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Quantum criticality and stability of three-body Coulomb systems

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We present quantum phase transitions and critical phenomena of three-body Coulomb systems with charges (Q, q, Q) and masses (M, m, M). Full numerical results, using the finite-size scaling method, for an arbitrary mass ratio $0 \leqslant \kappa = (1+m/M)^{-1} \leqslant 1$ over the range $1 \leqslant \lambda = |Q/q| \leqslant 1.25$, show that there exists a transition curve $\lambda_c(\kappa)$ through which all systems undergo a first-order phase transition from stable to unstable. Particularly, $\lambda_c(\kappa)$ has a minimum at $\kappa_m = 0.35$, which leads to a new proposed classification of the three-body Coulomb systems: moleculelike systems, $\kappa > \kappa_m$, such as Ps^- $(\kappa = 0.5)$ and atomlike systems, $\kappa < \kappa_m$, such as $\overline{p}pd$ $(\kappa = 0.33)$.

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The stability of three-body Coulomb systems is an old problem that has been treated in many particular cases [1–3], and several authors have reviewed this problem [4,5]. For example, the He atom $(\alpha e^- e^-)$ and $H_2{}^+$ (ppe^-) are stable systems, H^- $(pe^- e^-)$ has only one bound state [6], the positronium negative ion Ps^- $(e^+ e^- e^-)$ has a bound state [7], while the positron-hydrogen system $(e^- p e^+)$ is unbound and the proton-electron-negative-muon $(pe^- \mu^-)$ is an unstable system [8]. Here we show that all three-body ABA Coulomb systems undergo a first-order quantum phase transition from the stable phase of ABA to the unstable breakup phase of $AB+A$ as their masses and charges vary. Using the finite-size scaling method, we calculate the transition line that separates the two phases. For any combination of the three particles in the form ABA, one can read directly from the phase diagram if the system is stable or unstable. Moreover, the transition line has a minimum that leads to a new proposed classification of the ABA systems to moleculelike systems and to atomlike systems. This is very important in exploring the resonance spectrum and dynamics of three particles where there is neither an obvious point of reference as the heavy nucleus in H^- nor a line of reference as the internuclear axis in $H_2{}^+$. Rost and Wintgen [9] have shown that the resonance spectrum of the positronium negative ion Ps^- can be understood and classified with the $H_2{}^+$ molecule quantum numbers by treating the internuclear axis of Ps^- as an adiabatic parameter. Our approach gives a systematic classification of all ABA systems.

Let us consider the stability and quantum phase transitions of the three-body ABA Coulomb systems with charges (Q, q, Q) and masses (M, m, M). With the scale transformation $r \to fr$, where $f = \mu|Qq|$ and $\mu = mM/(m+M)$ is the reduced mass, the scaled Hamiltonian, $H \to \mu H/(f)^2$, reads [10]

$$H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{1}{r_1} - \frac{1}{r_2} - \kappa \boldsymbol{\nabla}_1 \cdot \boldsymbol{\nabla}_2 + \lambda \frac{1}{r_{12}}, \qquad (1)$$

where $0 \leqslant \lambda = |Q/q| \leqslant \infty$ and $0 \leqslant \kappa = 1/(1+m/M) \leqslant 1$. Here we have formally separated the motion of the center of mass, and the reference particle is the one with mass m. With this scaling transformation, the Hamiltonian depends linearly on the parameters λ and κ. We are interested in the study of the critical behavior of the Hamiltonian, Eq. (1), as a function of both parameters λ and κ. A critical point is defined as a point for which a bound state becomes absorbed or degenerate with a continuum [11]. The ABA system is stable if its energy is lower than the energy of the dissociation to $AB+A$. The critical behavior and stability of the ground-state energy as a function of λ for $\kappa = 0$ has been previously studied for the two-electron atoms [11] (with $Q=-1$, $M=1$, $m=\infty$ and $\lambda = 1/|q| = 1/Z$, where Z is the nuclear charge) and for the hydrogen moleculelike ions [10] (with $q=-1$, $m=1$, $M=\infty$ and $\lambda = |Q| = Z$).

