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Identification of atoms that can bind positrons

C. Harabati, V. A. Dzuba, and V. V. Flambaum
School of Physics, University of New South Wales, Sydney 2052, Australia

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Calculations of the positron binding energies to all atoms in the Periodic Table are presented and atoms where the positron-atom binding actually exists are identified. The results of these calculations and accurate calculations of other authors (which existed for several atoms only) are used to evaluate recommended values of the positron binding energies to the ground states of atoms. We also present the recommended energies of the positron excited bound levels and resonances (due to the binding of positron to excited states of atoms) which cannot emit positronium and have relatively narrow widths. Such resonances in positron annihilation and scattering may be used to measure the positron binding energy.

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I. INTRODUCTION

In this work we apply the relativistic linearized coupled-cluster single-double (SD) approximation to calculate positron binding energies for the atoms in the whole Periodic Table. Calculating the positron-atom bound states is a challenging theoretical problem due to the strong electron-positron correlation effects and virtual positronium (Ps) formation [1–3]. The existence of such states was predicted by many-body calculation [4] and verified variationally [5,6] more than a decade ago. Since that time a number of theoretical papers were published but only few atomic systems were studied. The most accurate calculations were performed for 11 positron-atom systems involving Li, Na, Ag, Cu, Au, Be, Mg, Ca, Zn, Sr, and Cd atoms [7–18]. A recent empirical fitted expression involving the polarizabilities (α), ionization potentials (I), and numbers of valence s electrons has also been based on the best calculations mentioned above [19]. A number of positron-atom bound states involving atoms with open d subshells were studied in our previous paper [20]. In spite of all these predictions no experimental evidence for positron-atom bound states has been found so far.

The situation is better for positron-molecule interaction since the resonant annihilation is observed for positrons in many polyatomic molecules [21]. The incident positron is captured into the bound state with the target molecule, with the excess energy being transferred to vibrations. Since the vibrational motion of the molecules is quantized, these transitions can only take place at specific positron energies. These energies correspond to vibrational Feshbach resonances of the positron-molecule complex [21–23]. The majority of the resonances observed are associated with individual vibrational modes of the molecule. The energy of the positron binding is then extracted from the downshift of the resonance energy, relative to the energy of the vibrational excitation [24,25]. Hence, by observing the resonances, the positron binding energy can be found. In this way, binding energies for over 60 polyatomic species have been determined [26–29] by measuring positron annihilation using a high-resolution, tunable, trap-based positron beam [30].

A similar effect in atoms has been proposed for experimental detection of positron-atom bindings in Ref. [31]. It was suggested that the resonances in the positron annihilation with atoms can be observed and associated with binding of the positron to a low-energy electronic excitation. These resonances can be found in open-shell atoms. If such atoms can bind a positron in the ground state, then it is very likely that they can bind a positron in the excited state of the same configuration. One can then consider the following process:

$$e^+ + A \rightarrow e^+A^* \rightarrow A^+ + 2\gamma. \tag{1}$$

First, a positron loses some energy by exciting the atom and becomes trapped to a bound state with the excited atom. Then, it annihilates with one of the electrons, and the resulting γ quanta can be detected. The first step of process (1) is obviously reversible. Hence, to estimate the efficiency of the resonant annihilation one needs to evaluate the rates of both positron annihilation (Γ_ν^a) and autodetachment (Γ_ν^e). One may estimate $\Gamma_\nu^e \sim 1$–10 meV for a Feshbach resonance at $\varepsilon \sim 1$ eV, populated through a quadrupole transition [31]. Hence, the resonances are sufficiently narrow to produce observable sharp features in the energy dependence of the annihilation rate Z_{eff}. For a binding energy $\varepsilon_b = 150$ meV, the estimated annihilation width is $\Gamma_\nu^a = 4 \times 10^{-7}$ eV and the branching ratio $\Gamma_\nu^e/\Gamma_\nu \approx 1$ (Γ_ν is the total width of the resonance). For a positron beam with the energy spread $\delta\varepsilon \sim 25$ meV, the peak resonant value of the annihilation rate is given by $Z_{\text{eff}} \sim 10^3$ in Ref. [31]. This indicates that the positron-atom resonances could be observed with a trap-based-beam technique similar to what was used for measuring resonances in the positron-molecule annihilation [25]. Resonances also manifest themselves in the positron scattering. Another method—measurement of the positron binding energies through laser assisted photorecombination—was suggested in Ref. [32].

We also would like to mention a possibility to capture the positron to a shallow bound level using a pulse of a very strong magnetic field. Such a field of the strength up to 100 T is available, for example, in the Los Alamos laboratory. Indeed, energy of an upper Zeeman component of the shallow positron-atom bound state may come above the ionization threshold and cross with the level of the free positron resulting in the positron capture (the same mechanism may be used to capture an electron to a negative ion state). This possibility deserves a separate publication, and we do not proceed any further in the present paper.

These possibilities to create the positron-atom bound states motivate us to survey the whole Periodic Table for positron binding and tabulate the results for experimentalists.

In the present paper we extend the study started in our previous paper [20] to all atoms in the Periodic Table up to uranium. Almost all previous calculations considered positron interacting with either a closed-subshell atom or an atom with a single electron above a closed-subshell core. The only exceptions are our recent works [20,31]. The reason for this is simple, there is no adequate theoretical method to perform accurate calculations for positron binding to open-shell atoms. In our previous paper [20] we suggested to use the linearized coupled-cluster single-double (SD) approach for this purpose. In this approach the interparticle interaction is included to all orders via an iterative procedure. The corresponding subset of terms includes the so-called *ladder* diagrams. This class of diagrams is very important in the positron-atom problem since it describes the effect of a virtual Ps formation. Summation of the electron-positron ladder-diagram series was performed earlier by solving a linear matrix equation for the electron-positron vertex function for hydrogen [33], noble-gas atoms [34], and halogen negative ions [35].

The linearized coupled-cluster method in its single-double approximation has been applied for a number of very accurate calculations for atoms and ions with one external electron above closed shells (see, e.g., [36–40]). Hence it is expected that the modified SD equations for the case of a positron interacting with a closed-shell atom should also give a reliable and accurate result.

A very brief summary of the SD equations for positron-atom interaction is provided in Sec. II. The details of the theory are given in our previous paper [20]. Comparison of our results for closed-shell atoms with the most accurate available calculations is described in Sec. III A. This provides us with an estimate of our accuracy. How the method is applied to the open-shell atoms is explained in Sec. III B where we also present positron binding energies to the ground state configuration of every atom in the Periodic Table. Determination of the energies of the resonances and excited bound states is explained in Sec. III C. The calculations for the positron binding to the excited electronic configurations of atoms are also presented in the same section. The paper ends with Sec. IV where all our results are summarized.

The recommended values of the positron binding energies are presented in Table V. The recommended values of the excited bound states and resonances are presented in Tables VI, VII, and X.

II. THEORY

Many-body atomic calculations for the positron-atom binding need construction of the single-particle basis sets separately for electron states and positron states. We use the relativistic Hartree-Fock (RHF) method and the B-spline technique [41] to do this. The self-consistent RHF procedure is initially done for the atom without a positron. Then full sets of single-electron and positron states are constructed using B-splines in a cavity of a reasonably large radius R. The radius must be larger than the size of the atom and should be chosen in such a way that the total positron-atom system fits into the cavity. We use $R = 30$ a.u. The effect of the finite cavity size on the positron-atom binding energy was studied and found to be negligible.

