

## Positronium scattering from Kr and Xe at low energies

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The scattering of orthopositronium from Kr and Xe is investigated with the fixed core stochastic variational method. The scattering lengths for Ps-Kr and Ps-Xe scattering in the fixed core approximation are  $3.18a_0$  and  $3.82a_0$ , respectively. Inclusion of core-polarization potentials leads to a significant reduction in the scattering lengths. The Ps-Kr and Ps-Xe scattering lengths were  $1.98a_0$  and  $2.29a_0$  for polarization potentials that were tuned to an average of the model electron-atom and positron-atom scattering lengths for the respective atoms. Other choices of the polarization potential resulted in scattering lengths that could be larger by  $0.3a_0$  or smaller by  $0.8a_0$ . The pick-off annihilation parameter  ${}_1Z_{\text{eff}}$  has also been computed as part of the analysis. The present values of  ${}_1Z_{\text{eff}}$  are about 3 to 10 times smaller than the accepted experimental values since short-range electron-positron correlations were ignored when the annihilation matrix element was evaluated.

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### I. INTRODUCTION

In the last year there has been considerable progress in the treatment of orthopositronium (Ps) scattering from atoms. On one hand, the fixed core stochastic variational method (FCSVM) has been adapted to perform scattering calculations within the framework of the stabilization method [1,2]. This has been used to generate *s*-wave phase shifts for the lighter rare gases, He, Ne, and Ar in the energy region just above threshold [3]. The *R*-matrix method has also been utilized to investigate ortho-Ps scattering from hydrogen and the rare gases [4,5]. One important result to emerge from this research has been agreement between the stabilization FCSVM and *R*-matrix scattering lengths for He, Ne, and Ar when they have been computed in the same approximation [3,4,6]. Given the difficulties associated with performing any sort of calculation of Ps-atom scattering this agreement can be regarded as a major step forward in the understanding of the Ps-atom scattering problem.

However, despite the progress for He, Ne, and Ar, there seem to be difficulties in determining the phase shifts for Xe [3]. Up to now, the only calculations so far reported for this system were computed in the static-exchange (SE) approximation using the *R*-matrix method [4]. The cross sections for Xe were very different in shape from those of the other rare gases. The cross sections had a minima below 0.5 eV incident energy, a sharp resonantlike feature between 1–2 eV, and another broad feature at about 10 eV. This cross section has been criticized on the grounds that (a) the two different *R*-matrix calculations that were done were inconsistent (b) and the shape of the cross section was completely different with the trends established for the other rare gases [6].

In order to shed further light on this situation, the stabilization FCSVM is applied to the calculation of the Ps-Kr and Ps-Xe phase shifts. The FCSVM phase shifts for Kr seem to be compatible with the *R*-matrix phase shifts, but the Ps-Xe phase shifts are completely different from the *R*-matrix phase shifts.

From the experimental perspective, there is very little information about the Ps-Kr and Ps-Xe cross sections close to threshold. While detailed examination of the  $\gamma$ -radiation

emitted in positron annihilation experiments has given estimates of the momentum-transfer cross sections for He, Ne, and Ar, the same is not true for Kr and Xe [7–9]. A beam experiment for Ps scattering from gases has been developed, but it is restricted to Ps energies above 10 eV [10]. The only experimental estimates of the low-energy Ps-Xe cross section are derived from the annihilation spectrum obtained from bubble states in high-density gases [11].

### II. CALCULATIONS AND RESULTS

The present calculations are based on a modified version of the FCSVM that was developed to handle scattering problems. The idea behind the approach is to diagonalize the system Hamiltonian in a large basis of square integrable states designed to provide a reasonable representation of a typical scattering state. The phase shifts and other information are then extracted from the positive energy pseudostates by projecting them with  $\Phi_{Ps}(\mathbf{r}_0 - \mathbf{r}_1)$  and fitting to the asymptotic form of the wave function, i.e.,  $\sin[k(|\mathbf{r}_0 + \mathbf{r}_1|/2) + \delta]$ , at large distances from the nucleus [1–3]. The method has been used to give estimates of the phase shifts and the pick-off annihilation parameter  ${}_1Z_{\text{eff}}$  close to threshold for Ps scattering from He, Ne, Ar,  $\text{Li}^+$ ,  $\text{Na}^+$ , and  $\text{K}^+$  [3,12].

