules. Therefore, it would be extremely useful to be able to determine, *a priori*, the bound state stability of a particular system, without detailed calculation. This is the aim of the present paper.

Reported here is the calculation of an “exact” stability bound for unit-charge three-particle Coulomb systems. This uses a novel variational approach formulated by Rebane and Kuzminskii for calculating the threshold mass of the detaching particle at dissociation of an atomic-molecular system<sup>8</sup> and is performed with a Laguerre-based wavefunction in perimetric coordinates. The results are presented on a reciprocal mass ternary diagram and compared to the lower bound stability boundary recently calculated in I, to consider the topology of the stability domain due to mass-symmetry breaking. Finally a simple algorithm is provided for predicting the stability of a given system.

## BOUND STATE STABILITY

In this work, a system is defined as stable if it has at least one bound state below the lowest continuum threshold. In the case of a three-particle system such as  $\{m_1^\pm m_2^\pm m_3^\mp\}$ , the lowest continuum threshold corresponds to dissociation into the heavier bound pair and an isolated particle at rest at infinity. Thus, the energy of the lowest dissociation threshold coincides with the ground-state energy of the two-particle heavier mass pair. In the case of three unit charges  $\{m_1^\pm m_2^\pm m_3^\mp\}$ , if we assume that  $m_1 \geq m_2$ , then the threshold energy,  $E_{th}$ , is simply the ground state energy of the hydrogen-like atom consisting

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of particles 1 and 3, i.e.,

$$E_{th} = E(m_1, m_3) = -\frac{1}{2}\mu_{13} = -\frac{1}{2}\frac{m_1 m_3}{m_1 + m_3} \\ = -\frac{1}{2}\frac{1}{m_1^{-1} + m_3^{-1}}. \quad (1)$$

Here, and throughout, atomic units are used. The critical mass of a third particle,  $m_2$ , sufficient to bind to a two-particle system, has been investigated in a number of ways. Assuming  $m_1 \geq m_2$  the following schemes have been employed:

- (i) Repeated energy calculations. For a given mass pair  $\{m_1^\pm, m_3^\mp\}$  the mass of  $m_2$  can be varied until  $E_0$ , the three-particle energy, coincides with  $E_{th}$ . Several authors have successfully used this method. However, it requires numerous variational energy calculations for a range of  $m_2$  values for each given mass pair.
- (ii) Mass-symmetry breaking. It is known that all symmetric systems (i.e.,  $m_1 = m_2$ ) are stable to dissociation.<sup>9</sup> Therefore, the Hamiltonian for an arbitrary system is written as a sum of symmetric (under  $1 \leftrightarrow 2$  exchange) and anti-symmetric terms, i.e.,  $\hat{H} = \hat{H}_S + \hat{H}_A$ . The variational principle is used to derive the ground state energy of the asymmetric system using the symmetric ground-state wavefunction,  $\psi_s$  of  $\hat{H}_S$ , as trial wavefunction. Using the relative excess binding energy of the symmetric three-particle system,  $(E_0 - E_{th})/E_{th}$ , as a function of the uniquely charged particle, Richard and co-workers<sup>10,11</sup> derived an explicit expression for the lower bound to stability, i.e., the boundary between stable and unstable unit-charge three-particle systems.
- (iii) Variational method for mass. Rebane and Kuzminskii have shown that it is possible to solve for the mass of  $m_2$  directly using a variational method.<sup>8</sup> Given that the energy is known at the boundary, i.e.,  $E_0 = E_{th}$ , this can be substituted into the Schrödinger equation. The Schrödinger equation can then be rearranged and solved as a generalised eigenvalue problem. This allows direct calculation of the threshold value of particle mass  $m_2^\pm$  via a single calculation for a given mass pair  $\{m_1^\pm, m_3^\mp\}$ .

In I we used scheme (ii) to calculate an accurate lower bound to stability using high accuracy non-relativistic symmetric energies. In this work, scheme (iii) is used to determine the mass  $m_2$  for a series of mass pairs  $\{m_1^\pm, m_3^\mp\}$ .