The single-particle basis states are found by constructing them as a linear combination of B-splines and diagonalizing the matrix of the RHF Hamiltonian:

$$h = c\alpha\cdot\mathbf{p} + (\beta-1)mc^2 - \gamma\frac{Ze^2}{r} + \gamma V_{\rm d} - \zeta V_{\rm exch}. \quad (2)$$

Here α, β are the Dirac matrices, and $V_{\rm d}$ and $V_{\rm exch}$ are the direct and exchange RHF potentials, respectively. The pair (γ,ζ) is taken (1,1) for electron and (−1,0) for positron. The wave function of an atom with a positron in state v can be written in the single-double (SD) approximation as an expansion

$$|\Psi_v\rangle = \Bigg[1 + \sum_{na}\rho_{na}a_n^\dagger a_a + \frac{1}{2}\sum_{mnab}\rho_{mnab}a_m^\dagger a_n^\dagger a_a a_b + \sum_{r\neq v}p_{rv}a_r^\dagger a_v + \sum_{rna}p_{rnva}a_r^\dagger a_v a_n^\dagger a_a\Bigg]|\Phi_v\rangle, \quad (3)$$

where $|\Phi_v\rangle$ is the zeroth-order wave function of the frozen-core atom in the relativistic Hartree-Fock approximation with the positron in state v. It can be written as

$$|\Phi_v\rangle = a_v^\dagger|0_C\rangle, \quad (4)$$

where $|0_C\rangle$ is the RHF wave function of the atomic core. Note that the following notations have been used to label the basis state in the rest of the paper: Indices a,b,c refer to electron states in the core, indices m,n,k,l refer to electron states above the core, indices v,r,w refer to positron states, and indices i,j refer to any states. The expansion coefficients ρ_{na} and ρ_{mnab} in Eq. (3) represent single- and double-electron excitations from the core. The coefficients p_{rv} represent excitations of the positron, and the coefficients p_{rnwa} represent simultaneous excitations of the positron and one of the electrons. The SD equations for the core excitation coefficients (ρ_{na} and ρ_{mnab}) do not depend on the external particle and they are the same in the electron and positron cases. These are well known equations from the linearized coupled-cluster theory, the details of the theory can be found, for instance, in Ref. [36]. The first step is to solve these equations iteratively to obtain the single-electron coefficients ρ_{ma} and the double-electron coefficients ρ_{mnab} for the core and to fix them in the rest of the calculation. The convergence of the core equations is maintained by observing the correlation correction to the energy of the core. One can refer to our previous paper [20] for the explicit form of the core equations.

After solving the SD equations for the core, one can start iterating the SD equations for the external particle. The SD equations for the positron can be obtained by substituting the state $|\Psi_v\rangle$ from Eq. (3) into the relativistic many-body Schrödinger equation,

$$H|\Psi_v\rangle = \epsilon_0|\Psi_v\rangle. \quad (5)$$

Projecting this equation onto $a_w^\dagger|0_C\rangle$ gives the equation for p_{wv},

$$(\epsilon_0 - \epsilon_w)p_{wv} = -\sum_{bm}q_{wbvm}\rho_{mb} + \sum_{bmr}q_{wbrm}p_{rmvb}. \quad (6)$$

TABLE I. Positron-atom binding energies relative to the channel $e^+ + \mathrm{A}$ (ε_b in meV) for closed-shell atoms obtained using the SD equations (SD) with the third-order correction (E3). I is the ionization energy from the ground state and α is the polarizability. The combination $S = m\alpha I^2/2\hbar^2$ is a dimensionless parameter called the potential strength. The best calculations in the literature are presented in the last column. The negative ε_b means the positron is not bound. Atoms with similar shells in their ground configurations are placed in the same group in increasing order of their atomic numbers Z. The first group is divided into two subgroups according to $I \lessgtr 6.8$ eV.

		Ground	I	α_d[a]		This work (meV)			Best other
Z	Atom	configuration	(eV)	(10^{-24} cm^3)	S	SD	E3	Total	calc. (meV)
20	Ca	$4s^2$	6.113	22.8	3.9	1382	50	1432	1201[b]
38	Sr	$5s^2$	5.695	27.6	4.1	1638	48	1687	1461[b]
56	Ba	$6s^2$	5.212	39.7	4.9	1974	48	2023	
70	Yb	$4f^{14}6s^2$	6.254	20.9	3.7	1359	43	1403	
88	Ra	$7s^2$	5.279	38.3	4.9	1902	40	1943	
2	He	$1s^2$	24.587	0.205	0.6	−145	0	−145	
4	Be	$2s^2$	9.322	5.6	2.2	187	27	214	86[e]
12	Mg	$3s^2$	7.646	10.6	2.8	596	39	636	464[c]
30	Zn	$4s^2$	9.394	5.75	2.3	211	23	235	103[f]
48	Cd	$5s^2$	8.993	7.36	2.7	273	79	352	178[d]
80	Hg	$6s^2$	10.437	5.7	2.8	64	61	126	
10	Ne	$2s^22p^6$	21.564	0.394	0.8	−145	0	−145	
18	Ar	$3s^23p^6$	15.759	1.641	1.9	−123	4	−119	
36	Kr	$4s^24p^6$	13.999	2.4844	2.2	−106	8	−98	
54	Xe	$5s^25p^6$	12.130	4.044	2.7	−68	14	−54	
86	Rn	$6s^26p^6$	10.748	5.3	2.8	−26	29	3	
46	Pd	$4d^{10}$	8.34	4.8	1.5	−39	9	−29	

[a] Ground state atomic static dipole polarizabilities from Ref. [43].

[b] The positron binding energies of 356 and 514 meV for atoms Sr and Ca, respectively, relative to the lowest threshold $\mathrm{A}^+ + \mathrm{Ps}$ have been obtained by the CI$_\infty$FC$_3$ method in Ref. [8]. Here FC$_3$ means fixed core with 3 particles treated explicitly, CI is the configuration interaction, and ∞ indicates an extrapolation to $l_{\max} \to \infty$ in the basis expansion. In the table the binding energies relative to the threshold $e^+ + \mathrm{A}$ are presented to compare with the present calculations.

[c] Calculation by the SVMFC$_3$ method from Ref. [8], where SVM means the stochastic variational method.

[d] Calculation by the CI$_\infty$FC$_3$ method from Ref. [9].

[e] Calculation by the SVM method from Ref. [10].

[f] Calculation by the CI$_\infty$FC$_3$ method from Ref. [12].

Projecting Eq. (5) onto $a_w^\dagger a_n^\dagger a_a |0_C\rangle$ gives the equation for the double-excitation coefficient p_{wnva},

$$\begin{aligned}(\epsilon_0+\epsilon_a-\epsilon_w-\epsilon_n)p_{wnva} &= q_{wnva} - \sum_{rm} q_{wnrm}p_{rmva} + \sum_{m} q_{wnvm}\rho_{ma} \\ &\quad - \sum_{b} q_{wavb}\rho_{nb} + \sum_{mb} p_{wmvb}\tilde{g}_{mabn} \\ &\quad + \sum_{rb} q_{warb}p_{rbvn} + \sum_{mb} q_{wmvb}\tilde{\rho}_{mabn}. \end{aligned} \tag{7}$$

In these equations $\tilde{g}_{mnkl} \equiv g_{mnkl} - g_{mnlk}$ and $\tilde{\rho}_{mnkl} \equiv \rho_{mnkl} - \rho_{mnlk}$. The coefficients g_{mnkl} and q_{wnva} are the Coulomb integrals for the electron-electron interaction and electron-positron interaction respectively. When solving these equations, the correction to the energy of the positron state v,

$$\delta\epsilon_v = -\sum_{mb} q_{vbvm}\rho_{mb} + \sum_{bmr} q_{vbrm}p_{rmvb}, \tag{8}$$

is used to control the convergence.

In contrast to the electrons-only case the calculations do not stop here. When the SD equations are used to calculate the energy and the wave function of the atom with single-valence electron above closed shells the RHF approximation is already a good approximation for the valence electron and only a small correction is needed. The correction is given by expressions similar to (6)–(8) (see, e.g., [36]). In the positron case there is no good zeroth-order approximation for the wave function of the bound positron. In the RHF approximation the positron-atom interaction is repulsive, and all of the single-particle positron basis states lie in the continuum. Since we cannot use a single positron RHF state as initial approximation we have to use all of them as a basis. The wave function of the positron bound to an atom is presented as a linear combination of the positron RHF states

$$\psi_p = \sum_v c_v\psi_v. \tag{9}$$

The energy ϵ_0 and the expansion coefficients c_v are found by solving the eigenvalue problem

$$\hat{\Sigma}X = \epsilon_0 X, \tag{10}$$

where X is the vector of expansion coefficients c_v, ϵ_0 is the lowest eigenvalue (which must be negative), and the elements of the effective Hamiltonian matrix $\hat{\Sigma}$ are given by

$$\sigma_{vw} = \epsilon_v\delta_{vw} - \sum_{mb} q_{wbvm}\rho_{mb} + \sum_{bmr} q_{wbrm}p_{rmvb}. \tag{11}$$

TABLE II. Positron-atom binding energies relative to the channel $e^+ + \mathrm{A}$ (ε_b in meV) for open-shell atoms obtained using the SD equations (SD) with third-order correction (E3). I is the ionization energy from the ground state. The combination $S = m\alpha I^2/2\hbar^2$ is called the potential strength. The negative ε_b means the positron is not bound. Atoms with similar shells in their ground configurations are placed in the same group in increasing order of their atomic numbers Z. The group with similar ground configurations is divided into two subgroups according to $I \lessgtr 6.8$ eV.