The actual calculations that are used to determine the scattering wave function were very similar to those described in Ref. [3]. Therefore, no details of the scattering calculation are presented apart from a brief description of the scattering Hamiltonian.

The FCSVM [13] has been used to describe the interaction of the projectile with the atom or ion. The FCSVM replaces the full Hamiltonian for the  $N_e$  electrons and a positron by a model Hamiltonian with the core electrons removed, viz.,

$$H = -\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - V_{dir}(\mathbf{r}_0) + V_{dir}(\mathbf{r}_1) + V_{p1}(\mathbf{r}_0) + V_{p1}(\mathbf{r}_1) + V_{exc}(\mathbf{r}_1) - \frac{1}{r_{01}} + V_{p2}(\mathbf{r}_1, \mathbf{r}_0) + \lambda \hat{P}, \quad (1)$$

where  $\mathbf{r}_0$  is the positron coordinate and  $\mathbf{r}_1$  is the electron coordinate. The direct potential ( $V_{dir}$ ) for the core is taken from a Hartree-Fock wave function and is the same (although opposite in sign) for the electron and the positron. The exchange potential ( $V_{exc}$ ) between the scattering electron and the Hartree-Fock core was computed exactly. The operator

$$\lambda \hat{P} = \sum_{i=1} \lambda |\phi_i\rangle\langle\phi_i|, \quad (2)$$

is an orthogonalizing pseudopotential that acts to produce wave functions orthogonal to the occupied core orbitals provided  $\lambda$  is a large positive number [14–16].

The polarization potential  $V_{p1}$  is defined with the functional form

$$V_{p1}(r) = -\frac{\alpha_d g^2(r)}{2r^4}. \quad (3)$$

The factor  $\alpha_d$  is the static dipole polarizability of the core and  $g^2(r)$  is a cutoff function designed to make the polarization potential finite at the origin. The same cutoff function was adopted for both the positron and electrons. Its form was chosen as

$$g^2(r) = 1 - \exp(-r^6/\rho^6), \quad (4)$$

where  $\rho$  is an adjustable parameter. The two-body polarization potential  $V_{p2}$ , is defined as

$$V_{p2}(\mathbf{r}_0, \mathbf{r}_1) = \frac{\alpha_d}{r_0^3 r_1^3} (\mathbf{r}_0 \cdot \mathbf{r}_1) g(r_0) g(r_1). \quad (5)$$

Inclusion of the two-body potential makes the polarization interaction reduce to a van der Waals type interaction when the Ps atom is at large distances from the nucleus.

While the static dipole polarizabilities, i.e.,  $\alpha_d$  for the rare gases are well known, there are naturally some uncertainties in the definition of the short-range form of the polarization potential. Therefore, three different forms of the polarization potential were constructed that depended on the physical criteria used to tune the cutoff parameter. First,  $\rho_-$  was defined by the requirement that the scattering length from a static-exchange +  $V_{p1}$  calculation of electron scattering from the rare-gas agree with the experimental scattering lengths for krypton,  $-3.35a_0$  [17] and xenon  $-6.5 \pm 0.1a_0$  [18]. Next,  $\rho_+$  was defined by using the procedure and values adopted in an earlier semi-empirical analysis of positron-atom scattering [19]. In effect, the polarized orbital calculations of McEachran, Stauffer, and Campbell [20] were used to tune the cutoff parameters. Finally,  $\rho_{av}$  was chosen by simply averaging  $\rho_+$  and  $\rho_-$ . The values of  $\rho_+$ ,  $\rho_-$  and  $\rho_{av}$  are listed in Table I.

