Critical stability of the three-body system (Z, e^-, e^+)

Dario Bressanini*
Dipartimento di Scienza e Alta Tecnologia, Università dell'Insubria via Valleggio 9, I-22100 Como Italy

(Received 16 October 2017; published 11 January 2018)

We studied the stability of the system (Z, e^-, e^+) as a function of the fixed nuclear charge Z. This system, which can be a model to study more complex systems such as positrons bound to atoms or charged excitons in semiconductors, is stable for $Z < 1$. We studied, using the diffusion Monte Carlo method, its ground-state energy $E(Z)$ as a function of the nuclear charge, giving a rigorous upper bound to the critical charge: $Z_c < 0.421$. We fitted the available data to give a nonvariational estimate of the critical charge: $0.418 < Z_c < 0.419$. We also studied a P^e bound excited state of unnatural parity and estimated its critical charge: $0.54 < Z_c < 0.55$.

DOI: 10.1103/PhysRevA.97.012503

I. INTRODUCTION

The stability of matter composed by particles with different charges and masses is a fundamental problem in many areas of physics. The ultimate goal is to understand more deeply the mechanism by which matter sometimes shows a collective binding instead of splitting into smaller fragments. Atomic and molecular physics were built on the studies of small quantum systems, like the helium atom or the hydrogen molecule. They served to define new concepts, to develop new computational techniques, and to get new insight on the properties of many-electron systems. After almost a century the problem of stability of these systems is still being explored, and only in recent years was a rigorous proof of the stability of the hydrogen molecule given [1].

Solid-state physics is another field where the problem of stability of charged excitons and biexcitons in semiconductors in different environments and geometrical setting is being actively studied both experimentally [2] and theoretically [3]. Here the behavior of electrons and holes is modeled using a fictitious system of particles with varying charges and masses.

The study of stability of exotic matter, such as the $td\mu$ molecule, that plays a crucial role in the process of muon catalyzed fusion, or systems of atoms and antiatoms such as the hydrogen-antihydrogen system [4], is another application of this fundamental problem.

Last but not least, in the last 20 years, hundreds of papers have been devoted to the study of the stability of positron-atom and positron-molecule systems in their ground [5] or excited states [6]. A few atoms and ions are able to bind a positron, while others can bind positronium, Ps (e^+,e^-), or both [7]. Sometime the structure of these systems seems well described by a positron orbiting an atom. In other cases, Ps is responsible for the binding. Unfortunately, our theoretical understanding of these systems is far from satisfactory.

In recent years, there has been a renewed interest in the stability of heliumlike systems as a function of the nuclear charge Z, considered as a real continuous variable. Of particular interest is the determination of the critical nuclear charge Z_c, the minimum value for which the system still has at least one bound state, while for $Z < Z_c$ the system loses an electron.

There has been a controversy in the literature on the value of the critical charge Z_c, which has finally been established by Estienne and co-workers [8] to be $Z_c = 0.911\,028\,224\,077\,255\,73$ and independently confirmed by Pilón and Turbiner [9].

The study of the two-electron atomic model has been fundamental in our understanding of the structure and properties of larger atoms, but no such fundamental model has been carefully studied in the field of systems containing a positron. The fact that a system composed of a proton, an electron, and a positron does not form a bound state [10] focused theoretical attention towards the stable four-body system PsH, which has been experimentally detected by Schrader and co-workers in 1992 [11] and to date is probably the most studied positronic system.

There is, however a rarely studied three-body system that is rich in features that, besides being of purely theoretical interest, could pave the way to a deeper understanding of positronic compounds. It is the Z-Ps system, composed of an electron and a positron moving in the field of a fixed nucleus of charge Z. This system could also be a model for an exciton bound to a screened charge.

In this paper we investigate, using the diffusion Monte Carlo (DMC) method, its energetic properties, with particular attention to the value of the critical charge Z_c for the ground and one excited state. Atomic units are used throughout the paper.

