# Configuration-interaction calculations of positron binding to zinc and cadmium

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The configuration-interaction method is applied to the study of positronic zinc ($e^+$Zn) and positronic cadmium ($e^+$Cd). The estimated binding energies and annihilation rates were 0.003 73 hartree and $0.42 \times 10^9$ sec$^{-1}$ for $e^+$Zn and 0.006 10 hartree and $0.56 \times 10^9$ sec$^{-1}$ for $e^+$Cd. The low-energy elastic cross section and $Z_{eff}$ were estimated from a model potential that was tuned to the binding energies and annihilation rates. Since the scattering lengths were positive ($14.5 a_0$ for Zn and $11.6 a_0$ for Cd) the differential cross sections are larger at backward angles than at forward angles just above threshold. The possibilities of measuring differential cross sections to confirm positron binding to these atoms is discussed.

## I. INTRODUCTION

Some of the first suggestions that positrons could bind to a neutral atom were made for group-IIB elements of the periodic table. The initial predictions of positron binding were made in a polarized orbital (PO) calculation of positron scattering from zinc and cadmium [1]. Results were presented for nonrelativistic and relativistic treatments of the atomic structure and scattering dynamics. One limitation of these calculations was that only the dipole component of the polarization potential was used even though it is known that the higher moments of the polarization potential are important in positron scattering calculations [2–4]. McEachran and Stauffer [5] did include the high-order moments of the polarization potential in a later PO calculation, but their model zinc atom had a dipole polarizability ($54 a_0^3$) that exceeds the experimental polarizability of $38.8 a_0^3$ [6] by 40% and could conceivably overestimate the strength of the polarization potential. The binding energies in both of the PO calculations were not calculated explicitly, rather they were deduced from the effective range relation $\varepsilon \approx 1/(2A^2)$ that is often used to relate the binding energy $\varepsilon$ to the scattering length $A$.

Many-body perturbation theory (MBPT) has also been used to predict the positron binding energy for Zn and Cd [7]. The strong electron-positron correlations makes the application of orthodox MBPT somewhat problematic [8]. However, the remedy adopted by Dzuba *et al.* to solve this problem is believed to result in an overestimation of the strength of the polarization correlation potential [9]. The MBPT binding energy of positronic magnesium given by Gribakin and King [10], 0.0362 hartree is about twice as large as the most recent estimates of the binding energy by the fixed core stochastic variational method (0.015 612 hartree [9]), the configuration-interaction method (0.001 62 hartree [11]), and the quantum Monte Carlo method (0.00168 hartree [12]). (Note all positron binding energies are given as positive numbers.)

The limitations of perturbative methods in accurately treating the strong correlations arising from the attractive

electron-positron interaction means that the binding energies resulting from these calculations are not expected to be very reliable. It is necessary to treat the $e^+$-$e^-$ correlations with a minimum of approximation in order to accurately determine the binding energy of positron binding systems. So far, three methods seem capable of achieving this. They are, the fixed core stochastic variational method (FCSVM) [13–15], the quantum Monte Carlo method (QMC) [12,16,17], and the configuration-interaction (CI) method [11,18–21]. Although, a FCSVM calculation of $e^+$Zn [22] and a CI calculation of $e^+$Cd [20] have already been reported, neither of these calculations were expected to give binding energies that were close to converged.

The FCSVM calculation for positronic zinc [22] gave a binding energy of 0.001 425 hartree. Although the FCSVM energy was far from converged, the prediction of binding within the constraints of the underlying model potential was rigorous since the determination of the binding energy was done variationally. The FCSVM calculations upon $e^+$Zn were extremely tedious and, to a certain extent, provided the initial stimulus to adapt the CI method to study positron binding atoms.

The initial CI calculations upon $e^+$Cd [20] used an orbital basis only about half the size as that adopted for the present calculation. Furthermore, the details of the core-polarization potential have been changed since the initial calculation. Despite these limitations, the previous CI calculations demonstrated the electronic stability of $e^+$Cd with a binding energy of 0.003 97 hartree [20]. The prediction of the stability of $e^+$Cd was quite reliable since binding was comfortably established with respect to a variety of potentials representing the core-valence interaction.

In the present work, the stability and structure of $e^+$Zn and $e^+$Cd have been established with large-scale CI calculations. Although extrapolations are used to estimate the binding energies, comparisons with previous work on $e^+$Be [21] (which has similarities in structure to $e^+$Zn and $e^+$Cd) suggest that the extrapolated binding energies should have accuracies of order 5%–10%. As part of our analysis, the binding energies of a number of states of Zn$^+$, Zn, Cd$^+$, and Cd are also computed and compared with experiment. The polarizabilities of the ground states of these systems are also com-

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TABLE I. The dipole polarizabilities ($\alpha_d$ in $a_0^3$) and cut-off parameters ($\rho_\ell$ in $a_0$) of the $Zn^{2+}$ and $Cd^{2+}$ core-polarization potentials.

| System | $\alpha_d$ | $\rho_0$ | $\rho_1$ | $\rho_2$ | $\rho_3$ | $\rho_{>3}$; $\rho_{p2}$ |
|---|---|---|---|---|---|---|
| $Zn^{2+}$ | 2.294 [22] | 1.63 | 1.80 | 2.30 | 1.60 | 1.83 |
| $Cd^{2+}$ | 4.971 [61] | 1.68 | 1.97 | 2.52 | 1.79 | 2.00 |

puted since the polarization potential is the primary dynamical mechanism leading to positron binding. Low-energy elastic cross sections and the annihilation parameter $Z_{eff}$ were estimated by using a model potential that was tuned to the binding energies and annihilation rates. Particular attention has been paid to the cross-section measurements that could be made to confirm positron binding to zinc or cadmium.

## II. DETAILS OF THE CALCULATION

The CI method as applied to positron-atomic systems with two valence electrons and a positron has been discussed previously [11,20,21], and the reader is referred to the preceding paper [11] for more details of the methodology. Briefly, the model Hamiltonian is initially based on a Hartree-Fock wave function for the neutral atom ground state. The core electrons (28 in the case of Zn and 46 in the case of Cd) are frozen. One- and two-body semiempirical polarization potentials are added to the potential field of the HF core. The parameters of the $\ell$-dependent core-polarization potentials defined with Eqs. (2)–(4) of [11] for Zn and Cd are listed in Table I. Table II gives a comparison of the experimental binding energies for $Zn^+$ and $Cd^+$ with those obtained by diagonalizing the model Hamiltonian. Inclusion of the core-polarization potentials dramatically improves the agreement of the fixed core Hamiltonian with experiment.