In order to obtain the stability diagram for the three-body Coulomb systems in the $(\lambda - \kappa)$ plane, one has to calculate the transition line $\lambda_c(\kappa)$ that separates the stable phase from the unstable one. To carry out the calculations we rely on the finite-size scaling method for quantum systems. With this method, for a given Hamiltonian, one should proceed with the following scheme [11]: (i) choose a convenient orthonormal basis set and calculate the matrix elements of the Hamiltonian; (ii) calculate the two leading eigenvalues $E_0^{(N)}(\lambda)$, $E_1^{(N)}(\lambda)$ of the finite Hamiltonian matrix of order N and their corresponding correlation length of the classical pseudosystem $\xi_N(\lambda)$,

$$\xi_N(\lambda) = -\frac{1}{\ln[E_1^{(N)}(\lambda)/E_0^{(N)}(\lambda)]}; \qquad (2)$$

(iii) use the phenomenological renormalization equation to obtain a sequence of pseudocritical parameters $\lambda^{(N)}$, which are the crossing points of the equation [12]

$$\frac{\xi_N(\lambda^{(N,N')})}{N} = \frac{\xi_{N'}(\lambda^{(N,N')})}{N'}, \qquad (3)$$

where N is the order of the Hamiltonian matrix and $N' = N-1$, except when there are parity effects, then one has to take $N' = N-2$; and finally (iv) extrapolate the values of the sequences, using extrapolating methods such as the algorithm of Bulirsch and Steor to obtain the critical parameters in the limit $N \to \infty$.

TABLE I. The critical parameters for different three-body Coulomb systems.

Systems	κ	λ_c	Systems	κ	λ_c
$^{\infty}$He	0	1.097 661	$ee\,\overline{e}$	0.5	1.084 831
He	0.000 013 7	1.097 649	$dd\,\overline{p}$	0.666 556 4	1.096 404
$\mu\mu p$	0.101 212 1	1.089 825	dde	0.999 727 6	1.230 653
$\overline{p}pt$	0.250 393 3	1.083 234	tte	0.999 818 1	1.231 663
$\overline{p}pd$	0.333 443 6	1.081 979	$^{\infty}H_2^+$	1	1.234 361

To carry out the variational calculations, we used the following complete basis set:

$$\Phi_{n,m,l}(r_1,r_2,r_{12}) = \phi_n(x)\phi_m(y)\phi_l(z),$$
$$\phi_n(x) = L_n(x)e^{-x/2}, \tag{4}$$

where L_n is the Laguerre polynomial of degree n and order 0 and $x=(\theta/k_x)(r_1+r_2-r_{12})$, $y=(\theta/k_y)(-r_1+r_2+r_{12})$, and $z=(\theta/k_z)(r_1-r_2+r_{12})$ are the perimetric coordinates [13]. Here we choose $k_x=1=k_y/2=k_z/2$ and $\theta=1.5$, which gives faster convergence results for the critical points.

Solving the Schödinger equation $H\Psi=E\Psi$, where $\Psi(r_1,r_2,r_{12})=\Phi(r_1,r_2,r_{12})+\Phi(r_2,r_1,r_{12})$, gives a sparse, real, and symmetric $M(N)\times M(N)$ matrix of order N. The symmetric matrix is expressed in a sparse row-wise format, reordered, and LU-decomposed [14]. Then, we employ the block-renormalization Lanczos procedure [15] to obtain the eigenvalues. From the leading two eigenvalues $E_0^{(N)}(\lambda)$ and $E_1^{(N)}(\lambda)$, we can obtain the correlation length, Eq. (2), for the classical pseudosystem $\xi_N(\lambda)$. Now we are in a position to apply the phenomenological renormalization equation, Eq. (3), to obtain a sequence of pseudocritical parameters $\lambda_c^{(N)}$ for different values of κ. The values of the parameter $\kappa=(1+m/M)^{-1}$ was varied in the interval [0,1] according to the different masses of the combined particles. The values, in atomic units, of the particle masses were taken from Ref. [16]: for electron $m_e=1.0$, proton $m_p=1\,836.152\,667\,5$, deuteron $m_d=3\,670.482\,955\,0$, tritium $m_t=5\,496.921\,617\,9$ [16,17], muon $m_\mu=206.768\,265\,7$, and helium $m_{\mathrm{He}}=7\,296.299\,508$. The values of κ for the different combinations of the three particles are listed in Table I. The extrapolated critical values of λ_c as obtained from the phenomenological renormalization equation, Eq. (3), are in complete agreement with the results of the first-order method. With this method, one defines $\lambda_c^{(N)}$ as the value in which the ground-state energy in the Nth-order approximation $E_0^{(N)}(\lambda)$ is equal to the threshold energy E_0^{th}. The results of the extrapolated critical values are listed in Table I, and are in good agreement with previous results for $^{\infty}$He [18] and $^{\infty}H_2^+$ [19].