II. THE Z-Ps SYSTEM

Consider a positive and a negative unit charge moving in a field generated by a fixed charge Z:

$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} + \frac{Z}{r_2} - \frac{1}{r_{12}}.$$

Z-Ps has two dissociation channels: $(Ze^-) + e^+$ and $Z + \mathrm{Ps}$ and two corresponding energy thresholds. For $Z \to 1$ from

*dario.bressanini@uninsubria.it

below, the (Z,e^-) hydrogenic system is negatively charged and can bind a positron: The first energy threshold is the energy of the hydrogenic system $E=-Z^2/2$. When $Z=1$ the system dissociates into $H+e^+$. When $Z\ll 1$ the system dissociates into a Z charge and a positronium Ps. This energy threshold is $E=-1/4$. In order to be chemically stable, disregarding the electron-positron annihilation, the energy of the system must be lower than both thresholds.

Harjiu and co-workers [12] described a simplified model of Z-Ps. Consider the electron positioned close to the Z charge. This system has energy $-Z^2/2$. The orbiting positron feels an effective charge of $Z-1$, with an energy of $-(Z-1)^2/2$.

The total energy of this simplified model is

$$E(Z)=-\frac{1}{2}+Z-Z^2=Z^2\left(-1+\frac{1}{Z}-\frac{1}{2Z^2}\right). \quad (1)$$

Note that $E(1)=-1/2$, correctly recovering the first dissociation limit. Going towards $Z\to 0$, the system dissociates into the fixed charge and the Ps system, with $E=-1/4$, but the simplified model does not describe the physical situation. Nevertheless the value of the threshold energy is reached for $Z=1/2$ and the three particles form a stable bound state for $1/2<Z<1$. The calculations of Harjiu and co-workers [12] showed that the stability domain extends somewhat for values of $Z<1/2$. They gave a first estimate of the critical charge $Z_c\approx 0.45$, but did not attempt a more accurate determination of the critical charge Z_c. The main objective of this paper is to give a more precise bound to Z_c.

III. CALCULATIONS

The wave function of an electronic system containing a positron, in most known cases, can be qualitatively understood considering the two limiting cases. $\Psi(e^+A)$, where a positron can be considered attached to the unperturbed A system, and $\Psi(\mathrm{Ps}A^+)$ where the positron detaches an electron, forming positronium, and the wave function describes Ps orbiting around the A^+ ion. The relative importance of the two structures depends on the ionization potential of the species A [13,14]. By varying the nuclear charge, Z-Ps can describe either a Ps or a positron bound to a core; this makes it an ideal model to study positronic systems. To this effect it is extremely important that the employed functional form for the wave function of Z-Ps has enough variational freedom to represent both limiting cases.

We employed a compact correlated wave function [6,15] to describe the ground state of Z-Ps for various Z charges:

$$\Psi=\sum_{i=1}^{L}\varphi_i, \quad (2)$$

$$\varphi_i=P_{i1}(r_1)P_{i2}(r_2)P_{i3}(r_{12}), \quad (3)$$

$$P(r)=e^{\frac{ar+br^2}{1+cr}}. \quad (4)$$

The wave functions, with $L=4$, were optimized using variational Monte Carlo (VMC) and then used in subsequent diffusion Monte Carlo (DMC) simulations. The ground-state wave function is positive everywhere and DMC is able to estimate the exact ground-state energy within a statistical error.