The Hamiltonian is then diagonalized in a CI basis constructed from a very large number of single-particle orbitals, including orbitals with $\ell = 10$. The CI basis was constructed by letting the two electrons and positron form all the possible $L=0$ configurations after populating the orbital basis subject to two selection rules, namely,

$$\max(\ell_0, \ell_1, \ell_2) \leq L_{max}, \qquad (1)$$

$$\min(\ell_1, \ell_2) \leq L_{int}. \qquad (2)$$

In these rules $\ell_0$, $\ell_1$, and $\ell_2$ are, respectively, the orbital angular momenta of the positron and the two electrons.

The diagonalization of the Hamiltonian matrix (with maximum dimensionalities up to 70 000) was performed using the Davidson algorithm [23]. Typically 500–1000 iterations have been required to diagonalize the Hamiltonians of positron binding atoms. However, the convergence of $e^+Cd$ was very slow and required more than 20 000 iterations before satisfactory convergence was reached.

Various expectation values were computed for these systems. The mean distances of the electron and positron from the nucleus are denoted by $\langle r_e \rangle$ and $\langle r_p \rangle$. The $2\gamma$ annihila-

TABLE II. Theoretical and experimental energy levels (in hartree) of some of the low-lying states of the $Cd^+$ and $Sr^+$ ions. The energies are given relative to the energy of the $Zn^{2+}$ or $Cd^{2+}$ core. The column $V_s$ gives the energies when only static terms are included in the core potential, while $V_{s+pol}$ adds the polarization potential to the core potential. The experimental energies for the spin-orbit doublets are statistical averages. The last row for each ion is the dipole polarizability (in $a_0^3$) of the $ns$ ground state (the core polarizability is added to the valence polarizability for the $V_{s+pol}$ calculation).

| Level | $V_s$ | $V_{s+pol}$ | Experiment [62,63] |
|---|---|---|---|
| | | $Zn^+$ | |
| $4s$ | −0.6162460 | −0.6603015 | −0.660180 |
| $4p$ | −0.4142650 | −0.4368332 | −0.436629 |
| $5s$ | −0.2477912 | −0.2553738 | −0.257230 |
| $4d$ | −0.2149902 | −0.2187392 | −0.218488 |
| $5p$ | −0.1913679 | −0.1963276 | −0.197577 |
| $6s$ | −0.1348695 | −0.1376028 | −0.138488 |
| $4f$ | −0.1251556 | −0.1258735 | −0.125887 |
| $5d$ | −0.1211429 | −0.1225399 | −0.122605 |
| $\alpha_d$ | 24.39 | 18.09 | |
| | | $Cd^+$ | |
| $5s$ | −0.5521406 | −0.6211981 | −0.621369 |
| $5p$ | −0.3808608 | −0.4128233 | −0.412730 |
| $6s$ | −0.2286586 | −0.2409554 | −0.243236 |
| $5d$ | −0.2065028 | −0.2122923 | −0.212292 |
| $6p$ | −0.1796120 | −0.1867128 | −0.187792 |
| $7s$ | −0.1259070 | −0.1307400 | −0.132470 |
| $4f$ | −0.1255450 | −0.1273414 | −0.127340 |
| $\alpha_d$ | 36.24 | 21.82 | |

tion rates for annihilation with the core and valence electrons are denoted $\Gamma_c$ and $\Gamma_v$, respectively.

The $L_{max} \to \infty$ limits were estimated with an extrapolation technique. Making the assumption that the successive increments $X_L$ to any expectation value $\langle X \rangle$ scale as $1/L^p$ for sufficiently large $L$ leads to

$$\langle X \rangle = \lim_{L_{max} \to \infty} \left( \sum_{L=0}^{L_{max}} X_L + \Delta \sum_{L=L_{max}+1}^{\infty} \frac{1}{L^p} \right). \qquad (3)$$

The power series is easy to evaluate, with $\Delta$ and the exponent $p$ given by Eqs. (11) and (12) of [11]. About 80% of the binding energies for $e^+Zn$ and $e^+Cd$ are obtained by the $L_{max} = 10$ calculations.

## III. CALCULATION RESULTS

### A. Tests of the model potentials

The ability of the underlying potential to give a good description of neutral zinc and cadmium is, of course, crucial in describing the interaction of the positron with these atoms. Table III reports energies, oscillator strengths, and the dipole polarizabilities of these systems and compares them with other calculations and experiments. The oscillator strengths

TABLE III. Energies levels (in hartree), oscillator strengths for the resonant transition ($f_{if}$), and dipole polarizabilities (in $a_0^3$ and includes the contribution from the core) for Zn and Cd. The energy of the ground state and the lowest $^1P^o$ excited state (relative to the energy of the $X^{2+}$ core) for CI basis sets with $L_{int}$ =0, 1, 2, 3, and 10. The number of configurations is given in the columns $N_{CI}$. The experimental energies are taken from [62] and [63].

| $L_{int}$ | $N_{CI}(^1S^e)$ | $E(^1S^e)$ | $N_{CI}(^1P^o)$ | $E(^1P^o)$ | $\Delta E$ | $f_{if}$ | $\alpha_d$ |
|---|---|---|---|---|---|---|---|
| | | | | Zn | | | |
| 0 | 136 | $-0.9736892$ | 192 | $-0.7762939$ | 0.1973953 | 1.687 | 50.46 |
| 1 | 214 | $-0.9935236$ | 336 | $-0.7897786$ | 0.2037450 | 1.512 | 40.66 |
| 2 | 292 | $-0.9949422$ | 432 | $-0.7910883$ | 0.2038539 | 1.537 | 41.18 |
| 3 | 328 | $-0.9953609$ | 496 | $-0.7914038$ | 0.2039572 | 1.542 | 41.23 |
| 10 | 580 | $-0.9955939$ | 880 | $-0.7916044$ | 0.2039895 | 1.544 | 41.25 |
| FCSVM [15] | | $-0.988586$ | | | | | |
| CI[a] | | | | | 0.213244 | 1.570 | 39.12 |
| CI[b] | | | | | 0.21508 | 1.563 | |
| Experiment | | $-1.005410$ | | $-0.792422$ | 0.212988 | 1.46(4) [28] | 38.8(8) [6] |
| | | | | | | 1.55(8) [29] | |
| | | | | | | 1.49(5) [27] | |
| | | | | Cd | | | |
| 0 | 120 | $-0.9240624$ | 210 | $-0.7394516$ | 0.1846108 | 1.662 | 57.46 |
| 1 | 225 | $-0.9370806$ | 392 | $-0.7509091$ | 0.1861714 | 1.484 | 49.42 |
| 2 | 316 | $-0.9385767$ | 509 | $-0.7525354$ | 0.1860413 | 1.506 | 50.04 |
| 3 | 361 | $-0.9391903$ | 581 | $-0.7529619$ | 0.1862284 | 1.511 | 50.07 |
| 10 | 613 | $-0.9394978$ | 965 | $-0.7532148$ | 0.1862830 | 1.513 | 50.09 |
| MCDF[c] | | | | | 0.198255 | 1.455 | |
| HFR[d] | | | | | | 1.388 | |
| Experiment | | $-0.951880$ | | $-0.752803$ | 0.199078 | 1.42(4) [31] | 49.6(16) [30] |
| | | | | | | 1.30(10) [32] | |