		Ground	I	α[a]		This work (meV)		
Z	Atom	configuration	(eV)	(10^{-24} cm^3)	S	SD	E3	Total
21	Sc	$3d4s^2$	6.561	17.8	3.5	908	129	1037
23	V	$3d^34s^2$	6.746	12.4	2.6	678	97	775
39	Y	$4d5s^2$	6.217	22.7	4.0	845	256	1102
57	La	$5d6s^2$	5.577	31.1	4.4	1223	324	1547
71	Lu	$5d6s^2$	5.426	21.9	2.9	222	245	470
89	Ac	$6d7s^2$	5.380	32.1	4.2	706	425	1131
90	Th	$6d^27s^2$	6.307	32.1	5.8	546	370	916
22	Ti	$3d^24s^2$	6.828	14.6	3.1	785	110	896
25	Mn	$3d^54s^2$	7.435	9.4	2.4	496	77	574
26	Fe	$3d^64s^2$	7.902	8.4	2.4	429	69	498
27	Co	$3d^74s^2$	7.881	7.5	2.1	360	61	422
28	Ni	$3d^84s^2$	7.635	6.8	1.8	295	55	350
40	Zr	$4d^25s^2$	6.634	17.9	3.6	729	209	939
43	Tc	$4d^55s^2$	7.119	11.4	2.6	461	133	594
72	Hf	$5d^26s^2$	6.825	16.2	3.4	305	198	503
73	Ta	$5d^36s^2$	7.549	13.1	3.4	274	166	441
74	W	$5d^46s^2$	7.864	11.1	3.1	235	141	377
75	Re	$5d^56s^2$	7.834	9.7	2.7	202	121	324
76	Os	$5d^66s^2$	8.438	8.5	2.8	167	105	273
77	Ir	$5d^76s^2$	8.967	7.6	2.8	137	91	229
59	Pr	$4f^36s^2$	5.473	28.2	3.8	1786	108	1895
60	Nd	$4f^46s^2$	5.525	31.4	4.4	1746	100	1846
61	Pm	$4f^56s^2$	5.582	30.1	4.3	1701	93	1794
62	Sm	$4f^66s^2$	5.644	28.8	4.2	1655	88	1743
63	Eu	$4f^76s^2$	5.67	27.7	4.1	1617	85	1702
65	Tb	$4f^96s^2$	5.864	25.5	4.0	1525	79	1604
66	Dy	$4f^{10}6s^2$	5.939	24.5	3.9	1490	76	1566
67	Ho	$4f^{11}6s^2$	6.02	23.6	3.9	1446	74	1521
68	Er	$4f^{12}6s^2$	6.107	22.7	3.9	1401	72	1474
69	Tm	$4f^{13}6s^2$	6.184	21.8	3.8	1354	71	1425
58	Ce	$4f5d6s^2$	5.538	29.6	4.1	1189	253	1442
64	Gd	$4f^75d6s^2$	6.149	23.5	4.0	816	284	1100
91	Pa	$5f^26d7s^2$	5.89	25.4	4.0	614	340	954
92	U	$5f^36d7s^2$	6.194	24.9	4.4	517	333	850
24	Cr	$3d^54s$	6.766	11.6	2.4	488	77	565
41	Nb	$4d^45s$	6.759	15.7	3.3	527	172	699
42	Mo	$4d^55s$	7.092	12.8	2.9	442	145	587
44	Ru	$4d^75s$	7.36	9.6	2.4	310	109	419
45	Rh	$4d^85s$	7.46	8.6	2.2	260	95	355
78	Pt	$5d^96s$	8.959	6.5	2.4	-10	57	47

[a]Ground state atomic static dipole polarizabilities from Ref. [43].

The first term on the right-hand side of Eq. (11) represents the positron energies in the static RHF approximation. The second and third terms describe the effect of the electron-positron correlations. The SD equations (6) and (7) must be iterated for every state in the expansion (9). Since these equations depend on the energy ϵ_0, which is found later from Eq. (10), we start with an initial guess for ϵ_0. The calculations are then performed iteratively, solving the SD equations (6) and (7) and diagonalizing the matrix (11) several times until ϵ_0 has converged.

The virtual Ps formation is described by an electron-positron ladder diagram series. They are included in SD equation in all orders. However, some third-order diagrams are missed by the SD method. It is well known that the missing third-order terms can give sizable corrections to the energy in atomic systems (see, e.g., Ref. [38]). Including these terms can

TABLE III. Positron-atom binding energies relative to the channel $e^+ + \mathrm{A}$ (ε_b in meV) for open p shell obtained using the SD equations (SD) with the third-order correction (E3). I is the ionization energy from the ground state. The combination $S = m\alpha I^2/2\hbar^2$ is the potential strength. The negative ε_b means the positron is not bound. Atoms with similar shells in their ground configurations are placed in the same group in increasing order of their atomic numbers Z. The group with similar ground configurations is divided into two subgroups according to $I \lessgtr 6.8$ eV.

		Ground	I	α[a]		This work (meV)		
Z	Atom	configuration	(eV)	(10^{-24} cm^3)	S	SD	E3	Total
13	Al	$3s^23p$	5.986	6.8	1.1	−38	38	0
31	Ga	$4s^24p$	5.999	8.12	1.3	−25	42	17
49	In	$5s^25p$	5.786	10.2	1.6	166	75	242
81	Tl	$6s^26p$	6.108	7.6	1.3	588	95	683
5	B	$2s^22p$	8.298	3.03	1.0	−136	3	−133
6	C	$2s^22p^2$	11.260	1.67	1.0	−139	1	−138
7	N	$2s^22p^3$	14.534	1.10	1.1	−141	0	−141
8	O	$2s^22p^4$	13.618	0.802	0.7	−143	0	−143
9	F	$2s^22p^5$	17.422	0.557	0.8	−144	0	−144
14	Si	$3s^23p^2$	8.151	5.53	1.7	−88	20	−68
15	P	$3s^23p^3$	10.486	3.63	1.8	−102	12	−90
16	S	$3s^23p^4$	10.360	2.90	1.4	−111	8	−103
17	Cl	$3s^23p^5$	12.967	2.18	1.7	−118	6	−112
32	Ge	$4s^24p^2$	7.899	5.84	1.7	−77	24	−53
33	As	$4s^24p^3$	9.789	4.31	1.9	−88	17	−71
34	Se	$4s^24p^4$	9.752	3.77	1.6	−95	13	−82
35	Br	$4s^24p^5$	11.814	3.05	1.9	−101	10	−91
50	Sn	$5s^25p^2$	7.344	7.84	1.9	−33	32	−1
51	Sb	$5s^25p^3$	8.608	6.6	2.2	−49	25	−24
52	Te	$5s^25p^4$	9.009	5.5	2.0	−57	20	−37
53	I	$5s^25p^5$	10.451	4.7	2.3	−63	17	−46
82	Pb	$6s^26p^2$	7.416	6.98	1.7	51	62	113
83	Bi	$6s^26p^3$	7.285	7.4	1.8	−2	46	45
84	Po	$6s^26p^4$	8.414	6.8	2.2	−16	38	22
85	At	$6s^26p^5$	9.350	6.0	2.4	−19	33	14

[a] Ground state atomic static dipole polarizabilities from Ref. [43].

lead to significant improvements in the accuracy of the results (see Sec. III). Consequently, we include these contributions for the positron-bound states with atoms in this work. The list of the missing third-order diagrams in SD equations and the corresponding perturbation-theory corrections to the energy of the positron state are derived and listed in Ref. [20].