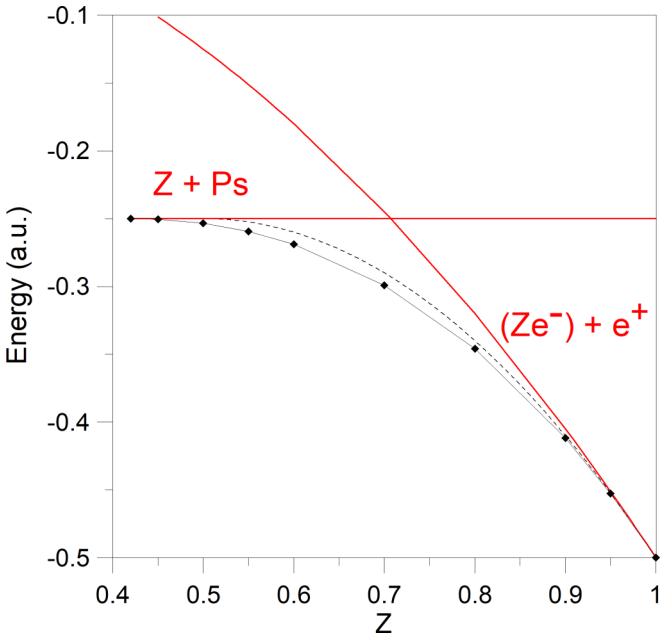

FIG. 1. DMC energy as a function of Z. The error bars are smaller than the symbol size. The dashed curve is the energy of the simplified model.

Short preliminary calculations in the range $Z=0.4$ to 1 with large steps verified that for $Z\to 1$ the system is always bound and correctly dissociates into $H+e^+$. Going in the opposite direction this preliminary scan found the system bound up to $Z=0.43$ while for $Z=0.42$ the statistical error was larger than the binding energy. Figure 1 shows the curve $E(Z)$ along with the energy of the simplified model.

IV. DETERMINATION OF Z_c

In order to give a more accurate estimate of the critical charge Z_c we performed much longer DMC simulations from $Z=0.420$ to 0.450 with steps of 0.001. The smallest value of Z where the estimated energy still lies below the dissociation threshold of -0.25 gives a rigorous upper bound to the value of the critical charge. The results in Table I, computed eliminating the time step bias on average, show that the system is still bound for $Z=0.421$. For $Z=0.420$ our DMC energy was statistically indistinguishable from the energy threshold so we cannot say if the system is still bound and we can only say that $Z_c<0.421$.

Estienne and co-workers [8] in their accurate estimation of the critical charge of two-electron atoms performed a linear extrapolation using six points very close to the critical point computing the variational energy at intervals of Z of 10^{-13} with quadruple precision arithmetic. This kind of accuracy is unattainable in DMC due to the inherent statistical error of the simulations, so to give a second estimate of the critical charge we follow a different route.

To estimate the critical point of the two-electron atom, Zamastil and co-workers [16] and Guevara and Turbiner [17] employed a Puiseux expansion with integer and half-

TABLE I. DMC energies in a.u. for $Z = 0.421$ to 0.450. The error bar on the last digits is in parentheses.

Z	E (a.u.) DMC
0.421	− 0.2500019(13)
0.422	− 0.2500040(14)
0.423	− 0.2500084(14)
0.424	− 0.2500127(15)
0.425	− 0.2500174(16)
0.426	− 0.250024(2)
0.427	− 0.250030(2)
0.428	− 0.250038(2)
0.429	− 0.250048(2)
0.430	− 0.250058(2)
0.431	− 0.250067(2)
0.432	− 0.250080(2)
0.433	− 0.250091(3)
0.434	− 0.250104(3)
0.435	− 0.250119(3)
0.436	− 0.250136(3)
0.437	− 0.250150(3)
0.438	− 0.250169(3)
0.439	− 0.250188(3)
0.440	− 0.250207(3)
0.441	− 0.250228(3)
0.442	− 0.250249(3)
0.443	− 0.250273(3)
0.444	− 0.250296(3)
0.445	− 0.250321(3)
0.446	− 0.250347(3)
0.447	− 0.250372(3)
0.448	− 0.250401(3)
0.449	− 0.250430(3)
0.450	− 0.250460(3)

integer powers of $Z - Z_c$. They confirmed the rigorous result obtained by Simon [18] that the energy expansion $E(Z) = \sum_{n=0}^{\infty} B_n (Z - Z_c)^{\alpha_n}$ around the critical charge lacks a square-root term $\alpha = 1/2$ but includes a linear term $\alpha = 1$ and an $\alpha = 3/2$ term.

As the first exploration step we performed a least-squares fit of the data using a quadratic model,

$$E(Z) = -\tfrac{1}{4} + a_2 (Z - Z_c)^2, \tag{5}$$

resulting in $Z_c = 0.4192$ and $a_2 = -0.484\,097$. This simple model is able to reproduce the fitted data with five decimal digits. When we added a linear term to the model the total square deviation of the fit did not statistically improve and the linear coefficient was quite small, of the order of 10^{-9}, statistically indistinguishable from zero. However, when we restricted the fit to the first ten points, closer to the critical charge, a linear term is no longer negligible and the estimate of Z_c is 0.4187.