[a]Relativistic CI with pseudopotential [25].
[b]CI with core excitations and relativistic shifts [26].
[c]Multiconfiguration Dirac-Fock with core excitations [33].
[d]Quasirelativistic CI with core polarization [33].

were computed with a modified operator [24]. The polarizabilities were determined by evaluating the usual oscillator strength sum rule (see Eq. (5) in [11]).

The energies listed in Table III are given with respect to a zero energy given by the energy of the system with both electrons removed. The two-particle energies of these systems are both about 1% smaller than experiment. Of more significance is the result that the energy difference for the resonant $ns^2$ $^1S^e \rightarrow nsnp$ $^1P^o$ transitions is about 5% smaller than experiment. Both zinc and cadmium are moderately heavy atoms and therefore relativistic corrections could be making contributions to the binding energies. While using the polarization potential will partly compensate for the energy shifts, some errors in the positions of the excited states can be expected.

The tendency to underestimate the energy difference for the resonant transitions can be expected to lead to polarizabilities that are somewhat too large. This does occur, but the effect is not as large as would be expected by considering the energy differences alone. The polarizability for Zn is about $2.5a_0^3$ larger than experiment while the polarizability for cadmium is about $0.5a_0^3$ larger than experiment. There are prob-

ably some fortuitous cancellations with errors in the dipole matrix elements partly compensating for the errors in the energy difference.

Since the present calculations report oscillator strengths as well as dipole polarizabilities, it is possible to try and correlate different determinations of the oscillator strength and dipole polarizability with each other. For zinc, the relativistic pseudopotential calculation of Ellingsen *et al.* [25] gave an oscillator strength of 1.57 while reproducing the experimental polarizability of $(38.8 \pm 0.8)$ $a_0^3$ [6]. The oscillator strength from a CI calculation explicitly allowing for core excitations and applying relativistic shifts to the energies was 1.563 [26]. These values are slightly larger than two early experimental measurements [27,28] while agreeing with the most recent measurement of $1.55 \pm 0.08$ by Martinson *et al.* [29]. Since the dipole polarizability is strongly influenced by the oscillator strength of the resonant transition (the present calculations indicate that 90% of the polarizability comes from the resonant transition, 5.5% from the core, and only 4.5% from the rest of the valence excitations), compatibility of the oscillator strength with the dipole polarizability requires an oscillator strength of about 1.56.

TABLE IV. Results of CI calculations for $e^+$Zn versus $L_{max}$ for a configuration basis with $L_{int}=3$. The total number of electron and positron orbitals are denoted by $N_e$ and $N_p$. The three-body energy of the $e^+$Zn ground-state (in hartree) system, relative to the energy of the $Zn^{2+}$ core is denoted by $E(e^+Zn)$, while $\varepsilon=|E(e^+Zn)|-|E(Zn)|$, gives the binding energy against dissociation into $e^+ + Zn$. Both $\langle r_e \rangle$ and $\langle r_p \rangle$, are given in $a_0$. The column $E(Zn)$ gives the two-body energy of neutral zinc. The $\Gamma_v$ and $\Gamma_c$ annihilation rates are given in units of $10^9$ sec$^{-1}$. The results in the row $\infty$ are from an $L_{max}\to\infty$ extrapolation with the exponent used for the extrapolation given in the row labeled $p$. The last two rows are results for $e^+$Be. The row labeled CI($L_{max}\to\infty$) includes the contribution from the $L_{max}\to\infty$ extrapolation and was taken from [21] while the FCSVM results are from [9].

| $L_{max}$ | $N_e$ | $N_p$ | $N_{CI}$ | $E(e^+Zn)$ | $E(Zn)$ | $\varepsilon$ | $\langle r_e \rangle$ | $\langle r_p \rangle$ | $\Gamma_c$ | $\Gamma_v$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 16 | 12 | 1632 | $-0.9718996$ | $-0.9736892$ | $-0.0017896$ | 2.76518 | 27.31482 | 0.000378 | 0.00028 |
| 1 | 28 | 23 | 4680 | $-0.9922076$ | $-0.9935236$ | $-0.0013159$ | 2.75449 | 24.29219 | 0.001185 | 0.00285 |
| 2 | 40 | 33 | 10680 | $-0.9943096$ | $-0.9949422$ | $-0.0006325$ | 2.75962 | 20.00150 | 0.004140 | 0.01600 |
| 3 | 48 | 41 | 16432 | $-0.9955615$ | $-0.9953609$ | $0.0002006$ | 2.77219 | 16.06161 | 0.009031 | 0.04689 |
| 4 | 56 | 49 | 22848 | $-0.9963557$ | $-0.9953609$ | $0.0009948$ | 2.78700 | 13.59318 | 0.013526 | 0.08653 |
| 5 | 64 | 57 | 29376 | $-0.9969903$ | $-0.9953609$ | $0.0016294$ | 2.79946 | 12.22965 | 0.016700 | 0.12449 |
| 6 | 72 | 65 | 36064 | $-0.9974672$ | $-0.9953609$ | $0.0021063$ | 2.80914 | 11.44745 | 0.018814 | 0.15729 |
| 7 | 80 | 73 | 42976 | $-0.9978170$ | $-0.9953609$ | $0.0024561$ | 2.81647 | 10.97122 | 0.020222 | 0.18457 |
| 8 | 88 | 81 | 49888 | $-0.9980725$ | $-0.9953609$ | $0.0027116$ | 2.82196 | 10.67105 | 0.021166 | 0.20685 |
| 9 | 96 | 89 | 56800 | $-0.9982602$ | $-0.9953609$ | $0.0028993$ | 2.82614 | 10.46265 | 0.021831 | 0.22523 |
| 10 | 104 | 97 | 63712 | $-0.9983995$ | $-0.9953609$ | $0.0030385$ | 2.82927 | 10.32455 | 0.022292 | 0.24023 |
| $p$ | | | | 2.83 | | 2.83 | 2.80 | 3.91 | 3.49 | 1.93 |
| $\infty$ | | | | $-0.999092$ | $-0.9953609$ | $0.003731$ | 2.8451 | 9.9139 | 0.02393 | 0.3927 |
| FCSVM [9] | | | | $-0.988586$ | $-0.990011$ | $0.001425$ | 2.85 | 12.36 | 0.0140 | 0.234 |
| $e^+$Be CI($L_{max}\to\infty$) | | | | $-1.014931$ | $-1.011848$ | $0.003083$ | 2.653 | 10.244 | 0.002112 | 0.3733 |
| $e^+$Be FCSVM | | | | $-1.015100$ | $-1.011953$ | $0.003147$ | 2.654 | 9.842 | 0.00222 | 0.418 |

