Stability of Coulomb systems as a function of the charges of the particles

T. K. Rebane

Physical Scientific-Research Institute, Leningrad State University

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The stability of Coulomb systems is investigated as a function of the charges of the particles. It is shown that every stable system gives rise to a region in which systems with varying charges of the particles remain unconditionally stable, and that every stable system that has only one bound energy level gives rise to a region in which such systems are unconditionally unstable. The regions of unconditional stability and instability of three-particle Coulomb systems are determined in explicit analytical form as a function of the charges of the particles. The boundaries of these regions are calculated for the systems obtained as functions of the constitutent charges of the atomic ion $H^-(\infty)$ with an infinitely heavy nucleus, the $\mu^+e^-e^-$ ion, and the positronium ion $e^-e^-e^+$. The boundaries of the region of unconditional stability are calculated for the systems obtained in an analogous manner from the mesomolecular ion $d^+d^+\mu^-$, the isotopic modifications $p^+p^+e^-$, $p^+d^+e^-$, and $d^+d^+e^-$ of the hydrogen-molecule ion, and the latter ion $H_2^+(\infty)$ with infinitely heavy nuclei. Account is taken of the motion of all the particles in the system, and of the associated correlation and nonadiabaticity effects. Bounds on the critical charge Z_{cr} and on the critical particle-coupling parameter λ_{cr} in the above systems are calculated. For all these systems these bounds are obtained for the first time, except in the case of the atomic ion $H^-(\infty)$. In the case of $H^-(\infty)$, the upper and lower bounds found for the critical charge of the nucleus are substantially more accurate than those obtained earlier by Hogreve. The results can be applied to the stability of various Coulomb systems and to the investigation of the convergence of perturbation theory in the coupling parameter λ characterizing the interaction of the like-charged particles in these systems.

INTRODUCTION

The problem of the stability of quantum-mechanical systems with Coulomb interaction of particles as a function of their charges occupies a central position in the theory of atomic and molecular ions. Reflected in this problem are the uncertainty principle (which prevents oppositely charged particles from completely coalescing and thereby prevents their Coulomb potentials from being completely screened), correlations in the motion of the particles (to which negative atomic and molecular ions entirely owe their existence), and, finally, the statistics of the particles (in boson systems negative ions can exist whose multiplicity is much greater than that of their electron analogs).

The investigation of the general properties of negative ions and the estimation of the maximum number of electrons that can be bound by one or more positively charged Coulomb centers have been the subjects of papers by a great many researchers. For example, in Refs. 1 and 2 it was shown that the negative hydrogen ion H^- has only one discrete energy level, so that this ion is stable only in its ground state and its excitation involves detachment of an electron. General estimates of the number N of electrons that can be bound in an atom with atomic number Z or in a molecule with K nuclei for which the sum of the atomic numbers is equal to Z can be found in Ref. 3: For an atom $N<2Z+1$ holds (it follows from this, for $Z=1$, that the doubly charged ion H^{--} is unstable), while for a molecule, $N<2Z+K$ (with $Z=1$ and $K=2$, this implies that the doubly charged molecular ion H_2^{--} is unstable).

In Ref. 4 the number N of electrons that can be bound in an atom with atomic number Z was considered for $Z\to\infty$, and it was found that the ratio of this number to the atomic number tends to unity ($N/Z\to 1$). This mathematically rigorous result is in agreement with the rule $N\leqslant Z+1$, which follows from experimental observations and almost completely rules out the possibility of the existence of doubly charged negative atomic ions. However, this rule, which is valid for electrons, does not hold for bosons. Model atoms containing boson analogs of electrons remain stable when the number N of these bosons is considerably greater than the atomic number Z. As the atomic number Z tends to infinity the ratio N/Z tends not to unity but to a value $\gamma\approx 1.26$ (Refs. 5, 6). Therefore, in the absence of the Pauli principle and of the resulting shell structure, the existence of negative atomic ions of very high multiplicity would be possible.

It is of considerable interest not only to analyze the stability of ions as a function of the number of particles constituting them, but also to investigate the stability of a system with a fixed number of particles when the masses or charges of the latter are changed. In Ref. 7, on the basis of variational calculations, the region in which a three-particle system with particle charges ± 1, ± 1, ∓ 1 in its ground state is unconditionally stable was established. In Ref. 8 this region was extended, and regions of unconditional stability of three-particle Coulomb systems in their excited states and with varying particles masses were found.

In the present paper we consider the stability of three-particle Coulomb systems as a function of the particle charges Z_1, Z_2, and Z_3. This problem is important in relation to the application of perturbation theory in the coupling parameter λ characterizing the interaction of the like-charged particles, which leads to representations of the wave function and energy of the system in the form of series in powers of the parameter λ. For example, for the energy of the ground state of a two-electron atom with a fixed nucleus

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22 coefficients in such a power series have been found.[9]

To establish the applicability of perturbation theory it is necessary to know the critical interaction-parameter value λ_{cr} at which the system loses stability and its discrete term moves into the continuous spectrum (where it can be transformed into an auto-ionization state). On the basis of an analysis of the perturbation-theory coefficients calculated in Ref. 9, Stillinger[10] determined that the critical value of the electron-interaction parameter in an atom with atomic number $Z=1$ is $\lambda_{cr}=1.0975$ (and also found the value $\lambda^*=1.1184$ at which the auto-ionization state disappears). But if we consider atoms with a fixed electron-interaction parameter $\lambda=1$ (the actual value), but with a continuously varying atomic number Z, the point of detachment of an electron corresponds to the critical atomic-number value $Z_{cr}=1/\lambda_{cr}=0.91116$. Variational calculations of the upper bound on the energy make it possible to determine an upper bound on the critical atomic number. For example, in Ref. 11 purely analytical variational calculations yielded $Z_{cr}\leqslant 868/901=0.9634$, while in Ref. 12, by means of a variational calculation with 476 basis functions, Baker *et al.* obtained[11] an extremely accurate upper bound on the critical atomic number ($Z_{cr}\leqslant 0.91103$), which agrees well with the nonvariational estimate of the quantity Z_{cr} from Ref. 10.

Two-electron systems with a fixed nucleus are the only example of a Coulomb system whose stability as a function of the particle charges has been investigated in detail.

Here we consider the stability of three-particle Coulomb systems with full allowance for the motion of all the particles (and for the correlation and nonadiabaticity effects associated with this motion). The systems to be investigated are not assumed to be symmetric in the masses or charges of the like-charged particles. At the basis of our approach lies the simple idea of varying the scale, which has made it possible to obtain useful inequalities for the total energies and components of the potential energy of atoms with varying atomic numbers[13] and lies at the basis of the convexity relation for the energies of quantum-mechanical systems.[14-16] Combining this approach with presently known results of highly accurate calculations of the energies and components of the potential energies of "standard" systems enables us to determine the region of unconditional stability of Coulomb systems as a function of the charges of the particles. Application of projection operators then allows regions to be established in which for the values of the particle charges under investigation the systems are unconditionally unstable.