III. RESULTS AND DISCUSSION

In our previous paper [20] we have reported the calculations of positron binding to 26 neutral atoms by using the current method. The rest of atoms in the Periodic Table are examined in this paper up to atomic number $Z = 92$ (uranium). All raw data are presented in Tables I to IV. Although there is no rigorous criterion for the positron binding to a neutral atom, it is widely accepted that the static dipole polarizability α and ionization potential I of the atom play an important role. Indeed, the positron feels a strong attractive polarization potential $-\alpha/2r^4$ outside the atom. Therefore, a large value of α and small radius of the atomic core increase the binding. Small radius of the atomic core corresponds to a large ionization potential I. Moreover, I and α may be combined as a single parameter which we have called the strength of the polarization potential [4]. It is a simple dimensionless parameter

$$S = \frac{m\alpha I^2}{2\hbar^2}. \tag{12}$$

The ionization potentials I from Ref. [42] and the static dipole polarizabilities α from Ref. [43] are shown in Tables I–IV for every atom in their ground state. In Tables I–IV we also present the values of the strength parameter S.

It seems natural to classify all atoms up to $Z = 92$ according to their ground state configurations, since they have similar positron binding for similar valence configurations. The arrangements of the first four tables are as follows. First, the atoms with similar valence shells are grouped and placed in the same table in increasing order of atomic number Z. A group with similar ground configurations is divided into two subgroups according to condition $I \lessgtr 6.80$ eV. For atoms with $I > 6.80$ eV, the Ps-formation channel is closed. The closest decay channel will be $e^+ + \mathrm{A}$. On the other hand, for $I < 6.80$ eV the lowest channel is $\mathrm{Ps} + \mathrm{A}^+$. In this work the positron binding energies have always been obtained with respect to the decay channel $e^+ + \mathrm{A}$, while in many papers the binding energies have been reported relative to the closest

TABLE IV. Positron-atom binding energies relative to the channel $e^+ + \mathrm{A}$ (ε_b in meV) for open s shell atoms obtained using the SD equations (SD) with the third-order correction (E3). I is the ionization energy from the ground state. The combination $S = m\alpha I^2/2\hbar^2$ is the potential strength. The negative ε_b means positron is not bound, – means the iteration of the SD equations does not converge for those atoms. Atoms with similar shells in their ground configurations are placed in the same group in increasing order of their atomic numbers Z. The group with similar ground configurations is divided into two subgroups according to $I \lessgtr 6.8$ eV.

		Valence	I	α[a]		This work (meV)			Best other
Z	Atom	configuration	(eV)	(10^{-24} cm^3)	S	SD	E3	Total	calc. (meV)
3	Li	$2s$	5.392	24.33	3.2	800	46	1015[b]	1477[d]
11	Na	$3s$	5.139	24.11	2.9	1042	48	1304[b]	1674[c]
19	K	$4s$	4.341	43.06	3.7	1746	72	2072[b]	
37	Rb	$5s$	4.177	47.24	3.8	–	–	–	
55	Cs	$6s$	3.894	59.42	4.1	–	–	–	
87	Fr	$7s$	4.073	47.1	3.6	–	–	–	
1	H	$1s$	13.598	0.667	0.6	−138	0	−138	
29	Cu	$4s$	7.726	6.2	1.7	125	40	166	170,[g] 152[h]
47	Ag	$5s$	7.576	6.78	1.8	172	75	247	123,[e] 159[f]
79	Au	$6s$	9.225	5.8	2.2	−25	49	24	−87[e]

[a] Ground-state atomic static dipole polarizabilities from Ref. [43].

[b] The positron binding energies of alkali-metal atoms are obtained by extrapolating to the values for $l_{\max} \to \infty$ (see, for instance, Fig. 1 for the extrapolation for Li).

[c] The positron binding energies of 13 meV for Na relative to the lowest threshold $\mathrm{Na}^+ + \mathrm{Ps}$ is obtained by the SVMFC$_2$ method in Ref. [17]. Here SVM means the stochastic variational method and FC$_2$ means fixed core with 2 particles treated explicitly. In the table the binding energy relative to the threshold $e^+ + \mathrm{Na}$ is shown to compare with the present calculation.

[d] The positron binding energies of 68 meV for Li relative to the lowest threshold $\mathrm{Li}^+ + \mathrm{Ps}$ is obtained by the SVM method in Ref. [18]. In the table the binding energy relative to the threshold $e^+ + \mathrm{Li}$ is shown to compare with the present calculation.

[e] Calculation by the CI + MBPT method, which is the relativistic configuration interaction plus many-body perturbation theory, from Ref. [13]

[f] Calculation by the SVMFC$_2$ method from Refs. [14,16].

[g] Calculation by the CI + MBPT method from Ref. [7].

[h] Calculation by the SVMFC$_2$ method from Refs. [15,16].

decay channel. The numbers are related by

$$\varepsilon_b = \varepsilon_{\mathrm{Ps}} - I + 6.80\ \mathrm{eV}, \tag{13}$$

where ε_b is the positron binding energy relative to the channel $e^+ + \mathrm{A}$, $\varepsilon_{\mathrm{Ps}}$ is the positron binding energy relative to the channel $\mathrm{Ps} + \mathrm{A}^+$, I is atomic ionization potential, and 6.80 eV is the binding energy of positronium.

The best calculations in the literature are presented in the last columns of Tables I and IV. There are 11 atoms studied accurately to predict the positron binding energies.

A. Closed-shell atoms

The results for a positron bound with closed-subshell atoms are shown in Table I. We use these atoms to test our method because these are the easiest systems from the computational point of view and a number of accurate calculations is available. The positron binding energies of 356, 514, 178, and 103 meV for Sr, Ca, Cd, and Zn atoms relative to the lowest thresholds ($\mathrm{A}^+ + \mathrm{Ps}$ for Sr and Ca and $e^+ + \mathrm{A}$ for Cd and Zn) have been obtained by the CI$_\infty$FC$_3$ method in Refs. [8,9,12] by Mitroy and co-workers. Here FC$_3$ means fixed core with 3 particles treated explicitly, CI is the configuration interaction, and ∞ indicates an extrapolation to $l_{\max} \to \infty$ in the basis expansion. All binding energies in the table are presented relative to the positron detachment threshold $e^+ + \mathrm{A}$. Equation (13) is used to convert the numbers when needed.

A stochastic variational method (SVM) was used for atoms with a small number of electrons. The positron binding energies of 464 and 86 meV were obtained for Mg and Be by the SVMFC$_3$ and SVM methods in Refs. [8,10]. The most accurate value is probably for the Be atom because it is the simplest system (four electrons in closed shells plus positron). Our calculations give the binding energy of 214 meV, which is 128 meV larger than the 86 meV energy obtained in Ref. [10]. A somewhat similar binding energy access is observed when comparing our results with available accurate calculations for other systems, see Table I (we will use this 128 meV correction to improve our results for a number of atoms where other accurate calculations are not available, see below). Note that the difference between our and the best earlier calculations for heavier atoms (Mg, Ca, Zn, Sr, and Cd) could be slightly larger due to the relativistic effects which have not been taken into account in the works by the Mitroy group. In contrast, our calculations are relativistic.

Our final raw results for the binding energy (ε_b) is the sum of the solution of the eigenvalue equation (10) (SD) and the third-order contributions (E3). The negative $\varepsilon_b < 0$ means that there is no positron binding to an atom. The positron-atom binding energy is very sensitive to the correlations. This leads to a large uncertainty in the calculations. Therefore, some negative values of ε_b might be within theoretical error bars.

As expected, increase of I and decrease of α lead to decrease of the positron-atom binding energy ε_b (see Table I). The first subgroup has larger ε_b than the rest of the table. This is also expected since atoms in this subgroup have larger potential strength S.

TABLE V. Recommended positron-atom binding energies (ε_b in meV) for all atoms in the Periodic Table up to uranium based on the current calculation and the most accurate values in the literature. The negative ε_b relative to any threshold shows that positron is not bound. Binding energies relative to the lowest dissociation threshold are shown in bold. A graphical presentation of this Table is in Fig. 2. Ionization potentials I are presented in Tables I–IV.