The present calculations gave a dipole polarizability that is about 1% larger than the experiment [30] for Cd. However, the present calculation underestimates the energy difference for the resonant transition by about 6.5%. Therefore, it would seem that an oscillator strength of 1.65 or larger would have to be used in the oscillator strength sum rule to get agreement with the experimental dipole polarizability of $(49.65 \pm 1.65)a_0^3$ by Goebel and Hohm [30]. The experimental oscillator strength measurements are smaller than 1.45 [31,32]. Similarly, two recent relativistic calculations gave resonance oscillator strengths of 1.39 and 1.455 [33]. The basis sets for both of these calculations were moderate in size when compared to the present calculation. There are obvious incompatibilities between the experimental oscillator strength and dipole polarizability. An earlier measurement of the polarizability by Goebel et al. [34] gave a smaller value, i.e., $(45.3\pm0.2)a_0^3$, but Goebel et al. regard this measurement as being less reliable [30]. The oscillator strength measurements are about 30 years old and the situation obviously demands a

modern determination of the oscillator strength to resolve this conundrum.

Our own opinion on the matter is that the dipole polarizability of Cd is probably about $45a_0^3$ (or smaller). There is no reason to believe that the present calculation should give the correct polarizability for cadmium when a similar model overestimates the polarizability of zinc by about 6%. Based on this analysis, it is expected that the present calculations will slightly overestimate the strength of the attractive interaction between the positron and these two atoms. This interaction is expected to be dominated by the polarization potential, and the polarizabilities of both atoms are probably slightly too large.

### B. Results for $e^+$Zn

The results of the sequence of calculations for $e^+$Zn with increasing $L_{max}$ are reported in Table IV. Positron binding is established by $L_{max}=3$ and the binding energy at $L_{max}=10$

TABLE V. Results of CI calculations for $e^+$Zn for the complete orbital basis (i.e., $L_{max}=10$) for different values of $L_{int}$. The organization of the table is the same as Table IV. The additional column reports $\alpha_d$ in $a_0^3$ (the contribution from the core polarizability is included).

| $L_{int}$ | $N_{CI}$ | $E(e^+Zn)$ | $E(Zn)$ | $\varepsilon$ | $\alpha_d$ | $\langle r_e \rangle$ | $\langle r_p \rangle$ | $\Gamma_c$ | $\Gamma_v$ |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 13856 | $-0.9808619$ | $-0.9736892$ | $0.0071728$ | 50.46 | 2.89878 | 8.11867 | 0.032533 | 0.37586 |
| 1 | 30020 | $-0.9964103$ | $-0.9935236$ | $0.0028868$ | 40.66 | 2.83243 | 10.47831 | 0.021542 | 0.23451 |
| 2 | 49736 | $-0.9979375$ | $-0.9949422$ | $0.0029953$ | 41.18 | 2.83016 | 10.36604 | 0.022058 | 0.23829 |
| 3 | 63712 | $-0.9983995$ | $-0.9953609$ | $0.0030385$ | 41.23 | 2.82927 | 10.32455 | 0.022292 | 0.24023 |

TABLE VI. Binding energies (in hartree) of positronic zinc and cadmium. Only the latest calculations of a given type by a particular group are listed in this table. References to earlier superseded works can be found in the text.

| System | Present CI explicit | Present CI extrapolated | MBPT [7] | Other |
|---|---|---|---|---|
| $e^+$Zn | 0.00304 | 0.00373 | 0.00845 | 0.001425,[a] $3.8\times10^{-7}$,[b] 0.00195[c] |
| $e^+$Cd | 0.00502 | 0.00610 | 0.0129 | 0.000056,[b] 0.003969[d] |

[a]FCSVM [22].
[b]Relativistic Polarized Orbital calculation, dipole only [1].
[c]Polarized orbital calculation [5].
[d]Earlier CI calculation with smaller basis [20].

is 0.003 038 5 hartree. When the extrapolation is applied, the binding energy increases by about 25%, and a binding energy of 0.003 73 hartree is indicated. Table V shows the convergence of the energy and other properties when $L_{int}$ increases from 0 to 3. The tabulations suggest convergence in most properties at the 1% level when $L_{int}=3$.

Positronic zinc is in many ways very similar to positronic beryllium. Neutral zinc and beryllium both have a valence $ns^2$ shell, with roughly the same binding energies and polarizabilities that are within 5% of each other (the polarizability of Be is about $37.76a_0^3$ [35]). Since zinc has a slightly larger polarizability than beryllium it is expected that $e^+$Zn would have a slightly larger binding energy and this is the case. The mean positron distance from the nucleus is $9.9a_0$, this is about the same distance from the nucleus as the positron in $e^+$Be.

Table VI reveals a rather large scatter amongst the other calculations of positronic zinc. The earlier FCSVM calculation was just not converged, and as such underestimated the binding energy. The initial PO calculation [1] only included the dipole component of the polarization potential and the system had a binding energy of less than $10^{-6}$ hartree. The later PO calculation which included higher-order multipoles of the polarization potential [5], can be best regarded as an approximation to the present ($L_{int}=0$, $L_{max}=10$) calculation. The PO binding energy was 0.001 95 hartree while the ($L_{int}=0$, $L_{max}=10$) calculation had a binding energy of 0.007 17 hartree. The PO calculation for positronic zinc seems to underestimate the strength of the electron-positron correlations. Although the PO method as applied by McEachran and co-workers seems to give a good description of positron-rare-gas scattering [2,36–38], its inherent limitations are exposed for the present systems with their stronger electron-positron correlations.