To illustrate the critical phenomena and stability of the three-body Coulomb systems, we consider in detail three different values of κ along the transition line: the He atom ($\kappa=0.000\,013\,7$), Ps^- ($\kappa=0.5$), and H_2^+ ($\kappa=0.999\,455\,7$). Figure 1 shows the crossing points, the pseudocritical points $\lambda_c^{(N)}$, obtained from the phenomenological renormalization equation, which means the crossing points of $[E_1^{(N)}(\lambda)/E_0^{(N)}(\lambda)]^N$ as a function of λ for He, Ps^-, and H_2^+ systems. At λ_c, the ground-state energy of each of the three systems becomes degenerate with the threshold of ionization for He and dissociation for Ps^- and H_2^+. Our numerical results show that the ground-state energy is a continuous function of $1.0\leqslant\lambda\leqslant1.25$ and $0\leqslant\kappa\leqslant1$, but bends over sharply at λ_c to become degenerate with the scaled lowest continuum at $E_0=-\frac{1}{2}$. By virtue of this behavior, we expect that the first derivative of the energy with respect to λ will develop a steplike discontinuity at λ_c. $H(\lambda_c)$ has a square-integrable eigenfunction, as κ varies, corresponding to a scaled threshold energy $E^{th}(\lambda_c)=-\frac{1}{2}$ [20]. $E(\lambda)$ approaches $E^{th}(\lambda_c)$ linearly in $(\lambda-\lambda_c)$ as $\lambda\to\lambda_c^-$ [20,21,18]. The behavior of the ground-state energy for the three systems and their first and second derivatives resembles the behavior of the free energy at a first-order phase transition. This behavior is universal for all ABA Coulomb systems.

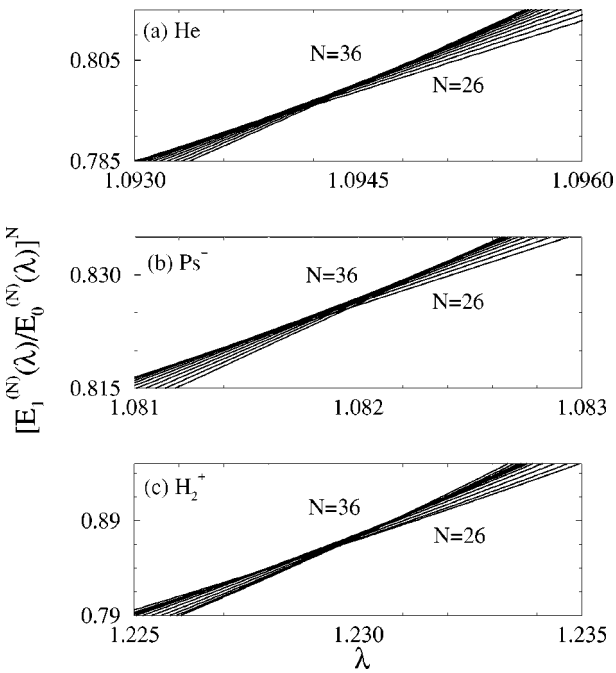

FIG. 1. The ratio between the ground-state energy $E_0^{(N)}(\lambda)$ and the second lowest eigenvalue $E_1^{(N)}(\lambda)$, raised to a power N as a function of λ for $N=26,27,\ldots,36$: (a) He atom ($\kappa=1.370\,557\,772\times10^{-3}$), (b) Ps^- ($\kappa=0.5$), and (c) H_2^+ ($\kappa=0.999\,455\,679$).

For the ABA Coulomb systems when $1\leqslant\lambda\leqslant\lambda_c$ the ratio of charges is sufficiently small enough to keep the three particles bound and the system at least has one bound state [6]. This situation remains until the system reaches a critical point λ_c, which is the maximum value of λ for which the Hamiltonian has a bound state. For $\lambda\geqslant\lambda_c$, one of the particles jumps to infinity with zero kinetic energy. Figure 2 presents a direct picture for the change in the mean value of the distance, $\langle r_{12}\rangle$, of the two like charge particles as λ varies. The steplike discontinuity at λ_c tells us about the jump of one of the particles and the breakup of the system. In Fig. 3 we plot the charge-density probability $|\Psi(r_1=a,r_2,r_{12})|^2$ for one of the protons of the numerically calcu-

