# Critical stability for two-electron ions with Yukawa potentials and varying $Z$

Sabyasachi Kar,[1,*] Yu-Shu Wang,[1] and Yew Kam Ho[2]
[1]*Department of Physics, Harbin Institute of Technology, Harbin 150001, People's Republic of China*
[2]*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei 106, Taiwan, Republic of China*

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We investigate the stability of two-electron ions interacting with Yukawa potentials with varying $Z$ using correlated exponential wave functions based on the Ritz variational method. The critical screening parameter $\mu_C$ as a function of the nuclear charge $Z$, the critical nuclear charge $Z_C$ as a function of the screening parameter $\mu$, and the ionization energies in terms of the screening parameter $\mu$ and $Z$ are reported. The critical charge for the bare Coulomb system ($Z$, $e$, $e$) obtained using 700-term correlated exponential wave functions is in reasonable agreement with the reported results in the literature. The critical screening parameter, critical nuclear charge, and ionization energy for the Yukawa system ($Z$, $e$, $e$) exhibit interesting behaviors. The possible existence of Borromean states and quasibound resonant states is also discussed.

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## I. INTRODUCTION

The problem of stability of a given quantum system made up of charged particles is of fundamental interest in many areas of physics such as atomic, molecular, and nuclear physics. The system might lose the stable configuration if the charge of one of the particles varies. Our study deals with the problem of stability of a two-electron system in which the nuclear charge has been considered as a real continuous variable. We aim to calculate the critical nuclear charge $Z_C$ for the ($Z$, $e$, $e$) system using correlated exponential wave functions in such a way that the system ceases to have a bound state when the charge $Z$ is less than critical nuclear charge $Z_C$. It is pertinent to mention here that the positive integer nuclear charges for the ($Z$, $e$, $e$) systems correspond to the stable systems. In recent years, there has been a renewed interest in studying the stability of two-electron systems as a function of the continuously varying nuclear charge $Z$ [1–5]. The precise determination of the critical nuclear charge $Z_C$ for the heliumlike system ($Z$, $e$, $e$) is of particular interest as it is the minimum value of $Z$ for which the system still has one bound state. In other words, the system ($Z$, $e$, $e$) does not support any bound state for $Z < Z_C$, and supports at least one bound state for $Z \geqslant Z_C$. The value of $Z_C$ has been reported in the literature by several authors [1–3,6–14] using a variety of sophisticated calculations, but the value of $Z_C$ obtained by Estienne *et al.* [1] based on a variational calculation using 2276 terms of a triple basis set is the most accurate one. The $Z_C$ reported by Estienne *et al.* [1] is accurate up to 17 decimal digits. An independent calculation by Pilón and Turbiner [3] using the Lagrange mesh method coincides with the best value of $Z_C$ [1] up to 11 decimal digits. A detailed survey of the critical stability of nonrelativistic systems in quantum mechanics is found in the review article of Armour *et al.* [12].

The knowledge of stability of a quantum system of charged particles under the influence of external environments is also of great importance in atomic, molecular, nuclear, and plasma physics, as summarized in recent reviews [15–17]. The atomic systems interacting with screened Coulomb potentials have also been a topic of considerable interest due to their importance in various branches of physical sciences. In view of the importance of the screened Coulomb potentials in several branches of physics and chemistry, it is of interest to investigate the critical screening parameter and the critical nuclear charge of the ($Z$, $e$, $e$) system interacting with screened Coulomb potentials. The atomic systems interacting with screened Coulomb potentials like the Yukawa atoms and the Debye atoms [4,5] can be defined, respectively, by the Yukawa potentials [18] and the Debye potentials [19]. Despite the similar mathematical forms, the Debye potentials are of interest to plasma physicists and the Yukawa potentials are of interest to nuclear physicists. At this point, it is of interest to refer to the atomic model without screening environments as the bare Coulomb atom. Apart from the works on the bare Coulomb atoms, the critical stability of one- and two-electron Yukawa atoms has been studied recently by Montgomery *et al.* [5] and Sen *et al.* [4]. However, more detail and independent study appears worthwhile with screening and without screening environments. It is imperative to point out two recent articles on the two-electron Debye atoms: the doubly excited states calculations by Ho [20] for the ($Z$, $e$, $e$) systems with varying nuclear charge, where the particle of charge $Z$ is assumed to have the mass of a positron, and the bound states calculations by Katriel *et al.* [21] for the ($Z$, $e$, $e$) systems where the mass of the particle with positive charge $Z$ is considered infinite.