The MBPT energy of Dzuba et al. [7], 0.008 45 hartree, is about twice as large as the present binding energy. As mentioned earlier, it is believed the MBPT calculation overestimates the strength of the polarization-correlation potential [9,11]. Therefore, a MBPT binding energy that is twice as large as the current CI binding energy is not an anomaly since it is consistent with the pattern established for positronic magnesium [9,11].

### C. Results for $e^+$Cd

The properties of $e^+$Cd are given in Table VII. The cadmium atom has a slightly smaller ionization potential ($I$), and a polarizability that is 20% larger than zinc. Therefore, it

TABLE VII. Results of CI calculations for $e^+$Cd versus $L_{max}$ with a configuration basis with $L_{int}=3$. The organization is the same as Table IV.

| $L_{max}$ | $N_e$ | $N_p$ | $N_{CI}$ | $E(e^+\text{Cd})$ | $E(\text{Cd})$ | $\varepsilon$ | $\langle r_e \rangle$ | $\langle r_p \rangle$ | $\Gamma_c$ | $\Gamma_v$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 15 | 12 | 1440 | −0.9223648 | −0.9240624 | −0.0016976 | 2.98690 | 27.6952 | 0.000505 | 0.00031 |
| 1 | 29 | 23 | 5010 | −0.9359202 | −0.9370806 | −0.0011604 | 2.99166 | 24.1689 | 0.001781 | 0.00311 |
| 2 | 42 | 33 | 12014 | −0.9382390 | −0.9385767 | −0.0003378 | 3.00016 | 19.1185 | 0.006607 | 0.01779 |
| 3 | 51 | 42 | 19457 | −0.9400166 | −0.9391903 | 0.0008264 | 3.01892 | 14.4648 | 0.015165 | 0.05551 |
| 4 | 59 | 50 | 26833 | −0.9411760 | −0.9391903 | 0.0019857 | 3.04051 | 11.9726 | 0.022512 | 0.10341 |
| 5 | 67 | 58 | 34161 | −0.9421108 | −0.9391903 | 0.0029205 | 3.05823 | 10.7451 | 0.027366 | 0.14894 |
| 6 | 75 | 66 | 41569 | −0.9428171 | −0.9391903 | 0.0036269 | 3.07199 | 10.0761 | 0.030481 | 0.18861 |
| 7 | 83 | 74 | 49121 | −0.9433380 | −0.9391903 | 0.0041477 | 3.08242 | 9.68952 | 0.032476 | 0.22184 |
| 8 | 91 | 82 | 56673 | −0.9437204 | −0.9391903 | 0.0045302 | 3.09038 | 9.43931 | 0.033818 | 0.24957 |
| 9 | 99 | 90 | 64225 | −0.9440029 | −0.9391903 | 0.0048126 | 3.09648 | 9.26897 | 0.034746 | 0.27264 |
| 10 | 107 | 98 | 71777 | −0.9442135 | −0.9391903 | 0.0050232 | 3.10113 | 9.15370 | 0.035391 | 0.29179 |
| $p$ | | | | 2.79 | | 2.79 | 2.58 | 3.71 | 3.44 | 1.77 |
| $\infty$ | | | | −0.945291 | −0.9391903 | 0.006100 | 3.1284 | 8.7819 | 0.03773 | 0.5273 |

is expected that the binding energy for Cd will be somewhat larger that that for zinc, and this is the case. The $e^+$Cd binding energy of 0.006 100 hartree is just over 50% larger than the binding energy of $e^+$Zn. A series of calculations for smaller $L_{int}$ were not done since the diagonalizations were very time consuming. It is expected that the convergence of the energy and annihilation rate with $L_{int}$ would be similar to that of $e^+$Zn.

Despite the larger binding energy, there are obvious qualitative similarities between the structures of $e^+$Cd and $e^+$Zn. The positron charge distribution for $e^+$Cd is diffuse with a mean positron radius of $8.78a_0$. This is about 10% more compact than the charge distribution of $e^+$Zn. The annihilation rate of $0.565 \times 10^9$ sec$^{-1}$ is about 40% larger than the annihilation rate of $e^+$Zn. Previous investigations have shown that parent atoms with smaller ionization potential generally have larger annihilation rates [39–41]. The larger annihilation rate occurs because the positron can more strongly attract an electron when the ionization potential (which is a measure of the interaction strength between the electron and the atomic core) is smaller. A reasonable summary of the structure of $e^+$Cd is that it is an analog of $e^+$Zn with a slightly more tightly bound positron.

The comparisons with other predictions of the binding energy (Table VI) are pretty much consistent with the pattern seen for zinc. The dipole-only PO calculation only predicts binding and the binding energy is about 100 times smaller than the present estimate. The MBPT binding energy is about twice as large as the present binding energy.

### D. Comments on the extrapolation procedure

Gribakin and Ludlow [42] recently used second-order perturbation theory to estimate the asymptotic dependence of the increments to the energy and annihilation energy with $\ell$. For the energy increments in Eq. (3) they gave $p_E = 4$ while $p_\Gamma = 2$ was deduced for the annihilation rate increments.

The CI calculations for $e^+$Zn and $e^+$Cd gave exponents for $p_E$ that were somewhat smaller than 4, presumably because the asymptotic region is not reached until $L_{max} > 10$. This raises the possibility that the present extrapolation correction to the energy is an overestimate. In a previous CI calculation involving $e^+$Ca and $e^+$Sr [21], the Gribakin-Ludlow analysis was used to develop improved estimates for $p_E$ and $p_\Gamma$. This more involved procedure was not adopted for the present work.