Table II gives the scattering length  $A$  and effective range for the different model calculations of Ps scattering from Kr and Xe. The results are presented as coefficients in the effective range expansion,

TABLE I. Parameters defining of the polarization potential. The dipole polarizability  $\alpha_d$  is given in  $a_0^3$  while the cutoff parameter  $\rho$  is given for both electron  $\rho_-$  and positron  $\rho_+$  scaling. The parameter  $\rho_{av}$  is the average of the electron and positron parameters.

System	$\alpha_d$	$\rho_-$	$\rho_+$	$\rho_{av}$
Kr	16.8	2.83	1.85	2.34
Xe	27.3	2.65	1.96	2.30

$$k \cot(\delta) = -\frac{1}{A} + \frac{1}{2} r_0 k^2, \quad (6)$$

extracted from a least squares fit to the FCSVM phase shifts for  $k < 0.3a_0^{-1}$ . The first point to be noted is that the present  $\alpha_d=0$  scattering length for Kr is about  $0.15a_0$  smaller than the deduced  $R$ -matrix scattering length for Kr (it has been assumed that the  $R$ -matrix calculation for Kr gives a positive  $A$ ). However, the FCSVM wave function has a greater degree of variational flexibility than the  $R$ -matrix SE calculation and therefore should have a slightly smaller scattering length. The comparisons for the different Ne and Ar scattering lengths in Table III reveal that a difference of about  $0.15a_0$  is expected between the FCSVM and  $R$ -matrix SE scattering lengths. Therefore, the FCSVM and  $R$ -matrix scattering lengths for Ps-Kr scattering are consistent when the difference in the effective channel space of the two calculations are taken into consideration.

With respect to xenon, there is no possibility of reconciling the  $R$ -matrix scattering length of  $\pm 1a_0$  with the FCSVM scattering length of  $3.82a_0$ . A plot of the  $R$ -matrix Ps-Xe elastic cross section (Fig. 16 in Ref. [4]) shows structures at low energies that are not present in the cross sections for any of the other rare gases. This led us to suspect the existence of errors in the  $R$ -matrix calculation of Blackwood, McAlinden, and Walters [6]. Concerns about the accuracy of the  $R$ -matrix calculation were communicated to Blackwood, McAlinden, and Walter's while the present manuscript was under review. Blackwood, McAlinden, and Walter's have reevaluated their Ps-Xe calculations and have concluded that numerical inaccuracies resulted in a Ps-Xe cross section that was incorrect [21].

The present calculation has a positive scattering length, indicating a repulsive potential. The sequence of frozen core FCSVM calculations for He, Ne, Ar, Kr, and Xe show a tendency for the scattering lengths to increase as the target atom gets larger. One interesting feature of Table III concerns an approximate relation between the FCSVM scattering lengths and the scattering lengths for electron and positron scattering. Defining  $A_-$  as the scattering length for electron scattering in the static-exchange approximation, and  $A_+$  as the scattering length for positron scattering in the static approximation, then it is noticeable that  $A_{\text{FCSVM}} \approx (A_+ + A_-)$ .

The calculations allowing for target polarization show that the impact of the polarization potential is quite substantial. The earlier calculations for Ar demonstrated that the core-polarization–van der Waals interactions could reduce the

TABLE II. The scattering length ( $A$  in  $a_0$ ), effective range ( $r_0$  in  $a_0$ ), zero energy cross section ( $\sigma$  in  $\pi a_0^2$ ), and the pickoff parameters  ${}_1Z_{\text{eff}}^{(0)}$  and  ${}_1Z_{\text{eff}}^{(1)}$  for Ps-Kr and Ps-Xe scattering. The uncertainty in the effective range fit to  $A$  are about  $\pm 1-2\%$  while the uncertainties in  $r_0$  are about  $\pm 30\%$ . The uncertainties in the fits to  ${}_1Z_{\text{eff}}^{(0)}$  are about  $\pm 1-2\%$  while the uncertainties in  ${}_1Z_{\text{eff}}^{(1)}$  are about  $\pm 30\%$ . The experimental  $\langle {}_1Z_{\text{eff}}^{(0)} \rangle$  are actually thermal averages obtained at room temperature.