A beautiful property of Coulomb Hamiltonians is the mass-scaling rule: scaling the masses by a factor  $x$  is equivalent to scaling the energy (and shrinking the length) by the same factor. The dissociation stability (or instability) remains unchanged. This means that a system containing  $N$  particles depends, at most, on  $(N - 1)$  mass ratios.<sup>11</sup> Furthermore, Martin *et al.*<sup>10</sup> have shown that all possible unit-charge three-particle systems can be represented on a ternary diagram in terms of the normalized reciprocal mass fraction coordinates:

$$a_i = \frac{1/m_i}{1/m_1 + 1/m_2 + 1/m_3}, \quad i = 1, 2, \text{ or } 3, \quad (2)$$

such that

$$a_1 + a_2 + a_3 = 1. \quad (3)$$

## METHOD

The non-relativistic Schrödinger equation for the S-states of unit charge, three-particle, Coulomb systems of the form  $\{m_1^\pm, m_2^\pm, m_3^\mp\}$ ,  $m_1 \geq m_2$  is considered. Rebane and Kuzminskii<sup>8</sup> formulated a method for the direct calculation of the threshold mass,  $m_2$ , by deriving the generalised eigenvalue equation (4) using the calculus of variations,

$$L\psi_j = \lambda_j M\psi_j, \quad j = 0, 1, 2, \dots, \quad (4)$$

where  $L$  is a self-consistent operator bounded from below,  $M$  is a positive, definite, self-conjugate operator, and the eigenvalues  $\lambda$  are extremal values resulting from the vanishing of the first variation. They showed that a particular case of (4) can be used to determine the threshold mass  $m_2$ , where the operators are defined as

$$L = -\frac{\nabla_1^2}{2m_1} - \frac{\nabla_3^2}{2m_3} + \frac{1}{r_{12}} - \frac{1}{r_{13}} - \frac{1}{r_{23}} - E_{th}(m_1, m_3), \\ M = -\frac{\nabla_2^2}{2}, \quad (5)$$

and the smallest eigenvalue  $\lambda$  corresponds to the threshold mass of particle 2, i.e.,

$$m_2 = -\frac{1}{\lambda}, \quad (6)$$

where this is the minimum mass of particle 2 for which the three-particle system is still stable.

This method is used in the present work to calculate the threshold value of  $m_2$  for a range of mass ratios  $m_1/m_3$ . As in I, the centre of mass motion is separated off and the translation-free coordinates are chosen to be the inter-particle distances  $r_1, r_2$  and  $r_3$  corresponding to the inter-particle distances 3-1, 3-2 and 1-2, with the origin at the third particle. The resulting equation of motion involves two (pseudo-)particles with reduced masses and a mass polarization interaction coupling the momenta of the particles at the origin of the coordinates. The equation is rearranged to the form (4) by factoring out the reciprocal mass of  $m_2$ . The problem is then recast in perimetric coordinates, defined as  $z_i = r_j + r_k - r_i$ , where  $i, j$ , and  $k$  denote cyclic permutation of 1, 2, and 3.

The resulting generalised eigenvalue equation is solved using a series solution method by expanding the wavefunction in a triple orthogonal set of Laguerre functions in scaled perimetric coordinates:

$$\psi(z_1, z_2, z_3) = e^{-\frac{1}{2}(\alpha z_1 + \beta z_2 + \gamma z_3)} \\ \times \sum_{l,m,n=0}^{\infty} A(l, m, n) L_l(\alpha z_1) L_m(\beta z_2) L_n(\gamma z_3). \quad (7)$$

This results in a 57-term recursion relation between the coefficients, which is used to form a sparse secular determinant that is solved in truncated form to give the eigenvalues as a function of basis set size  $N$ . For symmetric systems with fermionic exchange it was necessary to impose the constraint  $\alpha = \beta$  on the nonlinear variational parameters to take advantage of the useful quasi-orthogonal character of the wavefunction. However, no such constraint is necessary in this work

with non-identical like-charged particles, and all three non-linear parameters ( $\alpha$ ,  $\beta$ ,  $\gamma$ ) are varied. The parameters are optimised to minimize the mass using a conjugate gradients routine.<sup>12</sup> As in I, the mass of the lightest particle was set to 1, and the threshold energies were calculated using the most recent CODATA masses (in units of  $m_e$ ) for the muon, tauon, proton, deuteron, and triton, i.e.,  $m_\mu = 206.768\ 284\ 3$ ,  $m_\tau = 3477.15$ ,  $m_p = 1836.152\ 672\ 45$ ,  $m_d = 3670.482\ 965\ 2$  and  $m_t = 5496.921\ 526\ 7$ .<sup>13</sup>