In the present work, we are mainly interested in studying the critical stability of two-electron Yukawa systems ($Z$, $e$, $e$) as a function of the nuclear charge $Z$ as well as of the screening parameter. We determine the critical screening parameter and the critical nuclear charge as $Z$ varies for one- and two-electron Yukawa atoms using correlated exponential wave functions. It is to be noted that, by this term, we mean the

*skar@hit.edu.cn

 

TABLE I. The ground-state energies of two-electron ions $(Z, e, e)$ using 700-term exponential basis functions for selected values of $Z$ along with the available data and threshold energy.

| $Z$ | $E\,(Z, e, e)$ | $E\,(Z, e)$ |
|---|---|---|
| 1.0 | −0.52775101654[a] | −0.5 |
| | −0.52775101654438[b] | |
| 0.98 | −0.50084718003 | −0.4802000000000 |
| 0.95 | −0.46212469967 | −0.4512500000000 |
| | −0.4621246996838[b] | |
| 0.92 | −0.4254852816 | −0.4232000000000 |
| | −0.425485281676[b] | |
| 0.9110282243 | −0.4149862128 | −0.4149862127356 |
| 0.9110282242 | −0.4149862126 | −0.4149862126445 |
| 0.9110282241 | −0.4149862125 | −0.4149862125534 |
| 0.911028224077 25573(4)[c] | −0.414 986212532679[c] | |
| 0.91102822407(7) | −0.414 98621253[b] | |

[a]Kar and Ho [25].
[b]Pilón and Turbiner [3].
[c]Estienne *et al.* [1].

one-electron atoms and two-electron ions with varying or changing nuclear charge $Z$ with $Z < 1.0$. For the pure Coulomb case, the critical nuclear charge $Z_C$ for a two-electron system $(Z, e, e)$ obtained from the present calculation is in agreement with the reported results of Estienne *et al.* [1] and Pilón and Turbiner [3]. We exploit the Ritz variational method to obtain the ground-state energy using highly correlated exponential wave functions. The nonlinear variational parameters in the exponents of the proposed wave functions are simply generated using a pseudorandom technique. The ionization energies (IEs) as a function of the screening parameter are also reported.

## II. CALCULATIONS

To obtain the ground-state energy $E$ variationally in terms of the screening parameter and the nuclear charge for one- or two-electron Yukawa or Debye atoms, one needs to solve the Schrödinger equation:

$$H(Z, \mu)\Psi = E(Z, \mu)\Psi. \tag{1}$$

The Hamiltonian $H(Z, \mu)$ and wave function $\Psi$ for the two-electron Yukawa system $(Z, e, e)$ can be written as

$$H(Z, \mu) = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - Z\left[\frac{\exp(-\mu r_1)}{r_1} + \frac{\exp(-\mu r_2)}{r_2}\right] + \frac{\exp(-\mu r_{12})}{r_{12}}, \tag{2}$$

$$\Psi = \sum_{i=1}^{N_P} P_i[\exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}) + \text{exchange}]. \tag{3}$$

The parameter $\mu$ is known as the Yukawa or Debye screening parameter. For the free-atom case, we set $\mu = 0$. A full list of references on atomic systems interacting with Yukawa or Debye potentials can be found in the review articles [15–17,22]. The most convenient way to select the nonlinear variational parameters, $\alpha_i$, $\beta_i$, $\gamma_i$, can be written in the following matrix notation,

$$[\alpha_i\ \beta_i\ \gamma_i]^T = [\langle\langle k\sqrt{2}/2\rangle\rangle A\ \langle\langle k\sqrt{3}/2\rangle\rangle B\ \langle\langle k\sqrt{5}/2\rangle\rangle C]^T, \tag{4}$$

where $k = i(i+1)$ and $A$, $B$, $C$ are chosen randomly by the trial and error method. The symbol $\langle\langle x\rangle\rangle$ denotes the fractional part of a real number $x$.