System	$A$	$r_0$	$\sigma$	${}_1Z_{\text{eff}}^{(0)}$	${}_1Z_{\text{eff}}^{(1)}$
Ps-He					
FCSVM $\rho = \rho_{av}$ [3]	1.568	0.914	9.83	0.0378	-0.0152
Experiment [27]				$0.125 \pm 0.002$	
Ps-Ne					
FCSVM $\rho = \rho_{av}$ [3]	1.547	1.563	9.57	0.0922	-0.0717
Experiment [27]				$0.235 \pm 0.008$	
Ps-Ar					
FCSVM $\rho = \rho_{av}$ [3]	1.787	2.662	12.77	0.0964	-0.168
Experiment [27]				$0.314 \pm 0.003$	
Ps-Kr					
FCSVM $\alpha_d = 0$	3.18	2.20	40.5	0.0300	0.0247
FCSVM $\rho = \rho_-$	2.26	3.22	24.0	0.0647	-0.122
FCSVM $\rho = \rho_{av}$	1.98	4.02	15.6	0.0913	-0.211
FCSVM $\rho = \rho_+$	1.22	11.6	5.92	0.190	-0.880
$R$ -matrix [4]	3.32		44		
Experiment [27]				$0.478 \pm 0.003$	
Ps-Xe					
FCSVM $\alpha_d = 0$	3.82	2.25	58.5	0.0223	0.0165
FCSVM $\rho = \rho_-$	2.60	3.38	27.1	0.0638	-0.185
FCSVM $\rho = \rho_{av}$	2.29	4.03	20.9	0.0891	-0.318
FCSVM $\rho = \rho_+$	1.50	9.61	9.00	0.172	-0.926
$R$ -matrix [4]	$\approx \pm 1$		$\approx 5$		
Experiment [27]				$1.26 \pm 0.01$	

scattering length by almost 50%. The present calculations reveal an effect of similar magnitude. It is noticeable from Table III that the influence of van der Waals interactions becomes larger as the size of the target atom increases. So despite the fact that the scattering lengths for the fixed core model increase as the target atom gets heavier, there is a compensating trend for the van der Waals interaction to nullify this effect. At this point it is worth noting that a relatively small Ps-atom scattering length is consistent with positron annihilation experiments at high density. In order to explain the high-density positron annihilation data for He

and Ar, recourse is made to the concept of the positronium bubble [22,23]. It is believed that the repulsive interaction between Ps and these two rare gases permits the Ps atom to create a bubble, thus leading to a relatively long-lived component in the spectrum. The analysis of the annihilation spectrum in high-density Xe suggests a scattering length between 1.5 and  $3.0a_0$  [11]. The scattering lengths for the Ps-Xe calculations with polarization also tend to lie within this range.

Besides calculating the phase shifts, the pickoff annihilation parameter,  ${}_1Z_{\text{eff}}$  was also computed. The values listed in Table II were obtained by fitting the raw calculations of  ${}_1Z_{\text{eff}}$

TABLE III. Scattering lengths (in  $a_0$ ) for  $e^-$ ,  $e^+$  and ortho-Ps scattering from the rare gases. The  $e^-$ -atom  $A$  was obtained in the static-exchange approximation and the  $e^+$ -atom  $A$  was obtained in the static approximation. The  $R$ -matrix scattering lengths (in the SE approximation and with 22 Ps states) were estimated from the cross sections plotted in Ref. [4] and are generally assumed to be positive. The FCSVM scattering lengths with the core-polarization potential (labeled With pol) use the polarization potential with  $\rho = \rho_{av}$  [3].