Given the statistical noise of the available data at the moment it is not possible to safely establish the presence of a small linear term in the $E(Z)$ expansion around Z_c; however, it is likely that $0.418 < Z_c < 0.419$.

Additional calculations, with one of the computational techniques employed to study the helium atom with high accuracy, could be employed to completely resolve the matter studying the system sufficiently close to Z_c. We are planning to do such a study in the future.

Estienne and co-workers [8] found that the wave function at the critical point is not only square integrable, as theoretically predicted, but also remains localized at a finite distance from the nucleus. We computed the average distance of the electron and positron from the Z charge. We observed Ps detaching from the fixed charge as its value approaches Z_c. For $Z = 0.422$ the Ps is at about 70 bohrs from the positive charge.

All our calculations used a fixed positive charge of infinite mass. A finite mass decreases the binding energy of the system increasing the critical charge [19]. To give a rough estimate of the effect of a finite mass we use the result of Mitroy [20], who found that the critical mass of the system of unitary charges (m^+, e^-, e^+) is $m = 0.697\,78$. Assuming a linear dependence of the critical charge in the $E(Z, 1/m)$ plane and interpolating between our results and Mitroy's, we find that the critical charge using the mass of a proton increases slightly from 0.421 to 0.4212.

A future work could explore in detail the behavior of the system varying both the mass and the charge.

V. BEHAVIOR FOR $Z \to 1$

While the hydrogen atom cannot bind a positron, approaching $Z \to 1$ from below, there is an electrostatic interaction between the positron and the negatively charged (Z, e^-) system that can bind the positron into a stable three-body system. The simplified model gives a total energy of $E = -(1/2) - (Z - 1) - (Z - 1)^2$. We performed DMC simulations for $Z = 0.9$ to 0.99 with steps of 0.01 and fitted the energy with a quadratic model, $E(Z) = -1/2 + a_1(Z - 1) + a_2(Z - 1)^2$, with $a_1 = -1.002\,61$ and $a_2 = -1.203\,07$. Examining the positronic distribution for $Z = 0.99$ we find the dissociating positron at an average distance of more than 100 bohrs from the Z charge.

VI. THE P^e EXCITED STATE

H^- has only one true bound state. However, it also has an excited bound state, the $2p^2\,{}^3P^e$ state, of unnatural parity embedded in the continuum of natural parity. States of unnatural parity have also been found in various positronic systems [21]. The simplest known so far is the ${}^{2,4}S^o$ state of PsH [22]. We investigated the existence of a similar state for Z-Ps where formally the two particles are in $2p$ orbitals and together build a state of P^e symmetry. We omit the spin of the particles since they are irrelevant in this case as the wave function is not required to be either symmetric or antisymmetric with respect to the exchange of the leptons.

The trial wave function employed,

$$\Psi = (x_1 y_2 - y_1 x_2) \sum_{i=1}^{4} \varphi_i, \tag{6}$$

has the correct spatial symmetry, while the functional form of φ_i has been described above. We varied Z with steps of 0.01, optimizing the wave function at each point, and performed a subsequent DMC simulation. Since this excited state has a node, which might be different from the exact node of the

unknown exact wave function [23], DMC can only guarantee that the fixed node energy is an upper bound to the exact, unknown, energy.

Our DMC simulations show that the P^e state is below the dissociation threshold as $Z \to 1$. When Z is reduced we found a stable bound state up to $Z = 0.55$ with respect to dissociation into $Z + \mathrm{Ps}\ (2p)$, while for $Z = 0.54$ the state does not seem to be bound.

VII. CONCLUSIONS

We analyzed the Z-Ps three-body system, composed by a fixed positive charge Z, an electron, and a positron, showing that it is rich of features present also in many-body positronic systems. Figure 2 shows its stability diagram as a function of the nuclear charge Z. Below a critical value Z_c the system dissociates into Z and Ps. For $Z \geqslant 1$ the system dissociates into $e^+ + Ze^-$.