PRELIMINARY DISCUSSION OF THE STABILITY CONDITION

Suppose that the first two particles have charges Z_1 and Z_2 of the same sign, and that the third particle carries a charge Z_3 of the opposite sign. Since the particles 1 and 2 repel each other, the system can be stable only if the magnitude of the charge of the third particle, which plays a binding role, is sufficiently large. It is obvious that the system is stable when the charge of the third particle is greater in magnitude than the charges of the first and second particles, so that the inequalities

$$|Z_1/Z_3|<1, \quad |Z_2/Z_3|<1 \tag{1}$$

are fulfilled. In fact, in this case neither of the particles 1 and 2 can fully screen the Coulomb field of particle 3, and the system has infinitely many bound discrete levels, corresponding to the incompletely screened Coulomb potential of the third particle. We now consider the case when the charges Z_2 and Z_3 are fixed and the charge Z_1 of the first particle increases in magnitude without limit while remaining of the same sign. In this case, particles 1 and 3 are grouped into an atom-like ion, whose size (defined by the average distance between particles 1 and 3) tends to zero. In this limiting case, particle 2 will move in the field of an almost point charge (Z_1+Z_3), experiencing from the latter an infinitely strong Coulomb repulsion. Therefore, the system decays, with liberation of particle 2. We obtain an analogous result by fixing the charges of particles 1 and 3 and letting the magnitude of charge 2 tend to infinity. Thus, the three-particle system is certainly unstable in the limit

$$Z_2/Z_1\to 0, \quad Z_3/Z_1\to 0 \tag{2a}$$

or

$$Z_1/Z_2\to 0, \quad Z_3/Z_2\to 0\,. \tag{2b}$$

It is clear from what has been said that a three-particle system will be stable when the charge Z_3 of the binding particle 3 is sufficiently large and the charges Z_1 and Z_3 of the particles being bound are sufficiently small [ensuring fulfillment of the conditions (1)]. Loss of stability of the system occurs when the magnitude of the charge Z_3 decreases, or when the magnitudes of the charges Z_1 and Z_2 increase. In the next section these qualitative arguments will be made quantitative.

QUANTITATIVE STABILITY CRITERION

The Hamiltonian of the system being investigated is given by

$$H=-\frac{1}{2}\sum_{j=1}^{3}\frac{\Delta_j}{m_j}+\sum_{j>k}^{3}\frac{Z_jZ_k}{|\mathbf{r}_j-\mathbf{r}_k|}, \tag{3}$$

where the signs of the charges of the particles satisfy $Z_1Z_2>0$, $Z_1Z_3<0$, and $Z_2Z_3<0$. We use the atomic system of physical units: $|e|=m_e=\hbar=1$. After changing to relative particle coordinates

$$\mathbf{s}_1=\mathbf{r}_1-\mathbf{r}_3, \quad \mathbf{s}_2=\mathbf{r}_2-\mathbf{r}_3 \tag{4}$$

and separating out the nonquantum motion of the center of mass, we find that the Hamiltonian (3) takes the form

$$H=-\frac{1}{2}\left[\left(\frac{1}{m_1}+\frac{1}{m_3}\right)\Delta_{s_1}+\left(\frac{1}{m_2}+\frac{1}{m_3}\right)\Delta_{s_2}+\frac{2}{m_3}\nabla_{s_1}\nabla_{s_2}\right]+\frac{Z_1Z_2}{|\mathbf{s}_1-\mathbf{s}_2|}+\frac{Z_2Z_3}{s_2}+\frac{Z_3Z_1}{s_1}. \tag{5}$$

Its eigenvalues depend on the masses and charges of the particles. We denote by $E(m_1,m_2,m_3,Z_1,Z_2,Z_3)$ (or, more briefly, by E) the lowest of these eigenvalues. The system of particles in its ground state is stable when its energy is lower than the energy of both of the two atom-like systems into which it is transformed when particle 1 or particle 2 is removed from it. Therefore, a necessary and sufficient condition for stability of the system is that the following two strict inequalities be fulfilled simultaneously:

$$E<-\frac{m_1m_3(Z_1Z_3)^2}{2(m_1+m_3)} \tag{6a}$$

$$E<-\frac{m_2m_3(Z_2Z_3)^2}{2(m_2+m_3)} \tag{6b}$$

If just one of the inequalities (6a), (6b) is violated, the system is unstable against decay into an atom-like two-particle system and a free particle.

We change to the scale-transformed coordinates

$$\mathbf{t}=m_3Z_3^2\mathbf{s}_1, \quad \mathbf{u}=m_3Z_3^2\mathbf{s}_2. \tag{7}$$

In these coordinates the Hamiltonian (5) can be written, with allowance for the homogeneity properties of the kinetic-energy and potential-energy operators, in the form

$$H=m_3Z_3^4h(\mathbf{t},\mathbf{u};\mu,\nu,p,q). \tag{8}$$

Here we have introduced the new energy operator

$$h(\mathbf{t},\mathbf{u};\mu,\nu,p,q) =-\frac{1}{2}[(\mu+1)\Delta_t+(\nu+1)\Delta_u+2\nabla_t\nabla_u] -\frac{1}{pt}-\frac{1}{qu}+\frac{1}{pq|\mathbf{t}-\mathbf{u}|} \tag{9}$$

and are using the following notation for mass ratios and charge ratios:

$$\mu=m_3/m_1, \quad \nu=m_3/m_2, \quad p=-Z_3/Z_1, \quad q=-Z_3/Z_2. \tag{10}$$

The operator (9) depends parametrically on μ, ν, p and q, and its eigenvalues also depend on these parameters. We denote the lowest eigenvalue by $\varepsilon(\mu,\nu,p,q)$. It is related to the ground-state energy of the system by the equality

$$E(m_1,m_2,m_3,Z_1,Z_2,Z_3)=m_3Z_3^4\varepsilon(\mu,\nu,p,q). \tag{11}$$

The condition (6a), (6b) for stability of the system of particles reduces to the requirement that the following system of inequalities be fulfilled:

$$\begin{cases} \varepsilon(\mu,\nu,p,q)<-\dfrac{1}{2(\mu+1)p^2}, & \text{(12a)} \\ \varepsilon(\mu,\nu,p,q)<-\dfrac{1}{2(\nu+1)q^2}. & \text{(12b)} \end{cases}$$

The charges and masses of the particles appear in these conditions through the parameters μ, ν, p, and q (10). Therefore, the stability or instability of the system of particles is determined entirely by the charge ratios and mass ratios of the particles. Thus, if a system with a certain set of masses m_1, m_2, m_3 and charges Z_1, Z_2, Z_3 is stable (or unstable), the same property is also possessed by the system with proportionally changed particle masses and charges, equal to km_1, km_2, km_3 and lZ_1, lZ_2, lZ_3, where k and l are arbitrary positive, nonzero numbers.

CONDITION FOR CERTAIN STABILITY OF A COULOMB THREE-PARTICLE SYSTEM WITH VARYING PARTICLE CHARGES

Below, we assume that the particle-mass ratios μ and ν are fixed, and consider the stability of the system as a function of the charge parameters p and q. Accordingly, we use the abbreviated notation $\varepsilon=\varepsilon(p,q)=\varepsilon(\mu,\nu,p,q)$.

Suppose that the three-particle system with given particle-mass ratios μ and ν is stable when the ratios of the particle charges are equal to p_0 and q_0. Then, by virtue of continuity, in the neighborhood of the point p_0,q_0 there exists a certain region (an "island of stability") in which the system remains stable when the charge parameters p and q deviate from their initial values p_0 and q_0. The variational principle, in combination with variation of the scale, makes it possible to determine easily that part of the island of stability on which the three-particle system is unconditionally stable.