The Hamiltonian $H(Z, \mu)$ and wave function $\Psi$ for a one-electron $(Z, e)$ ion are as follows:

$$H(Z, \mu) = -\frac{1}{2}\nabla^2 - Z\frac{\exp(-\mu r)}{r} \tag{5}$$

and

$$\Psi = \sum_{i=1}^{N_Q} Q_i r^{i-1}\exp(-\delta r). \tag{6}$$

Here $\delta$, a nonlinear variational parameter, can be chosen randomly by the trial and error method. The parameters $P_i$ and $Q_i$ are linear coefficients. $N_P$ and $N_Q$ indicate the number of terms in the wave functions (3) and (6), respectively. The optimization for the upper bound to the true energy has been calculated here based on the Ritz variation principle. It is important to mention here that the wave functions in Eq. (3) are functionally similar to the Hylleraas-type wave functions [23] and can produce very accurate ground-state energy of negatively charged hydrogen ions correct up to 24 decimal digits depending on the computational resources [24]. According to our computational capacity, we can calculate the ground state of the negatively charged hydrogen ions correctly up to 11 decimal digits [25,26].

## III. RESULTS AND DISCUSSIONS

Following the above computational procedure, we calculate the upper bound to the ground-state energies of one-electron atoms and two-electron ions for different $Z$ and $\mu$ by diagonalizing the Hamiltonian using the proposed wave functions. For the bare Coulomb system $(Z, e, e)$, we are able

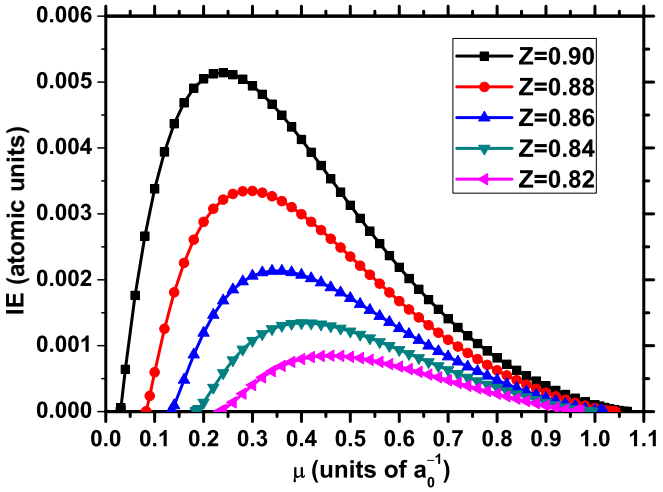


FIG. 1. The ground-state first ionization energies (IEs) for the two-electron ions at $Z = 0.90, 0.88, 0.86, 0.84, 0.82$.

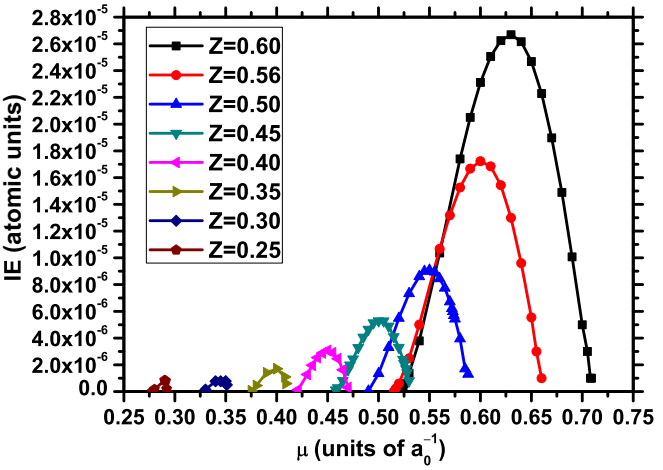


FIG. 3. The ground-state first ionization energies (IEs) for the two-electron ions at $Z = 0.60, 0.56, 0.50, 0.45, 0.40, 0.35, 0.30, 0.25$.