		ε_b (meV) to thresholds				ε_b (meV) to thresholds	
Z	Atom	$e^+ + \mathrm{A}$	$\mathrm{Ps} + \mathrm{A}^+$	Z	Atom	$e^+ + \mathrm{A}$	$\mathrm{Ps} + \mathrm{A}^+$
1	H	−138	6660	47	Ag	**123**[d]	899
2	He	−273	17514	48	Cd	**224**	2417
3	Li	1477	**68**	49	In	114	−900
4	Be	**86**[a]	2608	50	Sn	−129	415
5	B	−261	1237	51	Sb	−152	1656
6	C	−266	4194	52	Te	−165	2044
7	N	−269	7465	53	I	−174	3477
8	O	−271	6547	54	Xe	−182	5148
9	F	−272	10350	55	Cs	2767	−139
10	Ne	−273	14491	56	Ba	1895	**307**
11	Na	1674	**13**	57	La	1419	**196**
12	Mg	**464**[b]	1310	58	Ce	1314	**52**
13	Al	−128	−942	59	Pr	1767	**440**
14	Si	−196	1155	60	Nd	1718	**443**
15	P	−218	3468	61	Pm	1666	**448**
16	S	−231	3329	62	Sm	1615	**459**
17	Cl	−240	5927	63	Eu	1574	**444**
18	Ar	−247	8712	64	Gd	972	**321**
19	K	2400	−59	65	Tb	1476	**540**
20	Ca	1304	**617**	66	Dy	1438	**577**
21	Sc	909	**670**	67	Ho	1393	**613**
22	Ti	**768**	796	68	Er	1346	**653**
23	V	647	**593**	69	Tm	1297	**681**
24	Cr	437	**403**	70	Yb	1275	**729**
25	Mn	**446**	1081	71	Lu	282	−1092
26	Fe	**370**	1472	72	Hf	**375**	400
27	Co	**294**	1375	73	Ta	**313**	1062
28	Ni	**222**	1057	74	W	**249**	1313
29	Cu	**170**[c]	1092	75	Re	**196**	1230
30	Zn	**107**	2701	76	Os	**145**	1783
31	Ga	−111	−912	77	Ir	**101**	2268
32	Ge	−181	918	78	Pt	−81	2078
33	As	−199	2790	79	Au	−87[d]	2400
34	Se	−210	2742	80	Hg	−2	3635
35	Br	−219	4795	81	Tl	555	−137
36	Kr	−226	6973	82	Pb	−15	601
37	Rb	2528	−95	83	Bi	−83	402
38	Sr	1559	**454**	84	Po	−106	1508
39	Y	974	**391**	85	At	−114	2436
40	Zr	811	**645**	86	Rn	−125	3823
41	Nb	571	**530**	87	Fr	2578	-149
42	Mo	**459**	751	88	Ra	1815	**294**
43	Tc	**466**	785	89	Ac	1003	−417
44	Ru	**291**	851	90	Th	788	**295**
45	Rh	**227**	887	91	Pa	826	−84
46	Pd	−157	1383	92	U	722	**116**

[a] Calculation by the SVM method from Ref. [10] is recommended.

[b] Calculation by the SVMFC_3 method from Ref. [8] is recommended.

[c] The result of our earlier calculation by the CI + MBPT method (the relativistic configuration interaction plus many-body perturbation theory) from Ref. [7] as a recommended positron binding energy for the Cu atom.

[d] The results of our earlier calculations by the CI + MBPT method from Ref.[13] as a recommended positron binding energy for Ag and Au atoms.

B. Open-shell atoms

Tables II–IV show the positron binding energies to the ground state configurations of the open-shell atoms, which were suggested in our previous works [20,31] as good candidates for experimental detection of positron-atom bound states via resonant annihilation or scattering.

To deal with the positron binding to open-shell atoms with the SD approach we use an approximation in which open shells are treated as closed ones but with fractional occupation numbers [20]. For example, the ground state electron configuration of neutral Fe is $3d^64s^2$ above the Ar-like core. We treat it as a closed-shell system but reduce the contribution of the $3d$ subshell to the potential and CI matrix elements (11) by the factor 6/10. Both members of the fine-structure multiplet, $3d_{3/2}$ and $3d_{5/2}$, are included and corresponding terms are rescaled by the same factor (see Ref. [20] for more details). Note that the positron-atom binding has no strong sensitivity to the valence shell being open or closed because the Pauli principle is not applicable to the positron-electron interaction.

Table II shows the results of our calculations of positron binding energies ε_b for atoms with an open d shell and an open f shell. Their common feature is that they have an s orbital as the upper subshell in their ground configurations. Our numerical calculations have shown that this upper s shell provides a dominating contribution to the positron binding. As a result the positron is bound relative to the threshold of the channel $(\mathrm{A} + e^+)$ for all atoms. The situation is different for atoms in Table III where atoms with an open p shell are presented. Here only In and Tl have positron binding on their ground state configuration relative to the channel $(\mathrm{A} + e^+)$. However, In and Tl are still unstable against Ps formation, see Table V. All other atoms in Table III have no bound states with the positron. These results are also consistent with the magnitude of the strength parameter S which is $S \gtrsim 2.5$ in Table II and $S \lesssim 2.0$ in Table III.

Atoms in Table IV are different from the rest of the Periodic Table. First of all, they have very simple electronic configurations, one s electron above closed subshells, so they are the second simplest systems from the computational point of view after the closed-shell atoms in Table I. Two particles (an electron plus a positron) above closed shells can be treated using a sophisticated atomic many-body theory. Some best calculations are presented in the last column of the table. On the other hand, the Ps formation channel is open for alkali metals (the first set of atoms in Table IV) since $I < 6.80$ eV for them. Therefore, these systems are better described as positronium orbiting the positive ion A^+ [44] (a molecular type of bonding). Such systems are hard to describe in our present approach where a single-center basis with the origin on the atomic nucleus is used. To achieve a convergence, a very large number of partial waves $l_{\max}$ must be included to describe the total wave function. The fact that we could not get any convergent values for the positron binding energies to Rb, Fr, and Cs supports this argument. Comparison of our result for Li with the accurate variational calculation of Mitroy [18] shows that our method underestimates the positron binding energies for alkali-metal atoms. However, we obtained good agreements with the previous accurate calculations for Cu, Ag, and Au (see Table IV). Therefore, accurate description for alkali-metal atoms requires higher values of the maximum angular momentum $l_{\max}$. The value $l_{\max} = 10$ has been fixed in our computation for all atoms. Hence it is reasonable to estimate the extrapolated positron binding energies for alkali-metals in the limit of $l_{\max} \to \infty$. This is done by using the asymptotic formula

$$\varepsilon_b = \varepsilon_b(l_{\max}) - \frac{A}{(l_{\max} + 1/2)^3}, \tag{14}$$

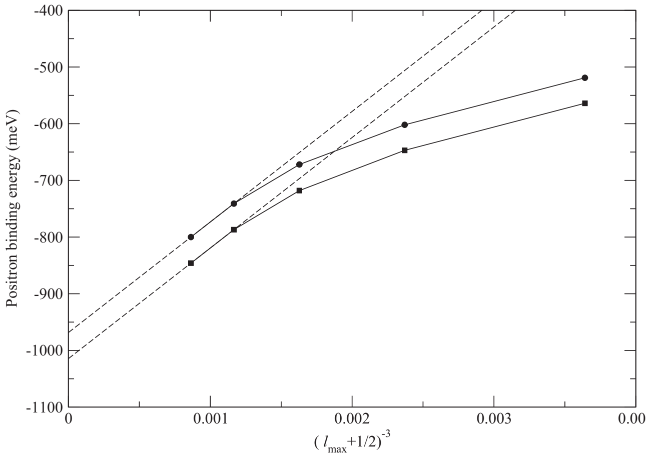

FIG. 1. Positron-Li binding energies relative to the channel $e^+ +$ A calculated using the SD equations (black dots) and with addition of the third-order correction (black squares) up to $l_{\max} = 10$. The dashed straight lines mark the extrapolated values on the energy axis for $l_{\max} \to \infty$.