The operator of the energy of the initial stable system is obtained from (9) with $p=p_0$ and $q=q_0$. It is equal to

$$h_0(\mathbf{t},\mathbf{u})\equiv h(\mathbf{t},\mathbf{u};\mu,\nu,p_0,q_0)=T-\frac{1}{p_0t}-\frac{1}{q_0u}+\frac{1}{p_0q_0|\mathbf{t}-\mathbf{u}|}, \tag{13}$$

where

$$T\equiv-\frac{1}{2}[(\mu+1)\Delta_t+(\nu+1)\Delta_u+2\nabla_t\nabla_u].$$

Since the initial system is stable, the lowest eigenvalue $\varepsilon_0=\varepsilon(p_0,q_0)$ of the operator (13) satisfies the inequalities obtained from (12a) and (12b) with $p=p_0$ and $q=q_0$:

$$\begin{cases} \varepsilon_0<-1/[2(\mu+1)p_0^2], & \text{(14a)} \\ \varepsilon_0<-1/[2(\nu+1)q_0^2]. & \text{(14b)} \end{cases}$$

We denote by $\psi_0(\mathbf{t},\mathbf{u})$ that normalized eigenfunction of the energy operator (13) of the initial system which pertains to its lowest eigenvalue ε_0. We go over to a system with arbitrary charge parameters p and q and set up the energy operator that is obtained from the energy operator (9) by changing the scale of the coordinates by a factor of α. Taking into account the homogeneity properties of the kinetic-energy and potential-energy operators, we obtain

$$h(\mathbf{t}/\alpha,\mathbf{u}/\alpha;\mu,\nu,p,q)=\alpha^2T-\alpha\left(\frac{1}{pt}+\frac{1}{qu}-\frac{1}{pq|\mathbf{t}-\mathbf{u}|}\right). \tag{15}$$

The lowest eigenvalue of the operator (15) is equal to ε, as for the energy operator (9). We now construct the mathematical expectation value of the energy operator (15) with the eigenfunction ψ_0 of the energy operator (13) of the initial stable system. According to the virial theorem, the contribution of the kinetic-energy operator [the first term in the right-hand side of (15)] to this mathematical expectation value is equal to $-\alpha^2\varepsilon_0$. Therefore, we have

$$\langle\psi_0(\mathbf{t},\mathbf{u})|h(\mathbf{t}/\alpha,\mathbf{u}/\alpha;\mu,\nu,p,q)|\psi_0(\mathbf{t},\mathbf{u})\rangle=-\alpha^2\varepsilon_0+\alpha\langle v\rangle. \tag{16}$$

We denote mathematical expectation values of physical quantities calculated with the eigenfunction ψ_0 of the energy operator (13) of the initial system simply by angular brackets. Then the quantity $\langle v\rangle$ is the expectation value of the potential energy of the interaction of the particles in the system under investigation [described by the energy operator (9)], calculated with the function ψ_0:

$$\langle v\rangle=\frac{1}{pq}\left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle-\frac{1}{p}\left\langle\frac{1}{t}\right\rangle-\frac{1}{q}\left\langle\frac{1}{u}\right\rangle. \tag{17}$$

By virtue of the variational principle, the mathematical expectation value of the operator $h(\mathbf{t}/\alpha,\mathbf{u}/\alpha;\mu,\nu,p,q)$, expressed by Eq. (16), is greater than or equal to its lowest eigenvalue, equal to $\varepsilon=\varepsilon(p,q)$. Therefore, for all positive values of the scale factor α, the following bound is valid for the ground-state energy of the system under investigation

with charge parameters p and q:

$$\varepsilon(p, q) \leqslant -\alpha^2\varepsilon_0 + \alpha\langle v\rangle. \tag{18}$$

The right-hand side of the inequality (18) depends on α. The optimum value of α, corresponding to the minimum of the right-hand side of (18), is easily found by differentiation. It is equal to

$$\alpha_0 = \langle v\rangle/2\varepsilon_0. \tag{19}$$

Substituting this value into (18), we obtain

$$\varepsilon(p, q) \leqslant \langle v\rangle^2/4\varepsilon_0. \tag{20}$$

This formula determines an upper bound on the lowest eigenvalue of the energy operator (9) of the system under investigation with charge parameters p and q in terms of an eigenvalue of the energy operator (13) of the initial stable system and the mathematical expectation value of the potential energy of the interaction of the particles in the system under investigation, calculated with an eigenfunction of the initial stable system.

For the bound (20) to be strong, the optimum value (19) of the scale factor α should be positive. The energy ε_0 of a bound state of the stable system is negative. Therefore, the mathematical expectation value of the potential energy in the numerator of Eq. (19) should be negative: $\langle v\rangle < 0$. This is ensured by a positive sign of the quantity α_0.

The condition for stability of a system of particles with charge parameters p and q is certainly fulfilled if in (12a) and (12b) we replace the exact energy eigenvalue $\varepsilon(p, q)$ of this system by its upper bound (20). Therefore, the system is certainly stable when the inequalities

$$\frac{\langle v\rangle^2}{2\varepsilon_0} < -\frac{1}{(\mu+1)p^2} \tag{21a}$$

$$\frac{\langle v\rangle^2}{2\varepsilon_0} < -\frac{1}{(\nu+1)q^2} \tag{21b}$$

and the condition $\langle v\rangle < 0$, which ensures positivity of the scale factor α_0, are fulfilled simultaneously. Substituting into (21a) and (21b) the explicit expression (17) for the mathematical expectation value of the potential energy, we bring these inequalities to the form

$$p\left\langle\frac{1}{u}\right\rangle + q\left[\left\langle\frac{1}{t}\right\rangle - \left(-\frac{2\varepsilon_0}{\mu+1}\right)^{1/2}\right] - \left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle > 0, \tag{22a}$$

$$p\left[\left\langle\frac{1}{u}\right\rangle - \left(-\frac{2\varepsilon_0}{\nu+1}\right)^{1/2}\right] + q\left\langle\frac{1}{t}\right\rangle - \left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle > 0. \tag{22b}$$

From our stipulation on the signs of the particle charges, the quantities p and q are positive. Therefore, fulfillment of the inequalities (22a) and (22b) implies fulfillment of the inequality

$$p\left\langle\frac{1}{u}\right\rangle + q\left\langle\frac{1}{t}\right\rangle - \left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle > 0, \tag{23}$$

which ensures a negative sign of the mathematical expectation (17) of the potential energy and, simultaneously, a positive sign of the scale factor (19). Therefore, the simultaneous fulfillment of the inequalities (22a) and (22b) is a sufficient condition that unconditionally guarantees the stability of a system with charge parameters p and q that are bound to be positive by virtue of our stipulation on the signs of the charges of the particles.

DETERMINATION OF THE REGION OF UNCONDITIONAL STABILITY OF A SYSTEM OF PARTICLES WITH VARYING CHARGES

On the plane of the variables p and q, all points whose coordinates satisfy the system of inequalities (22a), (22b) lie in a region in which the three-particle system (for given fixed particle-mass ratios μ and ν) is unconditionally stable under change of the particle-charge ratios p and q (10). It is possible to determine the boundaries of this region in explicit analytical form. We shall do this.

First we ascertain the sign of the coefficient of the quantity q in the inequality (22a) and the sign of the coefficient of p in the inequality (22b). According to (2a), the system of particles is unconditionally unstable when q has an arbitrary fixed value and $p \to 0$. Therefore, the system of inequalities (22a), (22b), fulfillment of which guarantees the stability of the three-particle system, cannot have a solution for $p = 0$, $q > 0$.