Using DMC we studied its ground-state energy $E(Z)$ as a function of the nuclear charge giving a rigorous upper bound to the critical charge $Z_c < 0.421$. We fitted the available data with a quadratic model to give a nonvariational estimate of the critical charge $0.418 < Z_c < 0.419$ We showed that this system has an additional P^e bound state of unnatural parity and estimated its critical charge to be $0.54 < Z_c < 0.55$.

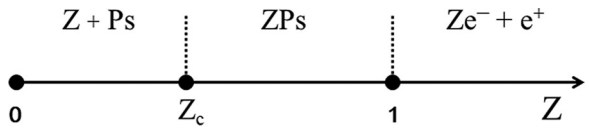

FIG. 2. Stability diagram as a function of Z for the system composed by a fixed positive charge Z, an electron e^-, and a positron e^+.

ACKNOWLEDGMENT

We wish to thank Mike Towler for his gracious hospitality at the TTI Institute during the "Quantum Monte Carlo in the Apuan Alps IX" conference where this work has begun.

[1] J.-M. Richard, J. Fröhlich, G.-M. Graf, and M. Seifert, Phys. Rev. Lett. **71**, 1332 (1993).
[2] B. Urbaszek, R. J. Warburton, K. Karrai, B. D. Gerardot, P. M. Petroff, and J. M. Garcia, Phys. Rev. Lett. **90**, 247403 (2003).
[3] D. Bressanini, M. Mella, and G. Morosi, Phys. Rev. A **57**, 4956 (1998).
[4] D. K. Gridnev and C. Greiner, Phys. Rev. Lett. **94**, 223402 (2005).
[5] G. G. Ryzhikh and J. Mitroy, Phys. Rev. Lett. **79**, 4124 (1997).
[6] D. Bressanini, Phys. Rev. Lett. **109**, 223401 (2012).
[7] X. Cheng, D. Babikov, and D. M. Schrader, Phys. Rev. A **85**, 012503 (2012).
[8] C. S. Estienne, M. Busuttil, A. Moini, and G. W. F. Drake, Phys. Rev. Lett. **112**, 173001 (2014).
[9] H. O. Pilón and A. Turbiner, Phys. Lett. A **379**, 688 (2015).
[10] E. A. G. Armour, Phys. Rev. Lett. **48**, 1578 (1982).
[11] D. M. Schrader, F. M. Jacobsen, N.-P. Frandsen, and U. Mikkelsen, Phys. Rev. Lett. **69**, 57 (1992).
[12] A. Harju, B. Barbiellini, and R. M. Nieminen, Phys. Rev. A **54**, 4849 (1996).
[13] D. Schrader, Nucl. Instrum. Methods Phys. Res., Sect. B **143**, 209 (1998).
[14] J. Mitroy, M. Bromley, and G. Ryzhikh, J. Phys. B: At., Mol. Opt. Phys. **35**, R81(R) (2002).
[15] D. Bressanini and G. Morosi, J. Phys. B: At., Mol. Opt. Phys. **41**, 145001 (2008).
[16] J. Zamastil, J. Cížek, L. Skala, and M. Šimánek, Phys. Rev. A **81**, 032118 (2010).
[17] N. L. Guevara and A. V. Turbiner, Phys. Rev. A **84**, 064501 (2011).
[18] B. Simon, J. Funct. Anal. **25**, 338 (1977).
[19] A. W. King, L. C. Rhodes, C. A. Readman, and H. Cox, Phys. Rev. A **91**, 042512 (2015).
[20] J. Mitroy, J. Phys. B: At., Mol. Opt. Phys. **33**, 5307 (2000).
[21] M. W. J. Bromley, J. Mitroy, and K. Varga, Phys. Rev. A **75**, 062505 (2007).
[22] J. Mitroy and M. W. J. Bromley, Phys. Rev. Lett. **98**, 063401 (2007).
[23] D. Bressanini, Phys. Rev. B **86**, 115120 (2012).