## RESULTS AND DISCUSSION

### Variational mass

The minimum mass of a third particle required to bind to selected two-particle atomic systems is given in Table I in electron atomic units. The masses presented are considered accurate to 2 significant figures (s.f.) and were calculated using a 3654-term basis; the rate of convergence, even for similar systems, is not uniform. Selected calculations were also performed using a 5456-term wavefunction but did not lower the mass significantly. The accuracy is several orders

of magnitude less than that achieved for the energy using the same methodology with much smaller matrices. Rebane and Kuzminskii had slightly greater success and reported mass values to 3 s.f. with a significantly smaller and more flexible exponential basis with 60 nonlinear parameters. However, it is still quite efficient to use large Laguerre-based wavefunctions as given the quasi-orthogonality, the non-diagonal elements of the Hamiltonian and overlap matrices are zero in most cases, and the accuracy reported is adequate for the purposes of the present paper.

### Stability boundary

A stability boundary is determined using the values in Table I and plotted on a reciprocal mass ternary diagram (Figure 1, green/solid line). This is referred to here as the “exact” stability boundary, as it is calculated using the exact threshold energy, with a precision determined by the accuracy of the threshold mass calculated variationally. It is to be compared with the lower bound stability calculated using the wavefunction of the symmetric systems (Figure 1, blue/dashed line). The proofs provided by Richard and

TABLE I. The smallest (threshold) value of mass  $m_2$  (in electron mass units) required for binding in atoms and molecules of the form  $\{m_1^\pm m_2^\pm m_3^\mp\}$  calculated using a 3654-term wavefunction, with selected systems calculated using a 5456-term wavefunction given after the slash; the uncertain digits are given in parentheses. The normalised reciprocal mass of the uniquely charged particle ( $a_3$ ) and the normalised reciprocal mass difference of the like-charged particles are also given.

$m_1$	$m_3$	$m_1/m_e$	$m_2$ threshold	$a_3$	$a_2 - a_1$
t	e	5496.9215267	2.2(19)	0.689299	0.310450
d	e	3670.4829652	2.2(17)/2.2(12)	0.689022	0.310602
$\tau$	e	3477.15	2.2(15)/2.2(12)	0.688846	0.310758
p	e	1836.15267245	2.2(15)/2.2(11)	0.688699	0.310550
$\mu$	e	206.7682843	2.2(06)	0.685787	0.307580
t	$\mu$	5496.9215267	43(9.0)	0.662837	0.287298
d	$\mu$	3670.4829652	42(8.8)	0.649983	0.276786
$\tau$	$\mu$	3477.15	42(7.1)	0.647837	0.275116
p	$\mu$	1836.15267245	39(7.7)	0.612589	0.249445
t	p	5496.9215267	25(87)	0.489268	0.183868
d	p	3670.4829652	20(94)	0.420686	0.158419
$\tau$	p	3477.15	20(27)	0.410850	0.155242
t	$\tau$	5496.9215267	34(17)	0.377345	0.145266
t	d	5496.9215267	34(75)	0.367097	0.142657
d	$\tau$	3670.4829652	25(40)	0.301559	0.127091
e	e	1	0.69(96)/0.69(87)	0.291542	0.125375
$\tau$	d	3477.15	24(59)	0.281830	0.123169
d	t	3670.4829652	27(37)	0.221925	0.113365
$\tau$	t	3477.15	26(03)	0.213107	0.113103
p	$\tau$	1836.15267245	14(00)	0.185976	0.109653
p	d	1836.15267245	14(04)	0.178161	0.109548
p	t	1836.15267245	14(36)	0.127852	0.106646
$\mu$	p	206.7682843	164.(8)/164.(6)	0.0475714	0.107537
$\mu$	$\tau$	206.7682843	16(4.9)	0.0257035	0.109802
$\mu$	d	206.7682843	16(4.9)	0.0243838	0.109909
$\mu$	t	206.7682843	16(4.9)	0.0164142	0.110845
e	$\mu$	1	0.79(93)	0.00214394	0.111257
e	p	1	0.79(70)/0.79(63)	0.000241490	0.112932
e	$\tau$	1	0.79(68)	0.000126197	0.122264
e	d	1	0.79(68)	0.000120809	0.113021
e	t	1	0.79(68)	$8.06709 \times 10^{-5}$	0.113037