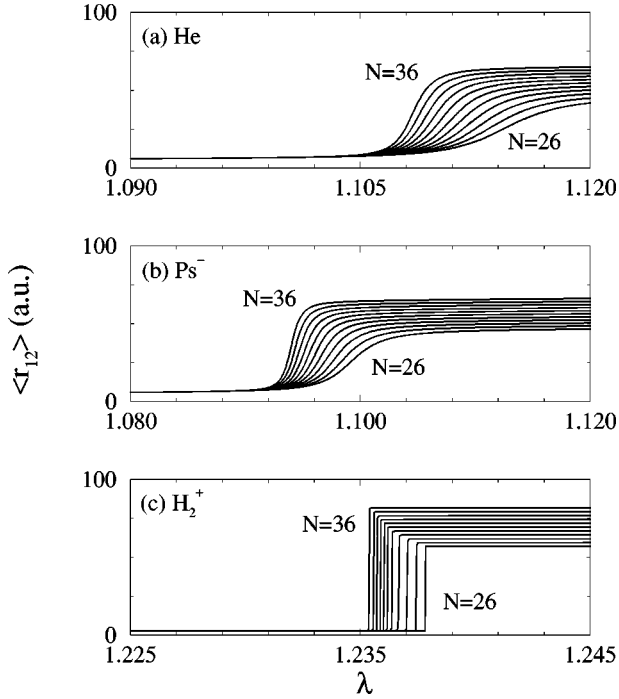

FIG. 2. The average distance between particle 1 and 2, $\langle r_{12}\rangle$ in atomic units, as a function of λ: (a) He atom, (b) Ps^-, and (c) $H_2{}^+$.

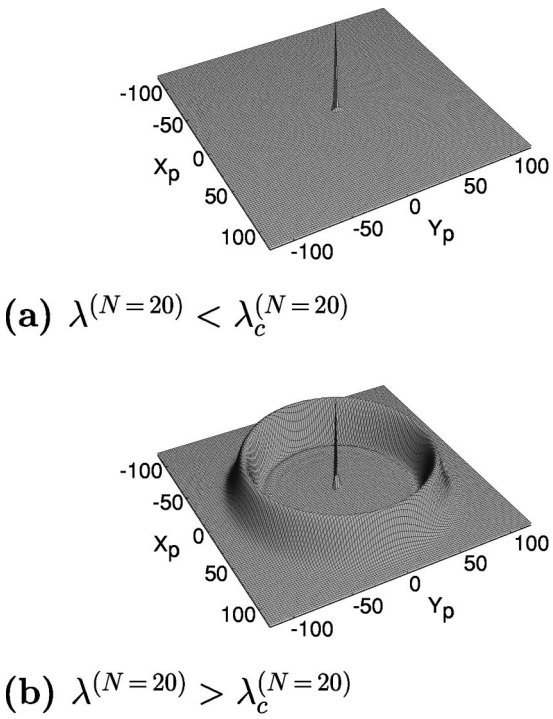

FIG. 3. The charge-density probability $|\Psi(r_1=a,r_2,r_{12})|^2$ for one of the protons of the $H_2{}^+$ like molecular ions, at fixed distance $a=3$. In this geometry, in the (X_p,Y_p) plane, the electron is fixed at the origin of the coordinates and the electron-proton distance is fixed at $a=3$ along the X_p axis. Here a, X_p, and Y_p are given in atomic units. In the upper part $\lambda^{(N=20)}=1.24<\lambda_c^{(N=20)}=1.2402$ and in the lower part $\lambda^{(N=20)}=1.241>\lambda_c^{(N=20)}=1.2402$.

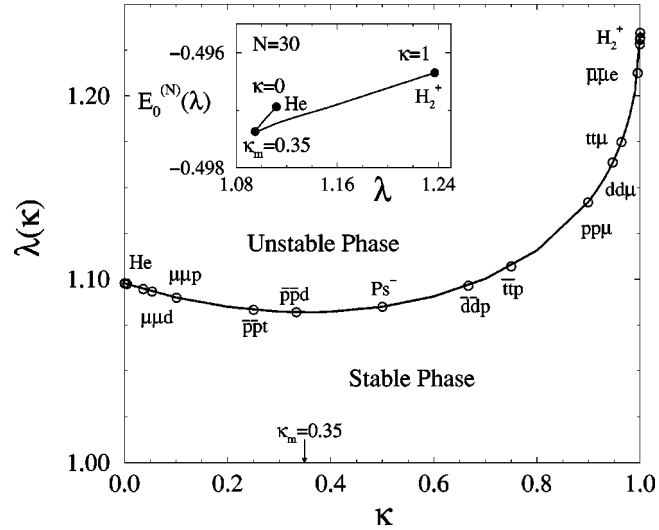

FIG. 4. The critical parameter λ_c as a function of κ in the range $0\leqslant\kappa\leqslant1$. The different three-body systems are shown along the transition line that separates the stable phase from the unstable one. Note the minimum value of $\kappa_m=0.35$; for $\kappa>\kappa_m$ we have moleculelike systems, while for $\kappa<\kappa_m$ the systems behave like atoms. The window in this figure shows the two branches in the $(E_0^{(N)},\lambda)$ plane as κ varies in the interval [0,1]. $E_0^{(N)}$ is given in atomic units.