We now assume that the coefficient of the quantity q in (22a) is positive. Setting $p = 0$, we find that the system of inequalities (22a), (22b) then has the solution

$$p=0, \quad q > \left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle \Big/ \left[\left\langle\frac{1}{t}\right\rangle - \left(-\frac{2\varepsilon_0}{\mu+1}\right)^{1/2}\right] > 0, \tag{24}$$

which contradicts what was said above. Therefore, the assumption made is incorrect, and the coefficient of q in (22a) is not positive. An analogous result can be obtained for the coefficient of p in (22b): For this it is sufficient to start from the relation (2b).[2)]

Thus, we have found that the following inequalities are valid:

$$\left\langle\frac{1}{t}\right\rangle - \left(-\frac{2\varepsilon_0}{\mu+1}\right)^{1/2} \leqslant 0, \tag{25a}$$

$$\left\langle\frac{1}{u}\right\rangle - \left(-\frac{2\varepsilon_0}{\nu+1}\right)^{1/2} \leqslant 0. \tag{25b}$$

The region of solutions of the system of inequalities (22a), (22b) on the plane of the variables p, q is bounded by straight lines, on which, respectively, the inequality (22a) or the inequality (22b) goes over into an equality. The first of these straight lines intersects the p axis at the point A, and the second intersects the q axis at the point B (see the figure). The coordinates of the points A and B are given by the following equalities:

$$p_A = \left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle \Big/ \left\langle\frac{1}{u}\right\rangle, \quad q_B = \left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle \Big/ \left\langle\frac{1}{t}\right\rangle, \quad q_A = p_B = 0. \tag{26a}$$

The point of intersection of these straight lines (point C) has coordinates

$$p_C = (1+\nu)^{1/2}\left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle \Big[(1+\mu)^{1/2}\left\langle\frac{1}{t}\right\rangle + (1+\nu)^{1/2}\left\langle\frac{1}{u}\right\rangle - (-2\varepsilon_0)^{1/2}\Big]^{-1},$$

$$q_C = (1+\mu)^{1/2}\left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle \Big[(1+\mu)^{1/2}\left\langle\frac{1}{t}\right\rangle + (1+\nu)^{1/2}\left\langle\frac{1}{u}\right\rangle - (2\varepsilon_0)^{1/2}\Big]^{-1}. \tag{26b}$$

As follows from (25a) and (25b), the denominators in (26a) and (26b) are positive, so that the point C is in the positive quadrant of the p, q plane. If we take into account the signs of the coefficients of p and q in (22a) and (22b), it is clear that the straight lines AC and BC have positive slopes. Therefore, the point C is located above and to the right of the points A and B. Taking the same signs into account, we can see that the inequality (22a) is fulfilled at points lying below the straight line AC, while the inequality (22b) is fulfilled at points lying above the straight line BC. Therefore, the region of solutions of the system of inequalities (22a), (22b) is the angle, shaded in the figure, with apex at the point C. This angle, opposite the angle ACB, is the region of unconditional stability of a three-particle system with varying charges—a region generated by specifying an stable initial system with coordinates p_0 and q_0. The boundaries of this region are fully determined by the coordinates of the points A, B, and C, which are expressed in terms of characteristics of the initial stable system by the formulas (26a) and (26b).

Returning, by means of Eqs. (7), (10), and (11), from the quantities $\mathbf{t}$, $\mathbf{u}$, μ, ν, p, q, and ε to the interparticle distances, the particle masses and charges, and the total energy E of the initial stable system, we can write the coordinates of the points A, B, and C in the form

$$p_A=\left\langle\frac{1}{r_{12}}\right\rangle\Big/\left\langle\frac{1}{r_{23}}\right\rangle, \quad q_A=0, \tag{27a}$$

$$p_B=0, \quad q_B=\left\langle\frac{1}{r_{12}}\right\rangle\Big/\left\langle\frac{1}{r_{13}}\right\rangle, \tag{27b}$$

$$\begin{cases} p_C=[m_1(m_2+m_3)]^{1/2}\left\langle\frac{1}{r_{12}}\right\rangle\Big/\Big[[m_1(m_2+m_3)]^{1/2}\left\langle\frac{1}{r_{23}}\right\rangle \\ \quad +[m_2(m_1+m_3)]^{1/2}\left\langle\frac{1}{r_{13}}\right\rangle-[-2m_1m_2m_3E]^{1/2}\Big], \\ q_C=[m_2(m_1+m_3)]^{1/2}\left\langle\frac{1}{r_{23}}\right\rangle\Big/\Big[[m_1(m_2+m_3)]^{1/2}\left\langle\frac{1}{r_{23}}\right\rangle \\ \quad +[m_2(m_1+m_3)]^{1/2}\left\langle\frac{1}{r_{13}}\right\rangle-[-2m_1m_2m_3E]^{1/2}\Big]. \end{cases} \tag{27c}$$

We restate the result obtained. If a certain initial system of three particles with masses m_1, m_2, and m_3 and charges $Z_1^{(0)}$, $Z_2^{(0)}$, and $Z_3^{(0)}$ is stable, so that its energy $E_0=E(m_1,m_2,m_3,Z_1^{(0)},Z_2^{(0)},Z_3^{(0)})$ satisfies inequalities of the form (6a) and (6b), then all three-particle systems in which the particle masses are equal to km_1, km_2, and km_3 and the particle charges are characterized by ratios $p=-Z_3/Z_1$ and $q=-Z_3/Z_2$ that fall in the shaded angle in the figure are also stable. The coordinates of the points A, B, and C are determined here by characteristics of the stable initial system from Eqs. (27a)–(27c), and k is an arbitrary positive factor.

According to the relation (1), formulated in our preliminary discussion of the condition for stability, three-particle Coulomb systems are unconditionally stable when the representative point p, q lies inside the infinite square whose lower left corner is located at the point G with coordinates $p_G=q_G=1$ (see the figure). Therefore, a Coulomb system of three particles with varying charges of the particles is unconditionally stable in the entire region marked by either type of shading.

REGIONS OF UNCONDITIONAL STABILITY OF SPECIFIC THREE-PARTICLE SYSTEMS

High-accuracy calculations of the energies of three-particle Coulomb systems have been the subject of a considerable number of papers by various authors (for a bibliography on this topic, see, e.g., Refs. 8 and 17). However, the number of three-particle systems for which highly accurate calculations have been made not only of the energy but also of the mathematical expectation values of the inverse distances between the particles is not great. Amongst such systems are:

1) the atomic hydrogen ion H^- with a fixed nucleus[18-20] [$H^-(\infty)$];

2) the positronium ion $e^-e^-e^+$ (Ref. 21);

3) the mesomolecular ion $d^+d^+\mu^-$ (Ref. 22);

4, 5, 6) hydrogen-molecule ions with moving nuclei[23,24]