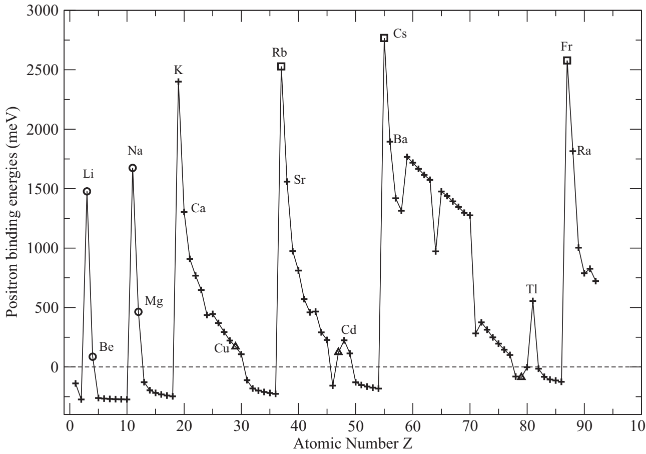

FIG. 2. Recommended positron binding energies from Table V relative to the dissociation threshold $e^+ +$ A. The results based on current study are shown with the + sign. The ○ shows the results of the previous best calculations based on configuration interaction (CI) or stochastic variational methods (SVM). △ shows the previous result of the relativistic method MBPT + CI for Cu, Ag, and Au in our group. The binding energies of Rb, Cs, and Fr are obtained by linear extrapolation of the values of Li, Na, and K with respect to the ion (A^+) radius, which are marked by a square □.

TABLE VI. Recommended values of excited bound states $\varepsilon < 0$ or resonance energies ($\varepsilon > 0$) in eV for the measurement of the positron-atom binding energies through resonant annihilation or scattering for atoms which have ionization potential (I) bigger than 6.8 eV (the ground state energy of Ps).

Z	Atom	Ground configuration	I (eV)	Excited states	E_{ex}[a] (eV)	ε_b (eV)	$\varepsilon = E_{\text{ex}} - \varepsilon_b$
26	Fe	$3d^64s^2$	7.902	$^5D_3$	0.052	0.370	−0.318
				$^5D_2$	0.087	0.370	−0.283
				$^5D_1$	0.110	0.370	−0.26
				$^5D_0$	0.121	0.370	−0.249
27	Co	$3d^74s^2$	7.881	$^4F_{7/2}$	0.101	0.294	−0.193
				$^4F_{5/2}$	0.174	0.294	−0.120
				$^4F_{3/2}$	0.224	0.294	−0.070
28	Ni	$3d^84s^2$	7.635	$^3F_3$	0.165	0.222	−0.057
				$^3F_2$	0.275	0.222	0.053
44	Ru	$4d^75s$	7.36	$^5F_4$	0.148	0.291	−0.143
				$^5F_3$	0.259	0.291	−0.032
				$^5F_2$	0.336	0.291	0.045
				$^5F_1$	0.385	0.291	0.094
				$^3F_4$	0.811	0.291	0.520
45	Rh	$4d^85s$	7.46	$^4F_{7/2}$	0.190	0.227	−0.037
				$^4F_{5/2}$	0.322	0.227	0.095
				$^4F_{3/2}$	0.430	0.227	0.203
				$^2F_{7/2}$	0.706	0.227	0.479
72	Hf	$5d^26s^2$	6.825	$^3F_3$	0.292	0.375	−0.083
73	Ta	$5d^36s^2$	7.549	$^4F_{5/2}$	0.249	0.313	−0.064
				$^4F_{7/2}$	0.491	0.313	0.178
				$^4F_{9/2}$	0.697	0.313	0.384
				$^4P_{1/2}$	0.750	0.313	0.437
				$^4P_{3/2}$	0.752	0.313	0.439
74	W	$5d^46s^2$	7.864	$^5D_1$	0.207	0.249	−0.042
				$^5D_2$	0.412	0.249	0.163
				$^5D_3$	0.599	0.249	0.350
				$^5D_4$	0.771	0.249	0.522
				$^3P2_0$	1.181	0.249	0.932
76	Os	$5d^66s^2$	8.438	$^5D_3$	0.516	0.145	0.371
				$^5D_2$	0.340	0.145	0.195
				$^5D_1$	0.715	0.145	0.570
				$^5D_0$	0.755	0.145	0.610
				$^3H_5$	1.778	0.145	1.633
77	Ir	$5d^76s^2$	8.967	$^4F_{3/2}$	0.506	0.101	0.405
				$^4F_{5/2}$	0.717	0.101	0.616
				$^4F_{7/2}$	0.784	0.101	0.683
				$^2G_{9/2}$	1.728	0.101	1.627
				$^2G_{7/2}$	2.204	0.101	2.103
				$^4P_{5/2}$	1.997	0.101	1.896

[a] Atomic excitation energy relative to the ground state from Ref. [42].

derived in Ref. [45] in the framework of the perturbation theory. Here $\varepsilon_b(l_{\max})$ is the binding energy for $l_{\max}$ and A is a constant which is different in different atoms. When the convergence is achieved for a given $l_{\max}$, all $\varepsilon_b(l > l_{\max})$ must lie on a straight line with respect to $1/(l_{\max} + 1/2)^3$. For instance, Fig. 1 shows that the positron binding energy for Li has not been convergent yet at $l_{\max} = 10$. However, we can estimate the extrapolated positron energy by assuming the straight line obtained from the last two points (for $l_{\max} = 9$ and $l_{\max} = 10$). We see that our extrapolated binding energies for Li and Na are still smaller than the previous accurate calculations shown in Table IV.

Now we will try to improve our predictions of the positron binding energies for all atoms based on comparison of our calculations and available accurate calculations for Be, Li, and Cu. Be is the simplest closed-shell atom that can bind a positron (see Table I), Li is the simplest alkaline atom that can bind a positron, and Cu has one electron above the closed-shell core (see Table IV). Each of them belongs to a different type of group in the Periodic Table. We assume that atoms in the same group or in a nearby similar group interact with the positron in the same way. The previous presumably accurate calculations of the positron binding to these three atoms (Be, Li, Cu) can be used to estimate the errors in the

TABLE VII. Recommended energies of the excited positron-atom bound states $\varepsilon < 0$ below Ps formation threshold ($\varepsilon < I - 6.8$ eV) for atoms which have ionization potential (I) less than 6.8 eV (the ground state energy of Ps).

Z	Atom	Ground configuration	I (eV)	Excited states	E_{ex}[a] (eV)	ε_b (eV)	$\varepsilon = E_{\mathrm{ex}} - \varepsilon_b$
21	Sc	$3d4s^2$	6.561	$^2D_{5/2}$	0.021	0.909	−0.888
22	Ti	$3d^24s^2$	6.828	$^3F_3$	0.021	0.768	−0.747
				$^3F_4$	0.048	0.768	−0.720
23	V	$3d^34s^2$	6.746	$^4F_{5/2}$	0.017	0.647	−0.63
				$^4F_{7/2}$	0.040	0.647	−0.607
				$^4F_{9/2}$	0.068	0.647	−0.579
39	Y	$4d5s^2$	6.217	$^2D_{5/2}$	0.066	0.974	−0.908
40	Zr	$4d^25s^2$	6.634	$^3F_3$	0.071	0.811	−0.74
				$^3F_4$	0.154	0.811	−0.657
				$^3P_2$	0.519	0.811	−0.292
				$^3P_0$	0.520	0.811	−0.291
				$^3P_1$	0.542	0.811	−0.269
				$^1D_2$	0.632	0.811	−0.179
41	Nb	$4d^45s$	6.759	$^6D_{3/2}$	0.019	0.571	−0.552
				$^6D_{5/2}$	0.049	0.571	−0.522
				$^6D_{7/2}$	0.086	0.571	−0.485
				$^6D_{9/2}$	0.130	0.571	−0.441
57	La	$5d6s^2$	5.577	$^2D_{5/2}$	0.130	1.419	−1.289
58	Ce	$4f5d6s^2$	5.538	$^3F_2^o$	0.028	1.314	−1.286
59	Pr	$4f^36s^2$	5.473	$^4I_{11/2}^o$	0.171	1.767	−1.596
				$^4I_{13/2}^o$	0.353	1.767	−1.414
60	Nd	$4f^46s^2$	5.525	$^5I_5$	0.140	1.718	−1.578
				$^5I_6$	0.293	1.718	−1.425
61	Pm	$4f^56s^2$	5.582	$^6H_{7/2}^o$	0.100	1.666	−1.566
				$^6H_{9/2}^o$	0.217	1.666	−1.449
				$^6H_{11/2}^o$	0.347	1.666	−1.319
62	Sm	$4f^66s^2$	5.644	$^7F_1$	0.036	1.615	−1.579
				$^7F_2$	0.101	1.615	−1.514
				$^7F_3$	0.185	1.615	−1.430
				$^7F_4$	0.282	1.615	−1.333
				$^7F_5$	0.388	1.615	−1.227
64	Gd	$4f^75d6s^2$	6.149	$^9D_3^o$	0.027	0.972	−0.945
				$^9D_4^o$	0.066	0.972	−0.906
				$^9D_5^o$	0.124	0.972	−0.848
				$^9D_6^o$	0.213	0.972	−0.759
65	Tb	$4f^96s^2$	5.864	$^6H_{13/2}^o$	0.344	1.476	−1.132
66	Dy	$4f^{10}6s^2$	5.939	$^5I_7$	0.513	1.438	−0.925
68	Er	$4f^{12}6s^2$	6.107	$^3F_4$	0.624	1.346	−0.722