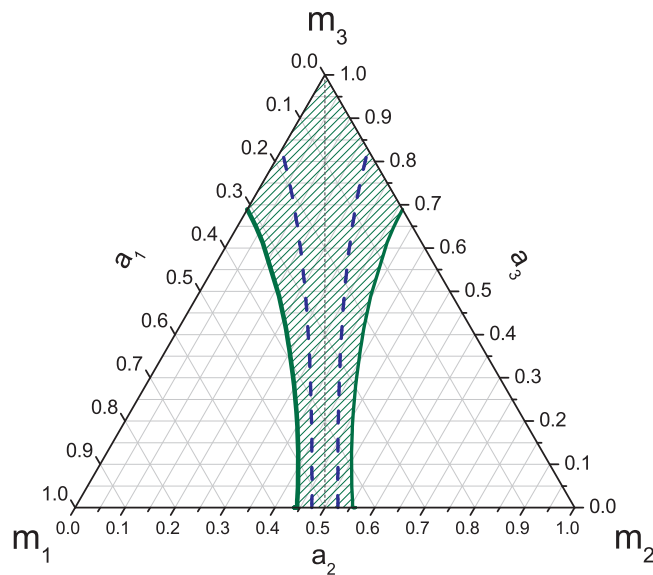


FIG. 1. The “exact” stability boundary (green/solid) calculated using the threshold mass of the third particle,  $m_2$ , in a three-particle system of the form  $\{m_1^\pm m_2^\pm m_3^\mp\}$  (data Table I), compared with the lower bound to stability (blue/dashed) derived from the binding energies of the systems along the central symmetry axis (grey/dotted). All systems within the green/solid boundary lines, sit within the stability domain (shaded green) and are stable to dissociation.

co-workers<sup>10,11</sup> regarding the topology of the stability domain remain valid; therefore all systems enclosed within the green boundary (shaded green) are stable to dissociation.

Prevalent species in chemical physics, such as  $\text{H}^-$ ,  $\text{H}_2^+$ , their isotopes and their muonic variants are found to cluster around the apex of the ternary diagram for molecular systems (such as,  $d^+ t^+ \mu^-$  known to catalyse nuclear fusion at room temperature<sup>14–16</sup>) and the central base of the triangle for atomic systems (such as  $e^- e^- \mu^+$ , observed as an impurity during muon spin resonance spectroscopy which is used to probe hydrogen impurities in semiconductors and a range of materials)<sup>17</sup> and are thus stable.

It is clear from Figure 1 that the lower bound stability underestimates the stability width, at large values of  $a_3$  as anticipated,<sup>10</sup> but also underestimates the width at small values of  $a_3$ . This is supported by the data in Table I, which provides  $a_3$ , the height of the point from the horizontal axis, and  $a_2 - a_1$ , which is proportional to the distance from the central symmetry axis and thus is a measure of stability. It indicates that molecular-like systems, i.e.,  $m_1, m_2 \gg m_3$ , are less affected by the mass difference of the like charged particles as the system remains stable when  $m_2 \ll m_1$ , than atomic-like systems,  $m_1, m_2 \ll m_3$ .