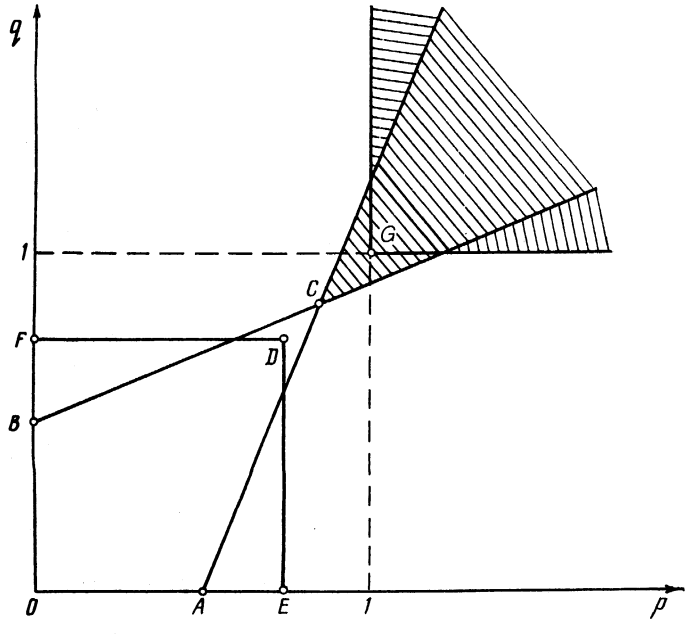

FIG. 1. Regions of unconditional stability and instability of three-particle Coulomb systems as a function of the charges of the particles. Plotted along the coordinate axes are the particle-charge ratios $p=-Z_3/Z_1$ and $q=-Z_3/Z_2$. The signs of the charges of the first two particles (Z_1 and Z_2) are the same, and opposite to the sign of the charge Z_3 of the third particle. The system is unconditionally stable in the shaded region inside the angle opposite the angle ACB, and inside the infinite square with lower left corner at the point G with coordinates $p_G=q_G=1$. The coordinates of the points A, B, and C are determined by Eqs. (27a)–(27c). The system is unconditionally unstable in the rectangle $OEDF$, the location of the corner D being determined by Eq. (46).

TABLE I. Physical characteristics of the stable three-particle Coulomb systems used as standards in the investigation of the stability of systems with varying particle charges.

Characteristics	System					
	H⁻ (∞)	$e^-e^-e^+$	$d+d+\mu^-$	$p+p+e^-$	$d+d+e^-$	H_2^+ (∞)
$m_1=m_2$	1	1	3670,481	1836,153	3670,479	∞
m_3	∞	1	206,769	1	1	1
$-E$	0,527751	0,262005	109,817	0,597139	0,598789	0,602634
$\langle r_{13}^{-1}\rangle=\langle r_{23}^{-1}\rangle$	0,683262	0,339831	150,43	0,84249	0,84562	0,852985
$\langle r_{12}^{-1}\rangle$	0,311022	0,155654	81,473	0,49071	0,49365	0,500703
$\langle r_{12}\rangle$	4,41269	8,546113	0,013743	2,0639	2,0441	1,9972

Note: The system $p^+d^+e^-$ that is symmetric in the particle masses has the following physical characteristics: $m_1 = 1836.153$; $m_2 = 3670.479$; $m_3 = 1$; $-E = 0.697818$; $\langle r_{13}^{-1}\rangle = 0.84372$; $\langle r_{23}^{-1}\rangle = 0.84414$; $\langle r_{12}^{-1}\rangle = 0.49205$; $\langle r_{12}\rangle = 2.0548$.

$[d^+d^+e^-, d^+p^+e^-, p^+p^+e^-]$;

7) the same ion with fixed, infinitely heavy nuclei[25] $[H_2^+(\infty)]$.

The symbols p^+, d^+, e^+, μ^-, and e^- denote the proton, deuteron, positron, negative muon, and electron, respectively. All the systems listed are stable in their ground state, and can be used as initial systems to determine the boundaries of the region of unconditional stability of analogous systems with the same particle-mass ratios, in accordance with the formulas of the preceding section. On the plane of the charge parameters p, q these systems correspond to the point G with coordinates $p = q = 1$. All these systems (except $p^+d^+e^-$) are symmetric in the masses. Their physical characteristics are given in Table I, and the characteristics of the nonsymmetric system $p^+d^+e^-$ are given in the note at the foot of this table.

According to what has been said in the preceding section, each of the above seven initial systems gives rise to a region of unconditional stability of systems with varying charges but fixed particle-mass ratios. The coordinates of the points A, B, and C that determine the boundaries of the regions of unconditional stability, calculated from the data of Table I by means of Eqs. (27a)–(27c), are given for the six mass-symmetric systems in the first four rows of Table II, while for the system $p^+d^+e^-$ that is asymmetric in the particle masses they are given in the note at the foot of this table.

Closeness of the point C to the coordinate origin is a measure of the stability of the system. In fact, from the definition of the charge parameters p and q it follows that there are two ways of giving a clear interpretation of the coordinate values p_C and q_C. If we consider a system that is symmetric in the masses of particles 1 and 2, with fixed unit charges of the first and second particles ($|Z_1| = |Z_2| = 1$), the lowest (in magnitude) third-particle charge that ensures the unconditional stability of the system is determined from the equality

$$|Z_3^{(+)}| = p_C = q_C. \tag{28}$$

Analogously, if we fix the charge of the third particle ($|Z_3| = 1$) and consider a system with varying particle charges $Z_1 = Z_2$, the largest value of the charge of either of these particles for which the system is unconditionally stable is equal to

$$|Z_1^{(-)}| = |Z_2^{(-)}| = 1/p_C = 1/q_C. \tag{29}$$

The quantity (28) is then an upper bound on the magnitude of the critical third-particle charge Z_{cr} at which the system loses its stability, while the quantity (29) is a lower bound on the critical value λ_{cr} of the interaction parameter:

$$Z_{cr} \leqslant |Z_3^{(+)}|, \quad \lambda_{cr} \geqslant |Z_1^{(-)}|. \tag{30}$$

It can be seen from the data of Table II that, for systems that are symmetric in the masses of particles 1 and 2, with increase of the particle-mass ratio $\mu = m_3/m_1 = m_3/m_2 = \nu$ the point C first moves away from the coordinate origin (going from the ion $H^-(\infty)$ to the positronium ion $e^-e^-e^+$),

TABLE II. Characteristic points A, B, C, and D determining the unconditional stability or instability of a three-particle Coulomb system as the charges of the particles are varied.

Coordinates of the characteristic points	Particle-mass ratio $\mu = m_3/m_1 = m_3/m_2 = \nu$					
	∞	1	0,055633	0,00054462	0,00027244	0
$p_A=q_B$	0,45520	0,45803	0,54160	0,58245	0,58377	0,58700
$p_B=q_A$	0	0	0	0	0	0
$p_C=q_C$	0,91707	0,92763	0,87123	0,828276	0,826815	0,823356
$p_C^{-1}=q_C^{-1}$	1,09043	1,07802	1,1478	1,20732	1,20946	1,21454
$p_D=q_D$	0,89090	0,90695	–	–	–	–
$p_D^{-1}=q_D^{-1}$	1,12246	1,10260	–	–	–	–

Note: The six columns of this table correspond to the six regions of unconditional stability generated by the six initial stable Coulomb systems described in Table I. A detailed description of the regions of unconditional stability or instability and of the characteristic points A, B, C, and D is given in the text. The mass-asymmetric system $p^+d^+e^-$ generates a region of unconditional stability with the following characteristic points: $p_A = 0.58290$; $q_A = 0$; $p_B = 0$; $q_B = 0.58319$; $p_C = 0.827532$; $q_C = 0.827645$.

TABLE III. Bounds on the critical charge Z_{cr} of the binding particle and on the critical parameter λ_{cr} characterizing the interaction of the like-charged particles being bound, and admissible limits of variation of the charge Z_2 of the second particle in Coulomb systems with various particle masses.