to obtain the critical charge $Z_C$ correct up to nine decimal digits. Table I shows the ground-state energy of the bare Coulomb system ($Z$, $e$, $e$) for selected values of $Z$ along with the threshold energy. The result for $Z = 1$ has been taken from earlier work [25] using the 700-term correlated exponential wave functions. Table I also exhibits the shift in energy eigenvalues for $Z > Z_c$. It is evident from Table I that the ground-state energies of the bare Coulomb system for $Z > Z_c$ are in good accord with the available results. The ground-state energies of the Yukawa systems ($Z$, $e$, $e$) and ($Z$, $e$) for selected values of $Z$ and $\mu$ are presented in Table A1 of the Supplemental Material [27]. We studied the convergence of our calculation with increasing number of terms in the basis functions and the stability of our computations with optimization using different sets of nonlinear parameters. The results presented in the tables are converged and stable up to the quoted digits. We restrict our calculations up to the 700-term wave functions for practical purposes.

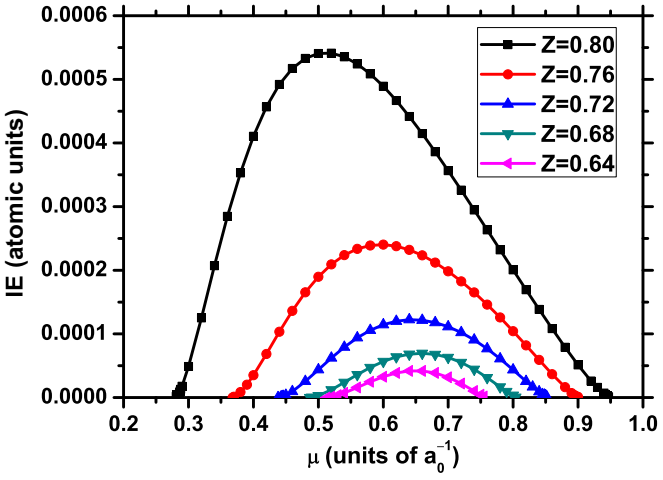


FIG. 2. The ground-state first ionization energies (IEs) for the two-electron ions at $Z = 0.80, 0.76, 0.68, 0.64$.

The ground-state first ionization energies (IEs) for different values of $Z$ as functions of the screening parameters are presented in Figs. 1–3. It appears from Figs. 1–3 and Table A1 in the Supplemental Material [27] that the IEs depend on $\mu$ nonmonotonically, rising from zero at a lower critical $\mu$, increasing up to a maximum value at $\mu = \mu_{\max}$, and then decreasing until they vanish at an upper critical $\mu$. Here we denote the critical $\mu$ as $\mu_C$ and the lower and upper $\mu_C$ as $\mu_L$ and $\mu_U$, respectively. The values of $\mu_{\max}$ at which the IEs approach a maximum in terms of $Z$ are listed Table A2 [27]. The upper and lower critical values are presented in Fig. 4. The $\mu_{\max}$ increases up to a point between $Z = 0.68$ and $Z = 0.64$, then starts to decrease with decreasing $Z$.

The values of $\mu_L$ for $Z = 0.90$ and 0.2 are determined, respectively, as 0.030 13 and 0.231. The detailed values in between are shown in Table A3 in the Supplemental Material [27]. The $\mu_L$ first increases up to about 0.60 with decreasing $Z$ and then starts to decrease and finally meets the curve for the upper critical value at $Z = 0.20$. It should be noted that the values of $\mu_U$ for $Z = 0.90$ and 0.2 are determined, respectively, as 1.066 and 0.231. The detailed values in between are

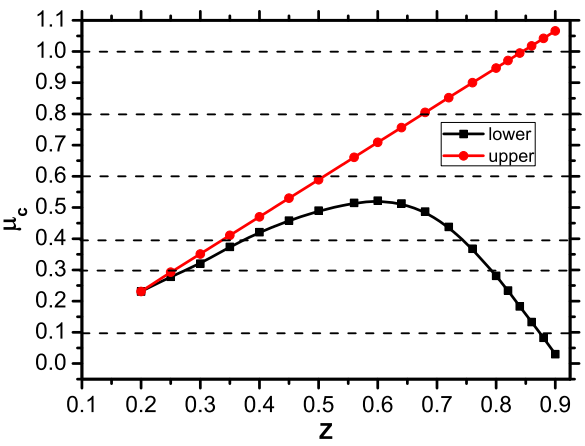


FIG. 4. The critical screening parameter $\mu_C$ (units of $a_0^{-1}$) vs the nuclear charge.