[a] Atomic excitation energy relative to the ground state from Ref. [42].

present calculations. Our method overestimates the binding energy for Be [10], underestimates it for Li [18], and is in good agreement with previous calculation for Cu [7]. Using these differences between our results and the most accurate results of other calculations, we derive recommended values for the positron-atom binding energies for the whole Periodic Table in Table V. The recommended binding energies for the atoms with closed shells or open f, d, or p shells are obtained by subtracting 128 meV from our results presented in Tables I–III. This is done to eliminate the difference between our value of 214 meV and the accurate result 86 meV [10] for the Be atom. The recommended positron binding energy to Mg has been taken from Ref. [8]. We use our previous accurate results for Cu, Ag, and Au obtained by the relativistic CI + MBPT method [7,13] as recommended values for these systems (170, 123, and −87 eV, respectively). The previous result for Cu is very close to the current calculation (166 eV) anyway.

The binding energies for Rb, Cs, and Fr are estimated by the linear extrapolation of the values for Li, Na, and K with respect to the ion (A^+) radius which is inversely proportional to the ion ionization potential ($r_+ \sim 1/I^+$). In this estimation we have used the literature results for Li and Na and the corrected result 2400 meV for K atom (our raw number 2072 meV is assumed to be underestimated similar to Li and Na). Note that all positron binding energies for Li, Na, and K lie on a straight line with respect to $1/I^+$. Using values of $1/I^+$ for the Rb^+, Cs^+, and Fr^+ ions we obtain the extrapolated positron binding energies for them by putting them on the same line (a linear extrapolation). We conclude that positron systems with K, Rb,

TABLE VIII. Positron-atom binding energies (ε_b^* in meV) for the excited states of configurations different from the ground state configurations which are obtained using the SD equations (SD) with the third-order correction (E3). E_{ex} is the excitation energy relative to the ground state.

		Valence	I	E_{ex}[a]	This work (meV)		
Z	Atom	configuration	(eV)	(eV)	SD	E3	Total
21	Sc	$3d^24s$	6.561	1.428	849	109	958
22	Ti	$3d^34s$	6.828	0.813	727	97	825
23	V	$3d^44s$	6.746	0.262	602	86	689
24	Cr	$3d^44s^2$	6.766	0.961	590	86	676
25	Mn	$3d^64s$	7.435	2.114	382	68	450
26	Fe	$3d^74s$	7.902	0.859	315	61	376
27	Co	$3d^84s$	7.881	0.432	243	53	297
28	Ni	$3d^94s$	7.635	0.025	173	46	220
29	Cu	$3d^94s^2$	7.726	1.389	240	49	289
39	Y	$4d^25s$	6.217	1.356	683	258	942
40	Zr	$4d^35s$	6.634	0.604	623	208	831
41	Nb	$4d^35s^2$	6.759	0.141	658	178	836
42	Mo	$4d^45s^2$	7.092	1.359	583	155	739
43	Tc	$4d^65s$	7.119	0.518	355	124	479
44	Ru	$4d^65s^2$	7.36	0.927	461	121	583
46	Pd	$4d^95s$	8.34	0.814	205	83	288
		$4d^85s^2$		3.112	361	97	459
56	Ba	$6s5d$	5.212	1.120	1345	389	1734
57	La	$5d^26s$	5.577	0.331	1237	324	1561
59	Pr	$4f^25d6s^2$	5.473	0.549	1120	286	1406
60	Nd	$4f^35d6s^2$	5.525	0.838	1060	285	1345
64	Gd	$4f^75d^26s$	6.149	0.790	544	288	832
65	Tb	$4f^85d6s^2$	5.864	0.035	749	284	1033
66	Dy	$4f^95d6s^2$	5.939	0.938	672	283	955
72	Hf	$5d^36s$	6.825	1.747	349	190	539
73	Ta	$5d^46s$	7.549	1.210	126	147	273
74	W	$5d^56s$	7.864	0.366	83	118	201
75	Re	$5d^66s$	7.834	1.457	51	96	147
76	Os	$5d^76s$	8.438	0.638	25	79	105
77	Ir	$5d^86s$	8.967	0.351	5	67	72
78	Pt	$5d^86s^2$	8.959	0.102	111	80	191
		$5d^{10}$		0.761	20	23	44

[a] Excitation energies relative to the ground states from Ref. [42].

TABLE IX. Recommended positron-atom binding energies (ε_b^* in meV) for excited states of all atoms in Table VIII. The negative ε_b^* relative to any threshold shows that positron is not bound. Binding energies relative to the lowest dissociation threshold are shown in bold. Ionization potentials I and electron excitation energies E_{ex} are presented in Table VIII.

		Valence	ε_b^* (meV) to thresholds	
Z	Atom	configuration	$e^+ + \mathrm{A}^*$	$\mathrm{Ps} + \mathrm{A}^+$
21	Sc	$3d^24s$	830	−837
22	Ti	$3d^34s$	697	−88
23	V	$3d^44s$	561	**245**
24	Cr	$3d^44s^2$	548	−447
25	Mn	$3d^64s$	322	−1157
26	Fe	$3d^74s$	**248**	491
27	Co	$3d^84s$	**169**	818
28	Ni	$3d^94s$	**92**	902
29	Cu	$3d^94s^2$	161	−302
39	Y	$4d^25s$	814	−1125
40	Zr	$4d^35s$	703	−67
41	Nb	$4d^35s^2$	708	**526**
42	Mo	$4d^45s^2$	611	−456
43	Tc	$4d^65s$	351	**152**
44	Ru	$4d^65s^2$	455	**88**
46	Pd	$4d^95s$	**160**	886
		$4d^85s^2$	331	−1241
56	Ba	$6s5d$	1606	−1102
57	La	$5d^26s$	1433	−121
59	Pr	$4f^25d6s^2$	1278	−598
60	Nd	$4f^35d6s^2$	1217	−896
64	Gd	$4f^75d^26s$	704	−737
65	Tb	$4f^85d6s^2$	905	−66
66	Dy	$4f^95d6s^2$	827	−972
72	Hf	$5d^36s$	411	−1311
73	Ta	$5d^46s$	145	−316
74	W	$5d^56s$	**73**	771
75	Re	$5d^66s$	19	−404
76	Os	$5d^76s$	−23	977
77	Ir	$5d^86s$	−56	1760
78	Pt	$5d^86s^2$	**63**	2120
		$5d^{10}$	−84	1314

Cs, and Fr atoms are unstable due to decay to positronium and positive ion (see Table V).

We also present in Table V the positron-atom binding energies relative to the Ps-formation threshold, $\mathrm{A}^+ + \mathrm{Ps}$. The closest decay channel is emphasized by the bold number in the Table V. We also present the results of the Table V in graphical form in Fig. 2.

Therefore, more than half of the atoms in the Periodic Table may bind the positron.