Initial system	Z_{cr}		λ_{cr}		Z_2	
	Lower bound	Upper bound	Lower bound	Upper bound	Lower bound	Upper bound
$H^-(\infty)$	0,8909	0,9171	1,0904	1,1225	0,9588	1,0817
$\mu^+e^-e^-$	0,8913	0,9174	1,0900	1,1219	0,9591	1,0812
$e^+e^-e^-$	0,9070	0,9276	1,0780	1,1026	0,9643	1,0706
$d^+d^+\mu^-$	–	0,8712	1,1478	–	0,9200	1,2116
$p^+p^+e^-$	–	0,8283	1,2073	–	0,8792	1,4069
$p^+d^+e^-$	–	0,8277	1,2082	–	0,8786	1,4111
$d^+d^+e^-$	–	0,8268	1,2095	–	0,8777	1,4160
$H_2^+(\infty)$	–	0,8234	1,2145	–	0,8741	1,4387

and then comes closer to the coordinate origin (going from the positronium ion to the mesomolecular ion $d^+d^+\mu^-$ and to isotopic modifications of the hydrogen-molecule ion). This corresponds to the fact that the point C is closer to the coordinate origin the greater is the difference between the mass of the binding particle 3 and the masses of the particles 1 and 2 being bound. The positronium ion plays here the role of a kind of "watershed" between atom-like and molecule-like systems.

Taking into account the data of Table II, from (28)–(30) we obtain the results given in Table III for upper bounds on the magnitude of the critical charge Z_{cr} of the third particle and lower bounds on the critical constants λ_{cr} characterizing the interaction of the like-charged particles in systems with various particle-mass ratios $\mu = m_3/m_1 = m_3/m_2 = \nu$.

For all these systems except $H^-(\infty)$, the bounds on the critical values of the charge of the binding particle and of the interaction constant of the like-charged particles being bound are obtained here for the first time. It should be recalled that our results rest on precision calculations of initial systems with charges $Z_1 = Z_2 = \pm 1$ and $Z_3 = \mp 1$. Therefore, they are valid when one takes account of the motion of all the particles in the system and the nonadiabaticity and correlation effects associated with this motion. In the case of $H^-(\infty)$ our upper bound for the critical atomic number (0.9171) is much better than the result $Z_{cr} \leqslant 0.9634$ obtained recently on the basis of an analytical investigation of the problem.[11] It is only a little worse than the most accurate values of the critical atomic number in $H^-(\infty)$ ($Z_{cr} = 0.91103$ and $Z_{cr} = 0.91116$), obtained, respectively, in Ref. 12 by means of a variational calculation with 476 basis functions and in Ref. 10 on the basis of a special technique for summing 22 terms of the perturbation-theory series in the electron-interaction parameter.

Also deserving of attention is the possibility of treating systems that are nonsymmetric in the charges of the particles, which stems from the specifying of the geometry of the region of unconditional stability and its characteristic points A, B, and C. For example, systems of the type $H^-(\infty)$ with particle masses $m_1 = m_2 = 1$ and $m_3 = \infty$ and with fixed charges of the first and third particles ($Z_1 = -1, Z_3 = +1$) remain certainly stable when the charge Z_2 of the second particle varies in the range from -0.9588 to -1.0817. Analogously, systems of the type of the mesomolecular ion $d^+d^+\mu^-$ with particle masses $m_1 = m_2 = 3670.481$ and $m_3 = 206.769$ and particle charges $Z_1 = 1$ and $Z_3 = -1$ remain unconditionally stable when the charge of the second particle is varied in the range from $+0.9200$ to $+1.2116$.

The important point is that all these conclusions are obtained by means of entirely elementary calculations from properties of the initial "standard" systems, viz., from the data of Table I.

CRITERION FOR UNCONDITIONAL INSTABILITY OF A SYSTEM OF THREE PARTICLES WITH VARYING CHARGES

We now derive a criterion for unconditional instability of a three-particle system. As before, we shall start from the fact that a certain "standard" system with charge parameters p_0 and q_0 is stable. We consider a system characterized by proportionally decreased values of the charge parameters $p = p_0/k$ and $q = q_0/k$, where $k \geqslant 1$. The energy operator for such a system is equal to

$$h(\mathbf{t},\mathbf{u}) = T - \frac{k}{p_0 t} - \frac{k}{q_0 u} + \frac{k^2}{p_0 q_0 |\mathbf{t}-\mathbf{u}|}, \tag{31}$$

and its lowest eigenvalue is equal to $\varepsilon(p_0/k, q_0/k)$. Dividing the coordinates $\mathbf{t}$ and $\mathbf{u}$ in (31) by the parameter k, we obtain the new energy operator

$$h\left(\frac{\mathbf{t}}{k}, \frac{\mathbf{u}}{k}\right) = k^2\left(T - \frac{1}{p_0 t} - \frac{1}{q_0 u} - \frac{k}{p_0 q_0 |\mathbf{t}-\mathbf{u}|}\right) \tag{32}$$

with the same eigenvalue $\varepsilon(p_0/k, q_0/k)$. This operator can be written in the form

$$h\left(\frac{\mathbf{t}}{k}, \frac{\mathbf{u}}{k}\right) = k^2\left[h_0(\mathbf{t},\mathbf{u}) + \frac{k-1}{p_0 q_0 |\mathbf{t}-\mathbf{u}|}\right], \tag{33}$$

where $h_0(\mathbf{t},\mathbf{u})$ is the energy operator (13) of the initial stable system with charge parameters p_0 and q_0. Consider the operator in the square brackets in Eq. (33):

$$g(\mathbf{t},\mathbf{u}) = h_0(\mathbf{t},\mathbf{u}) + \frac{k-1}{p_0 q_0 |\mathbf{t}-\mathbf{u}|}. \tag{34}$$

We denote its lowest eigenvalue by $\eta(p_0, q_0, k)$. Since, with $k = 1$, this operator coincides with the energy operator of the initial system, we have $\eta(p_0, q_0, 1) = \varepsilon(p_0, q_0) = \varepsilon_0$.

It follows from the operator equality (33) that the lowest eigenvalue of the energy operator (31) describing the system with proportionally decreased particle-charge ratios is related to the lowest eigenvalue of the operator (34) by

$$\varepsilon\left(\frac{p_0}{k}, \frac{q_0}{k}\right) = k^2 \eta(p_0, q_0, k). \tag{35}$$

Let us write down the stability condition (12a), (12b) for a system with charge parameters $p=p_0/k$ and $q=q_0/k$. With allowance for (35), it has the following form:

$$\eta(p_0, q_0, k)<\min\left[-\frac{1}{2(\mu+1)p_0^2}, -\frac{1}{2(\nu+1)q_0^2}\right]. \quad (36)$$

Direct application of this condition is difficult, since the dependence of the eigenvalue η of the operator (34) on the quantity k is unknown. Nevertheless, it is not difficult to construct for this eigenvalue a lower bound that makes it possible to establish the values of k for which a system of particles with charge parameters $p=p_0/k$ and $q=q_0/k$ is unconditionally unstable.