also shown in Table A3 [27]. It is worthwhile to mention here that the upper and lower critical parameters obtained from these calculations for $Z = 0.9$ are in agreement qualitatively with those reported by Sen *et al.* [4]. The values at $Z = 0.9$ reported by Sen *et al.* [4] are 0.029 83 and 1.001 68 for $\mu_L$ and $\mu_U$, respectively. The upper critical values are also the critical values for the Yukawa system $(Z, e)$.

We now provide an explanation for the phenomenon shown in Fig. 1. For the pure Coulomb case, the binding of the system results from the competition of the $Z$-dependent attractive potential $-Z(1/r_1 + 1/r_2)$ between the nucleus (the positively charged particle) and the electrons, with the $Z$-independent repulsive potential $+1/r_{12}$ between the two electrons. For $Z > Z_c$, the system is bound as the force due to the attractive potential is stronger than that of the repulsive potential. As $Z$ is decreased to below the critical charge, and as $Z$ only affects the attractive part, the force due to the repulsive potential hence overtakes the attractive contribution and the three-particle system becomes unbound. Next, this three-particle system is placed in a screening environment. The stability of the whole system now depends on the competition between the screened attractive potential and the screened repulsive potential. The screening effect is to reduce the strength of the interaction potential between any given pair of charge particles. Taking the case with $Z = 0.9$ as an example, the system is unbound for the pure Coulomb case, but when the screening effect is increased to $\mu > 0.030\,13$, for the first critical (lower) $\mu$, denoted as $\mu_L$, the system becomes bound again. This indicates that the screening has a stronger effect on the repulsive part of the potential than on the attractive part. As a result, the force due to the screened attractive potential overtakes that of the screened repulsive potential, and the system becomes bound with ionization energy increasing as $\mu$ increases. When $\mu$ is increased further to reach about $\mu = 0.24$ (for the case $Z = 0.9$), the ionization energy begins to decrease with increasing $\mu$, as both the attractive and repulsive potentials are reduced sufficiently, leading to the decrease of the overall ionization energy. When $\mu$ is increased further to values larger than 1.066, the upper critical $\mu_U$, the screening effect is so strong that the three-particle system becomes unbound again, as demonstrated in Fig. 1.

Next, when $Z$ is decreased further to $Z = 0.86$, for example, it is found that $\mu_L$ is increased to 0.1329 and $\mu_U$ is decreased to 1.018. For $\mu_L$, this is due to the fact that as $Z$ decreases, it would take a stronger screening strength (increasing $\mu_L$) to reduce the repulsive potential to make the system bound. For $\mu_U$, to achieve unboundedness it would need a weaker screening strength (decreasing $\mu_U$) for decreasing $Z$, as the system is a more loosely bound entity. The trend for $\mu_U$ continues to show decreasing behavior, like a straight line, for decreasing $Z$ (more on this issue later in the paper). For the lower critical screening parameter $\mu_L$, as seen in Fig. 4, the trend shows increasing behavior when $Z$ is decreased from 0.86 to about 0.6, but the trend for $\mu_L$ turns decreasing for decreasing $Z$ when $Z$ is decreased further from 0.6, and eventually these two curves for $\mu_L$ and $\mu_U$ meet each other at $Z = 0.20$. This phenomenon can be explained as follows. Figures 1–3 and Table A1 [27] show the ionization energies for various $Z$ values with different ranges of screening parameters. The IE for a given pair of $(Z, \mu)$ is the energy difference between the ground-state energy of the three-particle system and that of the two-particle system. When $Z$ is reduced to a sufficiently small value, such as a value lower than 0.6, the screening has a stronger reduction effect on the two-particle attractive potential than on the overall reduction to the three-particle potential. As a result, it would need a smaller screening parameter to yield a positive IE when $Z$ is decreased below the value of about 0.6, showing the decreasing behavior of $\mu_L$ for decreasing $Z$ (see Fig. 4).