There are two aspects where convergence can be incomplete. Besides the size of $L_{max}$, the number of LTOs for each value of $\ell$ could be increased. Using the value of $p_E$ taken from the $L_{max} = 8$, 9, and 10 calculations tends to yield a correction that is an overestimate. Using only 8 LTOs per partial wave tends to give a binding energy that is slightly too small. These effects do tend to cancel each other out. The application of exactly the same extrapolation procedure to the very similar $e^+$Be system, with a similar sized LTO basis, gave a binding energy 2% lower than a FCSVM calculation with almost identical physical content [21]. The current procedure is retained for the pragmatic reason that it was a good predictor for $e^+$Be.
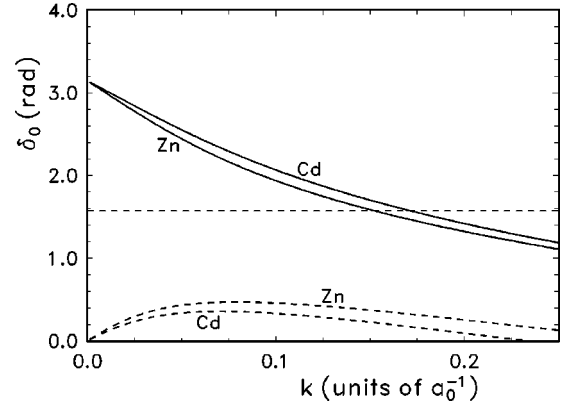


FIG. 1. The $s$-wave phase shifts as a function of $k$ (in units of $a_0^{-1}$) for $e^+$Zn and $e^+$Cd elastic scattering. The phase shifts corresponding to the potential tuned to support a physical state are shown as solid lines while the phase shifts for the virtual state case are shown as dashed lines. The horizontal dashed line marks $\delta_0 = \pi/2$.

## IV. SCATTERING OF POSITRONS FROM Zn AND Cd

Both zinc and cadmium have low melting temperatures and therefore it is possible that positron scattering experiments from these atoms could be done. Reasonable estimates of both the elastic scattering cross section and threshold $Z_{eff}$ can be obtained from the $e^+$Zn and $e^+$Cd binding energy and annihilation rate using a model potential technique [38,43]. The justification of the specific details of the model potential have been given elsewhere [38].

Besides the determination of the low-energy cross section, it is desirable to analyze the cross sections for features that could be used as indicators of positron binding in an experimental situation.

The positron-atom interaction consists of a short-range repulsive interaction and a long-range attractive interaction due to the $\alpha_d/(2r^4)$ polarization potential. The polarization potential ensures that phase shifts for the $\ell \geq 1$ partial waves are positive close to threshold. The large size of the polarizability for the systems under consideration, means that scattering lengths for the group-IIB atoms will generally be large, i.e., the positron will be weakly bound or just fail to be bound. The scattering length will be positive when the positron can be bound to the atom and negative when the system does not support the bound state. When the positron is bound and has a large positive scattering length, the zero-energy $s$-wave phase shift will be $\pi$ and will then decrease rapidly and eventually will pass through $\pi/2$ as the energy increases. When the scattering length is negative, the $s$-wave phase increases rapidly from zero until it reaches a maximum in the phase shift (the maximum phase shift cannot exceed $\pi/2$ [44]), and then begins to decrease.

Figure 1 shows the typical behavior of the $s$-wave phase shift for the cases when the potential supports a bound state and when the potential supports a virtual state. $S$-wave phase shifts that are in different quadrants will interfere differently with the higher $\ell$ partial waves and therefore the potentials leading to bound or virtual states can be expected to result in dis-similar differential cross sections. The completely differ-

TABLE VIII. The elastic cross section $\sigma_\rho$ (in units of $\pi a_0^2$) and the annihilation parameter $Z_{\mathrm{eff}}(k)$ as a function of $k$ (in $a_0^{-1}$). The cross sections at $k=0$ were obtained by extrapolation. The cross sections are unlikely to be reliable at energies above the Ps-formation threshold.

| $k$ ($a_0^{-1}$) | Zn | | Cd | |
| --- | --- | --- | --- | --- |
| | $\sigma_{el}$ | $Z_{\mathrm{eff}}$ | $\sigma_{el}$ | $Z_{\mathrm{eff}}$ |
| 0.00 | 843.9 | 110.7 | 535.8 | 80.14 |
| 0.01 | 857.3 | 108.8 | 557.9 | 79.04 |
| 0.02 | 838.7 | 104.4 | 563.0 | 76.75 |
| 0.03 | 794.1 | 98.19 | 552.1 | 73.75 |
| 0.04 | 733.1 | 91.00 | 529.6 | 70.28 |
| 0.05 | 664.2 | 83.45 | 499.7 | 66.60 |
| 0.06 | 593.9 | 76.04 | 465.5 | 62.91 |
| 0.08 | 464.7 | 62.91 | 394.4 | 56.18 |
| 0.10 | 361.0 | 52.78 | 330.1 | 51.02 |
| 0.12 | 283.4 | 45.56 | 278.2 | 47.72 |
| 0.15 | 205.9 | 39.04 | 223.7 | 45.81 |
| 0.20 | 138.8 | 34.89 | 172.9 | 46.30 |
| 0.25 | 105.5 | 33.33 | 138.3 | 45.00 |
| 0.30 | 82.77 | 31.36 | 107.8 | 41.03 |
| 0.40 | 51.46 | 26.63 | 64.93 | 33.12 |
| 0.50 | 34.11 | 23.51 | 42.97 | 28.98 |

ent behavior of the $s$-wave phase shifts close to threshold in these two cases can be exploited to verify experimentally whether the positron can bind to either atom. The boundary between the regions where the phase shifts change quadrants can be roughly estimated as $k \approx \pi/(2A)$.

### A. The model potential

The effective Hamiltonian for the positron moving in the field of the atom is approximated by the model potential

$$H = -\frac{1}{2}\nabla_0^2 + V_{dir}(\mathbf{r}_0) + V_{pol}(\mathbf{r}_0). \qquad (4)$$

The repulsive direct potential $V_{dir}$ is computed from the HF wave function of the target atom. The polarization potential is given by the form

$$V_{pol}(\mathbf{r}_0) = -\frac{\alpha_d[1 - \exp(-r^6/\rho^6)]}{2r^4}. \qquad (5)$$

The adjustable parameter $\rho$ is fixed by the requirement that the model potential has a bound state with a binding energy equal to that of the CI calculations. For Zn, the requirement that Eq. (4) gives $\varepsilon = 0.003\,731$ hartree gave $\rho = 2.593a_0$ when $\alpha_d = 41.23a_0^3$. For Cd, the requirement that Eq. (4) gives $\varepsilon = 0.006\,100$ hartree gave $\rho = 2.585a_0$ when $\alpha_d = 50.07a_0^3$. The elastic cross sections computed with this potential are denoted $\sigma_b$ and are given in Table VIII. The $s$-wave phase shifts corresponding to this case are shown in Fig. 1 as the solid lines.