By stipulation, $k\geqslant 1$. Therefore, the operator (34) differs from the energy operator (13) of the initial stable system by a term in the form of the product of the nonnegative quantity $(k-1)/p_0q_0$ with the positive-definite operator $1/|\mathbf{t}-\mathbf{u}|$. By virtue of the Cauchy–Bunyakovskiĭ inequality, we have

$$\langle\varphi|V|\varphi\rangle\langle\chi|V^{-1}|\chi\rangle\geqslant\langle\varphi|\chi\rangle\langle\chi|\varphi\rangle, \quad (37)$$

where V is a positive-definite operator and φ and χ are wave functions satisfying the condition for the existence of the corresponding matrix elements appearing in (37). Taking for χ the eigenfunction $\psi_0(\mathbf{t},\mathbf{u})$ of the ground state of the operator (13), we obtain from (37) the following lower bound on the mathematical expectation value of the operator V:

$$\langle\varphi|V|\varphi\rangle\geqslant\langle\varphi|\psi_0\rangle\langle\psi_0|\varphi\rangle/\langle\psi_0|V^{-1}|\psi_0\rangle. \quad (38)$$

Since this inequality is valid for any wave function φ, the following operator inequality holds:

$$V\geqslant\frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0|V^{-1}|\psi_0\rangle}. \quad (39)$$

In the numerator of the fraction is the projection operator onto the eigenfunction ψ_0 of the ground state of the system with energy operator (13). Setting $V=1/|\mathbf{t}-\mathbf{u}|$, we have

$$\frac{1}{|\mathbf{t}-\mathbf{u}|}\geqslant\frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0||\mathbf{t}-\mathbf{u}||\psi_0\rangle}. \quad (40)$$

We set up the auxiliary operator

$$\tilde{g}(\mathbf{t},\mathbf{u})=h_0(\mathbf{t},\mathbf{u})+\frac{k-1}{p_0q_0}\frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0||\mathbf{t}-\mathbf{u}||\psi_0\rangle}. \quad (41)$$

From (40) it is clear that this operator provides a lower bound on the operator (34):

$$\tilde{g}(\mathbf{t},\mathbf{u})\leqslant g(\mathbf{t},\mathbf{u}). \quad (42)$$

In particular, it follows from this that the lowest eigenvalue $\tilde{\eta}(p_0,q_0,k)$ of the operator (41) gives a lower bound on the lowest eigenvalue of the operator (34):

$$\tilde{\eta}(p_0, q_0, k)\leqslant\eta(p_0, q_0, k). \quad (43)$$

Let the initial system with charge parameters p_0 and q_0 be chosen so that it has only one bound state. Then the spectrum of the energy operator (13) consists of the discrete level ε_0 and the continuum, which starts at the point

$$\varepsilon_c=\min\left[-\frac{1}{2(\mu+1)p_0^2}-\frac{1}{2(\nu+1)q_0^2}\right] \quad (44)$$

and extends to $+\infty$. It is easy to see that the eigenfunctions of the auxiliary operator (41) coincide with the eigenfunctions of the operator (13), and that its continuous spectrum also starts at the point (44). Consider that eigenvalue of the operator (41) which corresponds to the ground-state eigenfunction ψ_0 of the initial system with energy operator (13). For $k=1$ it coincides with the lowest discrete energy level ε_0 of the initial system, and as k increases it increases monotonically and is given by the formula

$$\tilde{\eta}(p_0, q_0, k)=\varepsilon_0+\frac{k-1}{p_0q_0\langle\psi_0||\mathbf{t}-\mathbf{u}||\psi_0\rangle}. \quad (45)$$

When the parameter k reaches the value

$$k_c=1+p_0q_0\langle\varphi_0||\mathbf{t}-\mathbf{u}||\psi_0\rangle(\varepsilon_c-\varepsilon_0), \quad (46)$$

the eigenvalue (45) enters the continuous spectrum and with further increase of k it is absorbed by the continuum. Therefore, for $k\geqslant k_c$ the lowest eigenvalue of the auxiliary operator (41) is the boundary ε_c (44) of the continuous spectrum. It follows from the inequality (42) that in this case the operator (33) has no eigenvalues lying lower than the boundary ε_c of the continuous spectrum. Thus, for $k\geqslant k_c$ the condition (36) is not fulfilled and the three-particle system is unconditionally unstable.

We restate the result. If a certain initial three-particle system with particle-mass ratios μ and ν and with particle-charge ratios equal to $p_0=-Z_3^{(0)}/Z_1^{(0)}$ and $q_0=-Z_3^{(0)}/Z_2^{(0)}$ is stable and has only one discrete energy level, the analogous systems with the same particle-mass ratios and with particle-charge ratios equal to $p=p_0/k$ and $q=q_0/k$ are unconditionally unstable when the parameter k satisfies the inequality $k\geqslant k_c$, where the quantity k_c is given by Eq. (46).

This result admits a simple physical interpretation. It is clear that the "safety factor" of a stable system with respect to increase of the charges of the like-charged particles is greater the greater the depth of the discrete energy level of this system below the boundary of the continuous spectrum and the greater the average distance between the like-charged particles. The formula (46) gives quantitative confirmation of these considerations, by showing that the "distance" (equal to k_c-1) from the initial stable system with $k=1$ to the unconditionally unstable system with $k=k_c$ is proportional to the depth of the displacement of the initial discrete energy level from the boundary of the continuous spectrum and to the average distance between the like-charged particles in the initial stable system.

Since the negative hydrogen-atom ion $H^-(\infty)$ and the positronium ion $e^-e^-e^+$ have only one bound discrete energy level,[1,2,26] the criterion found here for unconditional instability is directly applicable to systems that can be obtained from these initial systems by change of the particle-charge ratios. Taking into account the values given in Table I for the energies of these systems and the average values $\langle r_{12}\rangle$ of the interparticle distances in these systems, we find that the three-particle system with particle masses $m_1=m_2$ and $m_3=\infty$ is unconditionally stable at the point D with coordinates $p_D=q_D=0.89090$; analogously, the system with all particles having the same masses ($m_1=m_2=m_3$) is unconditionally unstable at the point D with coordinates $p_D=q_D=0.90695$.[3)] This implies that for a two-electron

atom with a fixed nucleus the critical value of the atomic number is bounded from below by the inequality $Z_{cr} \geqslant 0.89090$, while for a system consisting of two electrons and a "positron" with variable charge (but with a fixed mass equal to the electron mass) the critical charge of the "positron" is bounded from below by the inequality $Z_{cr} \geqslant 0.90695$.

REGION OF UNCONDITIONAL INSTABILITY OF A THREE-PARTICLE SYSTEM

We now determine, on the plane of the charge parameters p, q, the region in which a Coulomb system of three particles is unconditionally unstable.

We shall consider functions in the form of the difference of the left- and right-hand sides of the inequalities (12a) and (12b):

$$f_1(p,q)=\varepsilon(p,q)+\frac{1}{2(\mu+1)p^2}, \tag{47a}$$

$$f_2(p,q)=\varepsilon(p,q)+\frac{1}{2(\nu+1)q^2}. \tag{47b}$$

Suppose that at a certain point D with coordinates p_D, q_D the three-particle system is unstable against decay along both possible channels $(1, 2, 3)\to(1, 3)+2$ and $(1, 2, 3)\to(2, 3)+1$. Then both inequalities (12a) and (12b) are violated simultaneously, and at the point D the functions (47a) and (47b) satisfy the relations

$$f_1(p_D, q_D)\geqslant 0, \tag{48a}$$

$$f_2(p_D, q_D)\geqslant 0. \tag{48b}$$

Consider first the consequences flowing from the inequality (48a). We form the derivatives of the function f_1 with respect to p and q. For the first of these quantities, taking into account the explicit form of the energy operator (9), the Hellmann–Feynman theorem, and the virial theorem, we find the following chain of equalities:

$$\begin{aligned}\frac{\partial f_1}{\partial p}&=\frac{\partial \varepsilon}{\partial p}-\frac{1}{(\mu+1)p^3}\\&=\frac{1}{p^2}\left\langle\frac{1}{t}\right\rangle-\frac{1}{p^2q}\left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle-\frac{1}{(\mu+1)p^3}\\&=-\frac{1}{p}\left[-\frac{1}{p}\left\langle\frac{1}{t}\right\rangle-\frac{1}{q}\left\langle\frac{1}{u}\right\rangle+\frac{1}{pq}\left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle\right.\\&\quad\left.+\frac{1}{(\mu+1)p^2}+\frac{1}{q}\left\langle\frac{1}{u}\right\rangle\right]\\&=-\frac{2}{p}\left[\varepsilon(p,q)+\frac{1}{2(\mu+1)p^2}\right]-\frac{1}{pq}\left\langle\frac{1}{u}\right\rangle.\end{aligned} \tag{49}$$