C. Excited states

In our calculations we do not distinguish between different electron states of the same configuration. If the positron is bound to an atom in a particular configuration, it is bound to all states of this configuration with approximately the same binding energy. Therefore, the energy splitting inside the ground state configuration is assumed to be the same for atoms with or without a positron. This assumption is supported by similar features of atomic scalar polarizabilities. The scalar polarizabilities have very close values for the different states of the same ground state configuration of many-electron atoms [46]. The values of the scalar polarizabilities determine the strength of the attractive polarization potential $-\alpha/2r^4$ acting on the positron. Therefore, it is natural to expect that if the polarizabilities are equal the positron binding energies will also be equal.

Since the energy splitting within a configuration is assumed to be the same for the atom with or without a positron, the energies of the excited states of the positron-atom system can be obtained as

$$\varepsilon = E_{\mathrm{ex}} - \varepsilon_b, \qquad (15)$$

where E_{ex} is the experimental value of the atomic excitation energy relative to the ground state and ε_b is the positron binding

TABLE X. Recommended positron-atom resonances $\varepsilon > 0$ and excited bound states $\varepsilon < 0$ below Ps formation threshold ($\varepsilon < I - 6.8$ eV) for atoms which can attach positron in its excited configuration from Table IX. The ground state ionization potentials I are also presented.

Z	Atom	Valence configuration	I (eV)	Excited states	$E_{\rm ex}$[a] (eV)	ε_b^* (eV)	$\varepsilon = E_{\rm ex} - \varepsilon_b^*$
4	Be	$1s^22s2p$	9.322	$^3P^o$	2.725		2.49[b]
23	V	$3d^44s$	6.746	$^6D_{1/2}$	0.262	0.561	−0.299
				$^6D_{3/2}$	0.267	0.561	−0.294
				$^6D_{5/2}$	0.275	0.561	−0.286
				$^6D_{7/2}$	0.286	0.561	−0.275
				$^6D_{9/2}$	0.301	0.561	−0.260
26	Fe	$3d^74s$	7.902	$^5F_5$	0.859	0.248	0.611
				$^5F_4$	0.915	0.248	0.667
				$^5F_3$	0.958	0.248	0.710
				$^5F_2$	0.990	0.248	0.742
				$^5F_1$	1.011	0.248	0.763
27	Co	$3d^84s$	7.881	$^4F_{9/2}$	0.432	0.169	0.263
				$^4F_{7/2}$	0.513	0.169	0.344
				$^4F_{5/2}$	0.581	0.169	0.412
				$^4F_{3/2}$	0.629	0.169	0.46
				$^2F_{7/2}$	0.922	0.169	0.753
				$^2F_{5/2}$	1.049	0.169	0.88
28	Ni	$3d^94s$	7.635	$^3D_3$	0.025	0.092	−0.067
				$^3D_2$	0.109	0.092	0.017
				$^3D_1$	0.212	0.092	0.12
				$^1D_2$	0.422	0.092	0.33
41	Nb	$4d^35s^2$	6.759	$^4F_{3/2}$	0.141	0.708	−0.567
				$^4F_{5/2}$	0.196	0.708	−0.512
				$^4F_{7/2}$	0.267	0.708	−0.441
				$^4F_{9/2}$	0.347	0.708	−0.361
				$^4P_{1/2}$	0.619	0.708	−0.089
				$^4P_{3/2}$	0.656	0.708	−0.052
43	Tc	$4d^65s$	7.119	$^6D_{1/2}$	0.518	0.351	0.167
				$^6D_{3/2}$	0.496	0.351	0.145
				$^6D_{5/2}$	0.458	0.351	0.107
				$^6D_{7/2}$	0.403	0.351	0.052
				$^6D_{9/2}$	0.318	0.351	−0.033
44	Ru	$4d^65s^2$	7.36	$^5D_4$	0.927	0.455	0.472
46	Pd	$4d^95s$	8.34	$^2[5/2]_3$	0.813	0.160	0.653
				$^2[5/2]_2$	0.961	0.160	0.801
				$^2[3/2]_1$	1.251	0.160	1.091
				$^2[3/2]_2$	1.453	0.160	1.293
74	W	$5d^56s$	7.864	$^7S_3$	0.365	0.073	0.292
78	Pt	$5d^86s^2$	8.959	$^3F_4$	0.102	0.063	0.039
				$^3F_3$	1.254	0.063	1.191
				$^3F_2$	1.921	0.063	1.858
				$^3P_2$	0.814	0.063	0.751

[a] Atomic excitation energy relative to the ground state from Ref. [42].

[b] The recent calculation of a resonant level from Ref. [11].

energy to the ground state. These excited states are also bound as long as $\varepsilon < 0$. Positive values of ε correspond to resonances in continuum. To close the positronium formation channel we also need the condition

$$\varepsilon < I - 6.80 \text{ eV}, \tag{16}$$

where I is the atomic ionization potential and 6.80 eV is the binding energy of the Ps ground state.

Using the condition for the excitation energy $E_{\rm ex} < \varepsilon_b + I - 6.80$ eV (stability against the positron emission) and the recommended positron binding energies ε_b from Table V we found the resonance and bound state energies for 26 atoms. Table VI shows resonances and bound states for the atoms with ionization potential larger than 6.8 eV, while Table VII is for atoms with $I < 6.8$ eV. Due to the limited accuracy of our calculations (~100 meV) the weakly bound positron states shown in Table VI may turn out to be low-lying resonances and vice versa.

The resonances and bound states in Tables VI and VII have been obtained for the positron binding to the excited states of the ground configurations. However, the positron may bind to a different electron configuration. It is known that helium excited state $1s2s\,^3S$ can bind a positron even though its ground state $1s^2\,^1S$ cannot. It has recently been calculated that the positron can attach to the $1s2s2p\,^4P^o$ excited state of Li [47]. Table VIII shows our calculations for excited state configurations that can bind a positron relative to the $e^+ + \mathrm{A}^*$ threshold, where A^* is the lowest excited state for a given configuration. We have found that 10 atoms in Table IX have excited bound states that are stable against both thresholds, $e^+ + \mathrm{A}^*$ and $\mathrm{A}^+ + \mathrm{Ps}$. The smaller binding energies are presented in bold in Table IX. Note that the positron does not bind to the ground states of Pd and Pt but both atoms bind in the excited states, see Table IX.

The energies of the positron resonances ($\varepsilon > 0$) and excited bound states ($\varepsilon < 0$) can be determined from the recommended positron binding energy ε_b^* for a particular configuration and excitation energies E_{ex} of the electronic states. Here E_{ex} should also satisfy the condition that $E_{\mathrm{ex}} < \varepsilon_b^* + I - 6.80$ eV (to stay below Ps formation threshold). The recommended energies of the positron bound states and resonances for excited configurations are presented in Table X. The results of the present work confirm the claim of Ref. [31] that many open-shell atoms do bind the positron not only in the ground state but also in excited states.

IV. CONCLUSION

The linearized coupled-cluster single-double approach with the third-order correction is used to calculate the positron binding energy for every atom in the Periodic Table. The fractional occupation number approximation is used to perform the calculations for open-shell atoms. To obtain the recommended values of the positron binding energies we introduce corrections which bring our results in line with the best available calculations which exist for 11 atoms only. We find that 49 atoms can bind the positron in the ground state. The recommended values of the binding energies are presented in Table V.

A number of atoms also have excited positron bound states and low energy positron resonances which may be used to measure the positron binding energy in the processes of the positron annihilation and scattering. The recommended values of these excited bound states and resonances are presented in Tables VI, VII, and X.

An order-of-magnitude estimate of the accuracy of our predictions is ∼100 meV. Due to the limited accuracy some of the calculated weakly bound states may be actually unbound and vice versa.

Finally, there are two problems for a future study. If the initial atomic angular momentum J_A is not zero the positron bound states form the doublets with the total angular momenta $J = J_A + 1/2$ and $J = J_A - 1/2$. The energy splitting is ∼1 meV.

If $J_A > 1/2$ the atom has an electric quadrupole moment Q and produces a long-range potential $eQ(3\cos^2\theta - 1)/(4r^3)$, which decays slower than the polarization potential $-e^2\alpha/r^4$. The quadrupole moment is large in atoms with several electrons in an open shell. The quadrupole potential may produce new features in the positron bound states such as localization of the positron wave function in the equatorial or polar areas depending on the sign of eQ. A similar effect may exist for an electron in a negative ion.

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