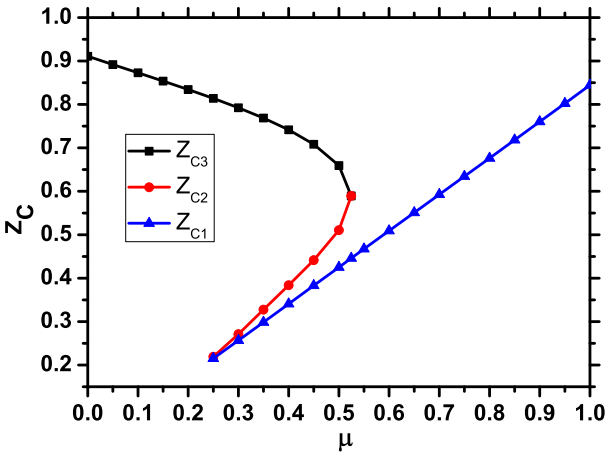


FIG. 5. The critical charge as a function of the screening parameter $\mu$ (units of $a_0^{-1}$).

Now, we comment on the "meeting" place between the curve for the upper critical $\mu_U$ and the curve for the lower critical $\mu_L$. We estimate that they "meet" around 0.20, and this $Z$ value is denoted as the "final critical charge, $Z_{\rm FC}$," This is the maximum $Z$ value below which no bound state can be found for any given screening strength with Yukawa-Debye interacting potentials. We also estimate the critical charge $Z_C$ for a given $\mu$ using a polynomial fitting based on the technique prescribed below. First, we draw the horizontal lines for $\mu$ (say 1.0, 0.8, etc.) in Fig. 4. The intersections between these horizontal lines and the two critical $\mu_C$ curves would indicate what the critical $Z$ should be for those $\mu_C$ values. For $\mu = 1.0$, 0.8, and 0.6, the place of intersection is denoted as $Z_{C1}$ for a given $\mu$. When $Z = 0.4$ or 0.3, the horizontal line would cross the two curves at three places, and we denote them as (from left to right) $Z_{C1}$, $Z_{C2}$, $Z_{C3}$. For $Z = 0.1$, the horizontal line crosses the line for the critical $Z$ curve at $Z_{C3}$.

We show our results in the form of $Z_C$ vs $\mu$ in Fig. 5, from which we can determine what the values of critical $Z$ are for a given $\mu$. For $\mu$ ranging from 0.0 to 0.2, the system is bound for $Z > Z_{C3}$. For $\mu$ ranging from 0.25 to 0.5247, the system is bound when $Z > Z_{C3}$ or $Z_{C1} < Z < Z_{C2}$. For $\mu$ ranging from 0.53 to 1.0, the system remains bound for $Z > Z_{C1}$. The values of $Z_{C1}$, $Z_{C2}$, $Z_{C3}$ obtained from the fifth-degree polynomial fittings of the data in Table A2 in the Supplemental Material [27] are plotted in Fig. 5 and listed in Table A4 [27]. We have also checked the values of $Z_C$ from the direct calculations, and those are correct up to an accuracy of four or five digits compared to the results obtained from the polynomial fitting. As we have shown in Table I, the $Z_C$ for the bare Coulombic system obtained from our work for $\mu = 0$ is 0.911 028 224 using 700-term correlated exponential wave

functions. Similarly the critical charges $Z_{C1}$ obtained from this work for $\mu = 0.05, 0.1$ are 0.891 81 and 0.87 85, respectively. As observed from a close look at Fig. 5, a critical screening parameter, say $\mu_X$, at a given $Z$ value can also inversely determine the critical charge $Z_C$ at $\mu = \mu_X$. It appears from Figs. 4 and 5 that the $\mu_C(Z)$ can also be written as $Z_C(\mu)$ directly using the method prescribed above. So the "curves" for $Z_{C1}(\mu)$ and $\mu_U(Z)$ have a similar nature.