lated eigenfunctions of the $H_2{}^+$-like molecular ions, at a fixed scaled distance $a=3$, which is the approximate distance between the electron and the other proton. In this geometry, in the (X_p,Y_p) plane, the electron is fixed at the origin of the coordinates and the electron-proton distance is fixed at $a=3$ along the X_p axis. For $\lambda^{(N=20)}=1.24<\lambda_c^{(N=20)}=1.2402$ the proton density peaks at $(X_p=-3,Y_p=0)$, as shown in the upper part of Fig. 3. For $\lambda^{(N=20)}=1.241>\lambda_c^{(N=20)}=1.2402$, the system breaks up and the proton jumps to a large distance; the proton density becomes localized at very large distance ($\simeq80$), as shown in the lower part of Fig. 3. When the size of the system increases, $N\rightarrow\infty$, the proton jumps to infinity.

The position of this steplike discontinuity in the $\langle r_{12}\rangle$ as a function of λ can be used as another possible definition of the pseudocritical $\lambda_c^{(N)}$. The extrapolated values of this sequence, using the Bulirsh and Stoer algorithm [11], as a function of κ are in complete agreement with the previous results of the crossing points of Eq. (3) and from the first-order method where $E_0^{(N)}(\lambda)=E_0^{th}$ [10]. The three groups of data for λ_c are consistent to an accuracy of better than 0.0005. The extrapolated values of λ_c as a function of κ are listed in Table I.

In Fig. 4 the transition line λ_c as a function of κ is shown. The parameter κ changes between $\kappa=1$, which corresponds to the $H_2{}^+$-like systems in the Born-Oppenheimer approximation and $\kappa=0$, which corresponds to the He-like atoms in the infinite mass approximation. Between the two limits $\kappa=0$ and $\kappa=1$, there are many stable three-particle systems, as shown in the figure. The transition line separates the three-particle systems into stable systems (with at least one bound state) and unstable systems. These numerical results confirm the general properties of stability domain discussed by Mar-

tin [8], the instability region in the λ-κ plane should be convex. Particularly, the transition curve has a minimum, which occurs at $\kappa_m = 0.35$, and hence all possible bound three-body systems are divided into two branches in the λ-κ plot, one with $0 \leqslant \kappa < \kappa_m$ and the other with $\kappa_m < \kappa \leqslant 1$. The two closest systems to κ_m are Ps^- with $\kappa = 0.5$ and $\overline{pp}d$ with $\kappa = 0.33$. The inset in Fig. 4 shows the two different branches in their ground-state energy as a function of the location of the pseudocritical points $\lambda_c^{(N)}(\kappa)$.

The observation of two different branches leads us to investigate the similarity between the moleculelike systems of the right branch, $\kappa > \kappa_m$, such as the Ps^-, and the atomlike systems of the left branch, $\kappa < \kappa_m$, such as $\overline{pp}d$. The parameter κ measures the strength of the mass polarization term, which is due to the motion of the two identical particles with respect to the third particle. The mass polarization term is then a measure of the momentum correlation of the two identical particles with respect to the third particle. If $\kappa \gg \kappa_m$, as in the case of a molecule such as $H_2{}^+$, the light particle with mass m and charge q tends to stay in the middle of the two heavy particles to achieve bonding, while for $\kappa \ll \kappa_m$, as in the case of the He atom, each light particle with mass M and charge Q is less localized and thus the momentum correlation is smaller. The fact that the resonance spectrum and dynamics of Ps^- ($\kappa = 0.5$) was understood and classified with the $H_2{}^+$ quantum numbers [9] is very encouraging and shows that the above proposed classification might shed some light on a systematic and concise picture of the dynamics of all ABA Coulomb systems.

In summary, we have shown that the ABA Coulomb systems exhibit a first-order quantum phase transition as the parameter λ varies. The transition line between the stable and the unstable phase was accurately calculated using the finite-size scaling method. The transition line $\lambda_c(\kappa)$ has a minimum at $\kappa_m = 0.352$ or $m/M = 1.84$, which separates the two branches in the $(E_0^{(N)}, \lambda)$ plane as κ varies between moleculelike systems and atomlike systems. This might be a powerful result, since it provides a rough picture of the dynamics for many exotic particle combinations that may be realized experimentally, such as $(e^- \mu^+ e^-)$, $(\mu^- p \mu^-)$, etc.

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