Atom	$e^\pm$ -atom		Ps-atom			
	$e^-$	$e^+$	$R$ -Matrix SE	$R$ -Matrix 22 states	FCSVM $\alpha_d = 0$	FCSVM With pol
He	1.48	0.425	1.91	1.82	1.84	1.57
Ne	1.07	0.774	2.16	2.01	2.02	1.56
Ar	1.49	1.35	2.98	2.83	2.85	1.79
Kr	1.59	1.59	3.32		3.18	1.98
Xe	2.01	1.92	$\sim \pm 1$		3.82	2.29

to the two-term form [3,24]

$${}_1Z_{\text{eff}} = {}_1Z_{\text{eff}}^{(0)} + {}_1Z_{\text{eff}}^{(1)}k^2. \quad (7)$$

The first thing to notice is the small size of  ${}_1Z_{\text{eff}}$  for the two  $\alpha_d=0$  calculations. The largely repulsive interaction prevents the Ps projectile from penetrating any appreciable distance into either atom, leading to the very small values of  ${}_1Z_{\text{eff}}$ . Inclusion of the core-polarization potentials introduces an attractive component into the Ps-atom potential. This allows the Ps projectile to penetrate further into the atomic volume. Despite the increase in the threshold  ${}_1Z_{\text{eff}}$ , the final estimates are still much smaller than the experimental values. Such a result also occurs for Ps-He, Ps-Ne, and Ps-Ar scattering [3]. One reason for this is that no consideration was given to short-range correlations between the positron and electron when  ${}_1Z_{\text{eff}}$  was computed.

However, there is an additional source of uncertainty in the experimental values quoted for  $\langle {}_1Z_{\text{eff}} \rangle$  (the  $\langle \rangle$  notation is used to designate that the experimental value is a thermal average). This parameter is derived from the long-time component in the annihilation spectrum. It has been recently suggested that the spin-orbit interaction (between the atom target and the Ps atom) could provide an additional mechanism for the quenching of Ps [25]. Evidence exists, in the form of a narrow component to the  $2\gamma$  angular correlation spectrum [26,25] to suggest that spin-orbit quenching does indeed contribute to the long-time decay of ortho-Ps. The present calculations give values of  ${}_1Z_{\text{eff}}$  for Xe no larger than 0.20, which is about six times smaller than the experimental  $\langle {}_1Z_{\text{eff}} \rangle$  of  $1.26 \pm 0.01$ . The difference between the  $\rho = \rho_{av}$  values of  ${}_1Z_{\text{eff}}$  and the experimental values listed in Table II become increasing larger as the size of the target atom increases. This is consistent with the idea of spin-orbit quenching since the strength of the spin-orbit interaction will increase as the target atom gets larger.

The other aspect of Table II worth noting is the sign of  ${}_1Z_{\text{eff}}^{(1)}$  for the different models. This parameter is a small positive number for the  $\alpha_d=0$  calculations. This suggests an

increase in kinetic-energy permits the Ps projectile to burrow deeper into the repulsive potential of the atom more effectively and thus the pickoff annihilation increases. This tendency for the  $\alpha_d=0$  calculation to give a positive  ${}_1Z_{\text{eff}}^{(1)}$  was also noted for He, Ne, and Ar. Including the polarization potentials into the calculation leads to a negative  ${}_1Z_{\text{eff}}^{(1)}$  and so in these cases the  $s$ -wave pickoff annihilation rate will decrease with increasing energy.

### III. CONCLUSIONS

To summarize, the stabilization FCSVM has been used to estimate the low-energy  $s$ -wave phase shifts for Ps scattering from Kr and Xe. The results of calculations in the fixed core model for Xe are at variance with  $R$ -matrix calculations [4]. The inclusion of the van der Waals interaction leads to substantial changes in the scattering length for both krypton and xenon. Although there is obviously some uncertainty in the definition of the short range form of the polarization-van der Waals potentials, the magnitude of the reduction in the scattering length gives strong support to the idea that inclusion of the van der Waals potential is necessary for a correct description of Ps-Kr and Ps-Xe scattering.

One interesting feature of the calculations is the tendency for the scattering lengths computed with the polarization potential to remain roughly the same magnitude as the target atom increases in size. The stronger repulsion in the static-exchange calculation of Ps-Xe and Ps-Kr scattering is to a large extent nullified by the increased strength of the van der Waals interaction.

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