It should be mentioned that in Ref. [5] the authors estimated $Z_{\rm FC}$ as 0.68. They also remarked that for the actual calculations "approaching this critical value would pose a significant computational challenge." In the present work, we extend calculations beyond $Z = 0.68$, and found that $Z_{\rm FC}$ should be 0.20. In Ref. [5], the authors scaled the screening parameter of two-body systems by the nuclear charge $Z$ for better optimization. In fact, exploiting the Rayleigh-Schrödinger $1/Z$ perturbation theory, if one resets the formulations of the proposed Yukawa system ($Z$, $e$, $e$) by the scaling transformation of coordinates $r \to r/Z$, screening parameter $\mu \to \mu/Z$, and energy $E(Z, \mu/Z) \to Z^2 E(Z, \mu/Z)$, the solution of the transformed Hamiltonian

$$\sum_{i=1}^{2}\left[-\frac{1}{2}\nabla_i^2 - \frac{\exp(-\mu' r_i)}{r_i}\right] + \frac{1}{Z}\frac{\exp(-\mu' r_{12})}{r_{12}} \tag{7}$$

can be obtained as

$$E(Z, \mu') = \sum_{n=0}^{\infty} E_n(\mu') Z^{-n}, \tag{8}$$

where $\mu' = \mu/Z$. Along this line, if one increases the electron-electron repulsion at a fixed threshold, say, near the lower critical stability, the three-body Yukawa system would not support a bound state. However, it is a common fact that the three-body Yukawa system is more and more loosely bound while approaching the threshold or approaching critical screening. The energy levels lying above the two-body system represent quasibound states. These quasibound states indicate the existence of shape resonances (see [28] for an example). One can find the quasibound states for the Yukawa system ($Z$, $e$, $e$), beyond the lower critical screening, using, for example, the complex scaling method [29]. However, it is outside the scope of the present investigation to study shape resonances in these three-particle systems. For the present study the upper critical screening parameters for the three-body Yukawa system are similar to the critical screening parameters for the two-body Yukawa systems, and it shows a straight line for $\mu_U$ vs $Z$ (see Fig. 4). In any case, the disagreement between our present finding for determining $Z_{\rm FC}$ and that reported in Refs. [4,5] suggested that further independent investigations on this issue are called for in order to shed light on this intriguing phenomenon.

Next, we present in brief the possible phenomena that occurred due to the Efimov [30,31] physics (see the review in Ref. [32] for details) while studying the bound states for two-body and three-body systems interacting with Yukawa potentials. It is a known fact that the Efimov effect, since its discovery, appears in several areas such as induced long-range interactions, discrete scale invariance, and Borromean binding. A three-body Yukawa system is defined as Borromean when it supports bound states for a fixed range of screening parameters (called the Borromean window) while none of their two-body subsystems are bound in such a range of screening parameters. From our present study, we may find the range for the Borromean binding [32–34] close to the upper critical screening parameter of the three-body Yukawa ($Z$, $e$, $e$) system, as the upper critical screening parameter for each $Z$ is similar to the critical screening of the respective two-body subsystem (see Table A1 in the Supplemental Material [27]). However, our calculations show that the Borromean window, if it existed, would be too narrow and close to the upper critical screening parameter. As for the region associated with the lower critical screening parameters, there is no Borromean binding. In other words, for a screening parameter that is less than the lower critical screening parameter of the three-body Yukawa system, the two-body system supports a bound state while the three-body system may support a quasibound state, and such a situation does not fall into the Borromean binding criteria.

## IV. CONCLUSIONS

In this article, we presented a calculation based on the Ritz variational method to obtain critical values of the screening parameter and the critical charge for two-electron ions interacting with Yukawa-Debye potentials, referred to throughout this paper as Yukawa systems ($Z$, $e$, $e$). The ground-state first ionization energies in terms of the nuclear charge and the screening parameters are also reported. The present study also confirms the best critical nuclear charge for the bare Coulomb system ($Z$, $e$, $e$) up to nine decimal digits using 700-term correlated exponential wave functions. We also conclude that the "final" critical $Z$, below which the two-electron ion would not form a bound state for any given screening strength under the influence of Yukawa-Debye potentials, is about 0.20. We hope our findings will serve as a benchmark reference for future studies on this topic.


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