There are two competing forces in any three-particle system as a result of the following properties of the Hamiltonian:<sup>18</sup>

- (1) The ground state energy is a concave function of each inverse mass. Thus, as  $m_2$  decreases the energy is destabilized. Therefore, for a fixed  $m_1$  and  $m_3$ , as  $m_2$  becomes lighter the system is destabilized. Physically,  $m_2$  ceases to have sufficient mass to be confined to the potential well resulting from the polarization interaction with the neutral atom  $\{m_1, m_3\}$ .<sup>8</sup>

- (2) The ground state energy of the symmetric ( $m_1 = m_2$ ) Hamiltonian has its energy lowered if a symmetry-breaking term ( $m_1 \neq m_2$ ) is added. When applying the variational principle to the asymmetric Hamiltonian with the symmetric ground state as trial wavefunction, the energy lowering of the symmetry breaking term is proportional to  $(m_2^{-1} - m_1^{-1})$ ; the difference being of second order in  $(m_2^{-1} - m_1^{-1})/2$ . Therefore, for fixed  $m_1$  and  $m_3$ , as  $m_2$  gets lighter, the difference becomes greater and the stabilization from the symmetry breaking increases.

Korobov and Richard have analysed mass-symmetry breaking in three-particle systems by estimating the first- and second-order perturbation terms calculated with the wavefunction of a symmetric configuration.<sup>18</sup> They conclude that the symmetric terms dominate for molecular-type systems, while the asymmetric terms win for atomic-like systems. This is illustrated nicely in the data presented in Table I. For example, in the case where  $m_1, m_2 \gg m_3$ , the molecular type systems  $\{d, m_2, e\}$ ,  $\{p, m_2, e\}$ , and even  $\{\mu, m_2, e\}$ , the mass  $m_2$  is fairly insensitive to the mass difference and the stability is controlled by the concavity. In these cases the Born-Oppenheimer approximation applies, with the consequence that decreasing the mass of one of the positive charges, i.e.,  $m_2$ , does not ruin stability as the heavy particles experience an effective two-body potential. Thus the stability depends primarily on the sum of the inverse masses, summarized as<sup>18</sup>

$$E(m_1, m_2, m_3) \geq \frac{E(m_1, m_1, m_3) + E(m_2, m_2, m_3)}{2}. \quad (8)$$

In the case where  $m_1, m_2 \ll m_3$ , the atomic-like regime, system stability is provided by the mass difference; however, with only small differences in the masses, the heavier of the two light like-charged particles binds tightly to the uniquely charged particle, thus screening the lighter particle,  $m_2$ , from the opposite charge of  $m_3$ . For example, in the case of  $\{e, m_2, p\}$  and  $\{\mu, m_2, p\}$ , the mass  $m_2$  varies greatly: 0.797 and 164, respectively, yet in both cases the ratio of  $m_2/m_1 \approx 0.79$ , essentially the particle becomes “too light” relative to the heavier like-charged particle. Thus the stability depends primarily on the symmetry-breaking term, not on the sum of the inverse masses, i.e.,<sup>18</sup>

$$E(m_1, m_2, m_3) < \frac{E(m_1, m_1, m_3) + E(m_2, m_2, m_3)}{2}. \quad (9)$$

This explains the shape of the stability boundary but not the increase in stability compared to the lower bound prediction.

To understand this observation we consider the Hamiltonian used to predict the lower bound to stability. In normalized reciprocal masses:

$$\hat{H}(a_1, a_2, a_3) = \hat{H}_S + \hat{H}_A = \left[ \frac{a_1 + a_2}{2} (\mathbf{p}_1^2 + \mathbf{p}_2^2) + a_3 \frac{\mathbf{p}_3^2}{2} + \hat{V} \right] + \left[ \frac{a_1 - a_2}{2} (\mathbf{p}_1^2 - \mathbf{p}_2^2) \right]. \quad (10)$$

The variational principle is used to derive the ground state energy of the asymmetric system using the symmetric

ground-state wavefunction,  $\psi_S$  of  $\hat{H}_S$ , as trial wavefunction, i.e.,

$$E_0(a_1, a_2, a_3) \leq \langle \psi_S | \hat{H}(a_1, a_2, a_3) | \psi_S \rangle \\ = E_0 \left( \frac{1}{2}(a_1 + a_2), \frac{1}{2}(a_1 + a_2), a_3 \right). \quad (11)$$