Taking (47a) into account, from this we obtain

$$\frac{\partial f_1}{\partial p}=-\frac{2f_1}{p}-\frac{1}{pq}\left\langle\frac{1}{u}\right\rangle. \tag{50}$$

For the derivative of f_1 with respect to q, taking the Hellmann–Feynman theorem into account we have

$$\frac{\partial f_1}{\partial q}=\frac{\partial \varepsilon}{\partial q}=\frac{1}{q^2}\left\langle\frac{1}{u}\right\rangle-\frac{1}{pq^2}\left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle. \tag{51}$$

We draw a straight line connecting the point D to an arbitrary point of the segment OF (this straight line is not shown in the figure). It is characterized by a nonnegative slope k, where

$$0\leqslant k\leqslant q_D/p_D \tag{52}$$

and is described by the parametric equation

$$p=p_D+s, \quad q=q_D+ks, \tag{53}$$

where s is the parameter whose variation corresponds to motion of the point with coordinates p, q (53) along the straight line. For the derivative of f_1 with respect to s, which determines the variation of the function f_1 as we move along the straight line under consideration, we have, with allowance for Eqs. (50), (51), and (53),

$$\begin{aligned}\frac{df_1}{ds}&=\frac{\partial f_1}{\partial p}\frac{dp}{ds}+\frac{\partial f_1}{\partial q}\frac{dq}{ds}\\&=-\frac{2f_1}{s}-\frac{k}{pq^2}\left\langle\frac{1}{|\mathbf{t}-\mathbf{u}|}\right\rangle-\frac{kp-q}{pq^2}\left\langle\frac{1}{u}\right\rangle.\end{aligned} \tag{54}$$

The second term on the right-hand side of (54), obviously, is negative. From (52) and (53) it follows that $kp-q=kp_D-q_D\leqslant 0$. Therefore, the third term in (54) is nonpositive. Discarding the second and third terms in (54), we obtain the inequality

$$\frac{df_1}{ds}\leqslant-\frac{2f_1}{p}. \tag{55}$$

By virtue of (48a), the function f_1 is nonnegative at the point D. The inequality (55) shows that as we move from the point D along any straight line inside the triangle ODF the function f_1 does not decrease. Thus, in the entire triangle ODF (see the figure) the following inequality holds:

$$f_1(p, q)\geqslant 0, \tag{56}$$

implying instability of the three-particle system.

We note now that for the function f_2 relations analogous to Eqs. (49)–(55) and differing from them only in interchange of the coordinates p and q are fulfilled. Therefore, it follows from the inequality (47b) that the system is unconditionally unstable in the entire triangle *OED*.

Let us combine these results. If a three-particle system is unstable at a certain point with coordinates p_D, q_D in respect of both possible decay channels, it is unconditionally unstable at all points whose coordinates simultaneously satisfy the inequalities $p\leqslant p_D$ and $q\leqslant q_D$, i.e., inside the rectangle *OEDF*.

The systems symmetric in the masses of particles 1 and 2, considered at the end of the preceding section and generated by the negative hydrogen-atom ion and the positronium ion, satisfy at the point D the conditions (47). Therefore, they are unconditionally unstable inside the rectangle *OEDF*, which in the given case is a square with side equal to 0.89090 [for systems of the type $H^-(\infty)$] or 0.90695 (for systems of the positronium-ion type).

CONCLUSION

The analysis performed here has shown that the method of variation of the scale makes it possible to determine the regions of unconditional stability and instability of Coulomb systems with varying particle charges for fixed ratios of the particle masses. Thus, three-particle Coulomb systems are unconditionally stable in the region shaded in the figure. The coordinates of the points *A*, *B*, and *C* on the plane of the

charge parameters $p = -Z_3/Z_1$ and $q = -Z_3/Z_2$ (the coordinates defining the region of stability) are related by Eqs. (27a)–(27c) to the total energy and to the component parts of the potential energy of the initial ("standard") stable system characterized by certain fixed values of the charges and masses of the particles.

The region of unconditional instability of three-particle systems with varying particle charges is the rectangle *OEDF* adjacent to the coordinate origin. The location of the corners of the rectangle is determined, using Eq. (46), from the values of the total energy and the average spacing between the like-charged particles in the initial system, which, in the given case, should have one (and only one) discrete energy level. Thus, every stable three-particle system generates a fully determined region of unconditional stability of systems with varying charges of the particles. In addition, every stable system that has only one discrete energy level also generates a fully determined region of unconditional instability of the systems that we are investigating.

Knowledge of these regions of stability and instability makes it possible, in particular, to find lower and upper bounds on the critical value $|Z_3| = Z_{cr}$ of the charge of the third (binding) particle at which the system with unit charges of the other particles ($|Z_1| = |Z_2| = 1$) loses its stability against decay, and also the corresponding bounds on the critical coupling parameter λ_{cr} (characterizing the interaction of the like-charged particles) at which the system with unit charge of the binding particle ($|Z_3| = 1$) loses its stability. These bounds are given in Table III for various three-particle systems that can be obtained from the initial systems indicated there by changing the particle charges. Also included in the table are data for the muon analog of the negative hydrogen-atom ion (the system $\mu^+ e^- e^-$), calculated taking the results of recent work[27] into account. In the last two columns of Table III we indicate the limits of the range of variation of the magnitude $|Z_2|$ of the charge of the second particle within which the system with unit charges of the other particles ($|Z_1| = |Z_3| = 1$) is unconditionally stable.

All these bounds (except the upper bound on the quantity Z_{cr} for H^-) are obtained here for the first time. They are quite accurate. For example, the upper bounds on the critical value Z_{cr} of the charge of the binding particle and on the critical value λ_{cr} of the interaction parameter of the particles being bound differ from the lower bounds by less than 3%. At the same time, Ref. 11 gives only a rough estimate of the bounds on Z_{cr} for the H^- ion: $1/2 < Z_{cr} < 868/901$, in which the upper bound amounts to 193% of the lower bound on the quantity being estimated.

The results obtained here can be applied to stability analysis and to the determination of the critical charge parameters and the regions of applicability of perturbation theory in the interaction of the particles in various Coulomb systems. They are a new confirmation of the usefulness of the method of variation of the scale in application to the study of the dependence of the energy of a quantum-mechanical system on the parameters appearing in its energy operator.

[1)] Ref. 12 is cited in the text of Ref. 11.
[2)] The validity of the inequalities (25a) and (25b) can also be proved purely analytically, starting from the relations obtained in Ref. 13 for the energy and the components of the potential energy of a Coulomb system with varying particle charges. The method used in the text is preferable by virtue of its brevity and clear physical meaning.
[3)] See Table II.

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