Since the important issue that an experiment will have to resolve is whether the scattering length is positive or negative, an additional calculation has been done for each atom. The cutoff parameter $\rho$ was tuned to give a scattering length that was negative but had the same magnitude. The values of $\rho$ were $4.216a_0$ and $5.0a_0$ for Zn and Cd, respectively. With these values of $\rho$ the model positron-atom interaction now supports a virtual state. The cross section derived from these calculations is denoted $\sigma_v$. The $s$-wave phase shifts for the virtual-state potentials are shown in Fig. 1 as the dashed lines.

### B. Positron annihilation

The annihilation of positrons in an atomic collision is most usually described by the annihilation parameter $Z_{\mathrm{eff}}$, which can be calculated from the scattering wave function [2,45,46]. The annihilation parameter for the model potential wave function is written as [38]

$$Z_{\mathrm{eff}} = \int d^3r[G_v\rho_v(\mathbf{r}) + G_c\rho_c(\mathbf{r})]|\Phi(\mathbf{r})|^2, \qquad (6)$$

where $\rho_c(\mathbf{r})$ and $\rho_v(\mathbf{r})$ are the electron densities of the core and valence electrons of the target atom, and $\Phi(\mathbf{r})$ is the positron scattering function. In the plane-wave Born approximation, the positron wave function is written as a plane wave and the annihilation parameter is equal to the number of atomic electrons, i.e., $Z_{\mathrm{eff}} = N_e$.

The enhancement factors $G$ are introduced to take into consideration the impact that electron-positron correlations will have upon the annihilation rate. The attractive nature of the electron-positron interaction leads to electron-positron correlations that increase the electron density at the position of the positron, and consequently increases the annihilation rate. Such enhancement factors are routinely used in the calculation of the annihilation rate of positrons in condensed-matter systems [47–49]. The enhancement factor for valence and core electrons is treated differently. For core orbitals, $G_{core}$ is simply set to 2.5 due to reasons outlined in [38]. The valence enhancement factor $G_{valence}$ is computed by the simple identity

$$G_{valence} = \frac{\Gamma_v^{CI}}{\Gamma_v^{model}}, \qquad (7)$$

where $\Gamma_v^{CI}$ is the annihilation rate of the positron with the valence orbitals as given by the CI calculation and $\Gamma_v^{model}$ is the valence annihilation rate predicted by the model potential calculation with $G = 1$.

### C. Effective range estimates

Before using the model potential to determine the threshold cross section and phase shifts, it is instructive to apply effective range theory to this problem [38]. The real part of the scattering length $A$ is given by

$$A = \frac{1}{\sqrt{2|\varepsilon|}} \qquad (8)$$

while at zero energy $Z_{\text{eff}}$ becomes

$$Z_{\text{eff}}(k=0) = 4.401\,53 \times 10^{-11} \frac{\Gamma}{\sqrt{|\varepsilon|^3}}. \qquad (9)$$

In these equations, $\varepsilon$ is the binding energy expressed in hartree while the annihilation rate is given in sec$^{-1}$. A similar equation has been derived by Gribakin [50] using a different technique. Applying these equations to Zn and Cd yields scattering lengths of $11.6a_0$ and $9.05a_0$, respectively. The threshold values of $Z_{\text{eff}}$ were 80.6 for Zn and 52.3 for Cd.

The estimates of $Z_{\text{eff}}$ are relevant to the existing debate regarding the mechanisms responsible for positrons annihilation in collisions with gases [3,38,50–53]. Tabulations of $Z_{\text{eff}}$ for a number of gases (mainly molecules with single bonds) have suggested the empirical formula [51,53,54]

$$\ln(Z_{\text{eff}}) \approx B|I - E_{Ps}|^{-1}, \qquad (10)$$

where $B \approx 33$ when $I$ is given in eV. Using Eq. (10) as a guide, there have been speculations that metal vapors such as Zn and Cd could have $Z_{\text{eff}}$ of order $10^6$ [53]. The results of the effective range analysis seem to rule out such large values of $Z_{\text{eff}}$.

### D. Model potential calculations

The low-energy elastic cross sections and $Z_{\text{eff}}$ are given for momenta up to $0.5a_0^{-1}$ in Table VIII. The scattering lengths for Zn and Cd were $14.5a_0$ and $11.6a_0$, respectively. The effective range estimates from the preceding section are about 20% smaller than the model potential values. When it comes to $Z_{\text{eff}}$, the effective range estimates are about 40% smaller than the model potential values.

One of the more interesting features of the energy dependence of the elastic cross section is that it increases very close to threshold. This occurs because of the interaction of the scattering length term and polarizability term in the effective range expansion [55],

$$\tan(\delta) = -Ak - \frac{\pi\alpha_d k^2}{3} + \cdots \qquad (11)$$

close to threshold. The resulting cross section can be approximated as

$$\sigma_{el} = \frac{4\pi A^2}{\left(1 - \frac{\pi\alpha_d k}{3}\right)^2 + A^2 k^2}. \qquad (12)$$

A negative scattering length leads to a cross section that decreases from threshold. But when the scattering length is positive the cross section increases because of the linear term in the denominator. Gribakin [52] has suggested that the rate at which the cross section changes, $d\sigma/dE$ can be used to identify positron binding. The clearest signature occurs very
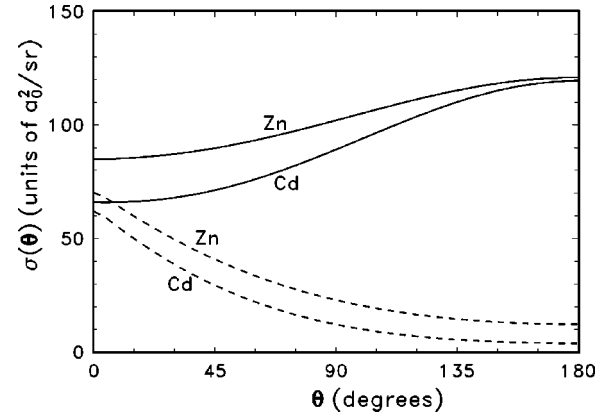


FIG. 2. The differential cross sections (in $a_0^2$/sr) for positron scattering from zinc and cadmium at $k = 0.09a_0^{-1}$ (energy $= 0.1102$ eV). The DCS for the bound state potentials are plotted as a solid line while the DCS for the virtual state potentials are plotted as a dashed line.

close to threshold where the cross section increases with increasing energy. However, this behavior only occurs for $k < 0.02a_0^{-1}$ (i.e., $E \leqslant 0.006$ eV) and therefore would be difficult to measure with existing positron beam technology. At higher energies the difference between the bound and virtual state case is not so obvious.