The symmetric energy is expressed in terms of the relative excess binding energy due to the addition of a third particle  $m_2$  to  $\{m_1, m_3\}$  as a function of the reciprocal mass of the uniquely charged particle,  $a_3$ . It is then recast in terms of the symmetry breaking term  $a_1 - a_2$  by taking the ratio of the symmetric threshold energy to the actual threshold energy. This term can then be used to derive the width of the stability band in terms of the symmetric systems by elimination. However, explicit consideration of the anti-symmetric terms in the Hamiltonian is not included in this treatment and gives rise to the additional width of the stability band at all values of  $a_3$ . In terms of a perturbative treatment around the stable symmetric bound state,<sup>18</sup> the anti-symmetric term enters at second order and is sufficient for systems where the mass difference is small (e.g., in the atomic-like systems) but underestimates the full contribution at larger differences as occurs for molecular-like systems.

### Stability prediction

Predicting the stability of a particular three-particle system simply requires the calculation of its position in the ternary diagram, using the definitions of the reciprocal masses given in (2). If it falls within the stability domain it is stable to dissociation. Given that the critical masses used to define the stability boundary are converged to 2 s.f., the error on the boundary is at best  $\pm 0.005$  in scaled units.

However, even within this limited accuracy, it would be useful to be able to determine the threshold mass for stability of the third particle with any particle pair. In order to do this it is necessary to calculate the crossing point of the stability boundary with the line of constant mass ratio for the two-particle system. The coordinates in the ternary diagram, are  $x = (a_2 - a_1)/\sqrt{3}$  and  $y = a_3$ . Following I, it is possible to fit the boundary to a function of  $a_3$ , the reciprocal mass of the uniquely charged particle, and express the line of constant mass ratio  $a_1/a_3$  in these coordinates, and solve simultaneously. However, a much simpler method is to use the coordinate system,<sup>8</sup>  $x = m_3/(m_1 + m_3)$  and  $y = m_3/(m_2 + m_3)$  as this eliminates  $m_2$  from the independent variable. Using this coordinate system, the stability boundary is fitted to a function of the form used in I, i.e.,

$$y = f(x) = \sum_{i=0}^5 c_i x^{\frac{i}{2}}. \quad (12)$$

This results in an excellent fit with an  $R^2$  value of 0.999 999 83. The optimised values for this fit are:  $c_0 = 0.310 672 03$ ,  $c_1 = 0.677 996 13 \times 10^{-2}$ ,  $c_2 = 0.195 965 44$ ,  $c_3 = -0.609 288 42 \times 10^{-1}$ ,  $c_4 = 1.359 881 3$ ,  $c_5 = -0.812 377 64$ . Substituting  $x = m_3/(m_1 + m_3)$  into  $y = f(x)$  for a given mass pair  $m_1$  and  $m_3$  provides the lightest  $m_2$  mass possible for binding to the two-particle system.

## CONCLUSIONS

The smallest like-charge particle mass for which a three-particle system remains stable has been used to calculate an “exact” stability boundary. The upper bound of the particle mass corresponding to the exact threshold energy for a given two-particle system was calculated using the variational principle.<sup>8</sup> The generalised eigenvalue equation was solved using a series solution method for the three-particle system in translation-free internal coordinates using a wave function expanded in a triple orthogonal set of Laguerre functions with three nonlinear parameters. This work demonstrates the utility of the series solution method, but indicates that the wavefunction, so successful in energy calculations, does not adequately capture the physics of the variational mass problem resulting in very slow convergence. The “exact” stability bound, with limited precision of 2 s.f., was used to compare with the lower bound to stability recently calculated in I. The shape and increased region of stability was discussed and the latter attributed to the important anti-symmetric terms in the Hamiltonian. Finally, a functional fit to the data in a judicious choice of mass coordinates provided a simple analytical expression for the calculation of the critical mass of a third particle required for binding to any two-particle system.

## ACKNOWLEDGMENTS

The authors would like to thank Professor J.-M. Richard and Professor E. A. G. Armour for a helpful communication regarding their excellent review,<sup>11</sup> and Professor B. T. Sutcliffe and Professor A. J. McCaffery for valuable comments on the paper.

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