### E. Differential cross section

The differential cross section (DCS) is particularly interesting to determine since signatures of a positive scattering length are much more apparent in the differential cross section than in the integrated cross section. Comments about using the differential cross section to identify positron binding have been made previously but without presenting the results of any numerical calculations [56].

The differential cross section is written

$$\sigma(\theta) = |f(\theta)|^2, \qquad (13)$$

where the scattering amplitude is

$$f(\theta) = \frac{1}{2ik} \sum_{\ell} (2\ell+1)[\exp(2i\delta_\ell) - 1]P_\ell(\cos\theta). \qquad (14)$$

The shape of the DCS changes dramatically when the scattering length changes sign from negative to positive. The phase shifts for $\ell \geqslant 1$ are positive and to a first approximation given by [55]

$$\tan(\delta_\ell) \approx \frac{\alpha_d \pi k^2}{(2\ell+3)(2\ell+1)(2\ell-1)}. \qquad (15)$$

A positive scattering length, giving a phase shift between $\pi/2$ and $\pi$, results in a DCS that is larger at backward angles than at forward angles. This is shown in Fig. 2 where the DCS for positron scattering from zinc is plotted. The potential supporting the bound state has a cross section that increases slowly as the scattering angle is increased. The po-
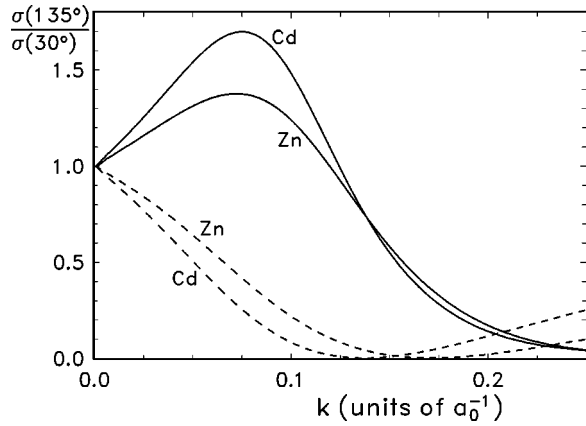
FIG. 3. The DCS ratio $R = \sigma_b(135°)/\sigma_b(30°)$ is plotted as a function of $k$ (in $a_0^{-1}$) for positron scattering from zinc and cadmium (solid lines). The cross-section ratios computed from the virtual state potential $R = \sigma_v(135°)/\sigma_v(30°)$ are shown as the dashed lines.

tential with a negative scattering length has a DCS that is strongly peaked in the forward direction. There is an order of magnitude difference between the two sets of cross sections at a backward angle such as 135°.

The differences between a positive and negative scattering length are also very noticeable in Fig. 3 where the DCS ratio, $R = \sigma(135°)/\sigma(30°)$ is plotted. The bound state potential gives a ratio that initially increases from threshold. The virtual state potentials give a ratio that decreases steadily from threshold. A measurement of the DCS ratio at positron energies from 0.060 eV to 0.30 eV should provide experimental evidence of the stability of $e^+$Zn and $e^+$Cd.

Differential cross section measurements of this type could conceivably be used to determine whether mercury will bind a positron. Positron binding to mercury was predicted by Dzuba *et al.* [7] who estimated a binding energy of 0.001 65 hartree. However, as we have seen, the MBPT calculation tends to overestimate the attraction of the positron to the atom. The polarizability of mercury, namely, $33.91 \pm 0.34 a_0^3$ [57] is smaller than that of Be and Zn which bind the positron weakly. With the available theoretical information, it is not possible to definitely determine whether positron binding is possible or not. Deciding this question theoretically will be difficult since a fully relativistic calculation would be necessary. It is quite likely that the best way to determine the stability of the positron-mercury system will be a DCS experiment.

The stability of positronic magnesium could also be investigated in a DCS experiment. The positron-magnesium system has a smaller scattering length and a larger dipole polarizability [38] so the peaking of the DCS toward backward angle should be even larger than in cadmium or zinc.

The disadvantage of magnesium is that the production of an atomic vapor requires a cell capable of higher temperatures.

## V. SUMMARY AND FUTURE PERSPECTIVES

The CI method has been used to compute the binding energies and annihilation rates for $e^+$Zn and $e^+$Cd. These two systems, together with $e^+$Be, form a set of very similar exotic atoms. The positron is found at moderately large distances from a largely undisturbed atom, and is weakly bound to the atom by polarization forces. About 20% of the binding energy is derived from an extrapolation to the $L_{max} \rightarrow \infty$ limit. Previous work on $e^+$Be suggests that the net error in the binding energy associated with this extrapolation will be of the order of 5% [21].

The specification of the core-polarization potential is one of the largest sources of uncertainty in the calculation. Since zinc and cadmium are both moderately heavy atoms, it is likely that the core-polarization potential is also compensating for small relativistic energy shifts. However, the core-polarization potential does not have much of a direct influence on the positron, rather it influences the motion of the valence electrons which in turn affects the motion of the positron (e.g., adding a core-polarization potential for a parent atom with $I > 6.8$ eV causes the positron binding energy to decrease [15,58]). The sensitivity of the bound state to changes in the underlying core-polarization potential was tested in a calculation with the $Zn^{2+}$ polarizability increased to $3.90 a_0^3$ while everything else remained unchanged. When this was done, the total polarizability of neutral zinc dropped to $35.84 a_0^3$ and the two-body energy of Zn changed to $-1.044 28$ hartree. However, the positron still remains bound with a binding energy of about 0.002 232 hartree and a total annihilation rate of $0.327 \times 10^9$ s$^{-1}$.

The low-energy elastic-scattering calculations indicate that measurement of the differential cross sections should permit verification that zinc and cadmium can bind a positron. It will be necessary to take measurements at positron beam energies below 0.15 eV. Positron sources capable of achieving this do exist, so such an experiment is definitely feasible [53,59]. Besides verifying positron binding to zinc and cadmium, a differential cross section experiment would also be able to determine whether positron binding to mercury is possible.

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