Positronium scattering from closed-shell atoms and ions

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The scattering of orthopositronium from He, Ne, Ar, Li^+, Na^+, and K^+ is investigated with the fixed-core stochastic variational method. The scattering length for Ps-He scattering was $1.57a_0$, a value consistent with the threshold cross sections derived from three positron lifetime experiments. The scattering lengths for the Ps-Ne and Ps-Ar systems were $1.55a_0$ and $1.79a_0$, respectively. That there was only a 15% variation among the scattering lengths is compatible with the experiment of Coleman *et al.* [J. Phys. B **27**, 981 (1994)], who found the low-energy cross sections for He, Ne, and Ar to be about the same size. The scattering lengths for Ps scattering from Li^+, Na^+, and K^+ were $12.9a_0$, $28.5a_0$, and $-1.9a_0$. The relatively small magnitude of the Ps-K^+ scattering length strongly supports previous suggestions that the Ps-K^+ system does not support a bound state. The annihilation parameter $^1Z_{eff}$ has also been computed as part of the analysis. The present values of $^1Z_{eff}$ are about 2.5–3 times smaller than the accepted experimental values since short-range electron-positron correlations were not taken into consideration when the annihilation matrix element was evaluated.

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I. INTRODUCTION

The positronium-atom scattering problem is one of the most difficult problems in atomic-collision theory. The source of the difficulty lies in the fact that both the projectile and the target are composite objects with an internal structure. This means that the interaction matrix elements involve multicenter integrals that are difficult and time consuming to evaluate [1]. Particular sources of concern are the evaluation of the exchange matrix element involving the electrons in the target and the electron forming part of the positronium. An even more formidable problem is the inclusion of the Van der Waals interaction between the positronium (Ps) projectile and the atomic target. There have been few calculations of Ps-He scattering that have permitted simultaneous excitation of the He target and the Ps projectile and even then the channel spaces were restricted in size [2].

The motivation for the present investigation is provided by an examination of the available information for the Ps-He system. The different measurements of the threshold cross sections cover a range from $2.6\pi a_0^2$ to $13\pi a_0^2$ [3–6]. Most of the measurements of the cross section are indirect determinations at threshold, derived from the analysis of positron-lifetime experiments. Only in the last few years has it been possible to make beams of Ps suitable for scattering experiments [7]. However, the beam experiments on Ps-He scattering have been done at energies greater than 10 eV [7], and so cannot be used to resolve the discrepancies in the crucial threshold region. Similarly, there is also a good deal of variation in the different calculations of Ps-He scattering [8–17,19] with recent calculations giving threshold cross sections ranging from $3.3a_0^2$ [13] to $13\pi a_0^2$ [16]. A reasonable assessment of the current situation for Ps-He scattering is that there is some confusion as to the precise value of the threshold cross section [20].

In this article, a modification of the fixed-core stochastic variational method [21–26] (FCSVM) is applied to the calculation of Ps-atom scattering from the rare gases He, Ne, and Ar, and the closed-shell alkali ions Li^+, Na^+, and K^+ for the $L=0$ partial wave. While there have been experiments quoting cross sections for Ps-Ne and Ps-Ar scattering [3,6,27,28], there have been only a few calculations [14,29]. The application of the FCSVM to Ps-He scattering has been described previously in an abbreviated form [21]. Extension of the method to neon and argon was very easy and the additional calculations took hardly any computer time. Besides determining the scattering phase shifts, the parameter characterizing the pick-off annihilation rate, namely, $^1Z_{eff}$, has been been reported for He, Ne, and Ar. The scattering of Ps from the positive ions, Li^+, Na^+, and K^+ was studied in order to highlight the link to bound states of the positron-atom complex. There have been no scattering calculations of the Ps-Li^+, Ps-Na^+, or Ps-K^+ systems at threshold energies as such, although there have been a number of calculations of the cross sections for the alternative e^+-alkali entrance channel [30,31].

II. CALCULATION TECHNIQUE

The method as applied is not a traditional scattering calculation, rather it uses stabilization ideas [21,32–36] to extract the phase shifts from the positive-energy pseudocontinuum that results from the SVM diagonalization of the Hamiltonian. A more detailed exposition of the method has been given recently [36], so the present discussion is somewhat abbreviated. The SVM uses explicitly correlated Gaussians (ECGs) as basis functions, viz.,

$$\Psi = \exp\left(-\frac{1}{2} \sum A_{ij} \mathbf{x}_i \mathbf{x}_j \right), \tag{1}$$

$\mathbf{x}_i$ being coordinates of the ith particle, and has the advantage that evaluation of the exchange (and other) matrix elements is easily accomplished.

The present calculation scheme is now described. The configuration space is divided into two regions, an inner or interaction region and a scattering region. In the inner region,

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the SVM is used to define an ECG basis (of dimension K) that gives an accurate solution of the Schrodinger equation for the lowest-energy state. For a system like Ps-Li^+, which supports a bound state, this amounts to a standard bound-state calculation. However, the Ps-He system does not support a bound state and the procedure must be modified. In this case the exponents α_i of the Gaussians connecting the electron and positron to the nucleus are restricted to be larger than a certain minimum size, say $\alpha_i > 0.01$. This constrains the electron and positron to be localized reasonably close to the nucleus and results in an SVM iteration procedure that effectively solves the Schrödinger equation in some sort of box.

Once the inner wave function has been obtained, a set of ECGs designed to represent positive-energy Ps were added to the basis. First an 8-Gaussian representation of the P ground state $\Phi_P(\mathbf{r}_0,\mathbf{r}_1)$, where $\mathbf{r}_0$ and $\mathbf{r}_1$ are the positron and electron coordinates, was constructed (the energy obtained was $-0.249\,997\,2$ hartree). Then a series of ECGs were constructed by multiplying the Ps Gaussians with a Gaussian with the Ps center-of-mass coordinate as its argument,

$$\Phi_{ij} = \phi^j_{Ps}(\mathbf{r}_0,\mathbf{r}_1)\exp(-\beta_i R^2), \tag{2}$$

where $\mathbf{R}$ is the coordinate of the center of mass of the Ps atom and ϕ^j_{Ps} is one of the Gaussians used in the expansion of the Ps ground state. The exponents β_i of the center-of-mass Gaussians were chosen to form an even-tempered sequence, viz.,

$$\beta_i = \frac{\beta_1}{T^{i-1}}. \tag{3}$$

Numerical experiments have shown that the factor T should be made as close to 1.0 as possible [36]. In all the calculations reported in this work β_1 was set to 3.84, T was chosen to be 1.40 and 30 values of β_i were used. With this choice the smallest value of β_1 was about 1.6×10^{-4}. This choice of β_1 and T was based on considerations discussed in [36] and numerical experiments performed during the present series of calculations.

The inner and outer basis functions were then checked for linear dependence and ECGs having large overlaps with existing basis functions were excluded giving a final basis of dimension M. The basis was diagonalized by standard techniques and the phase-shift information extracted.

The overlap of the Ps ground state with the positive-energy pseudostate was computed at a succession of values of R, the Ps center-of-mass coordinate. Effectively, the positive-energy wave functions $\Psi(\mathbf{r}_0,\mathbf{r}_1)$ were multiplied by $\delta[(\mathbf{r}_0+\mathbf{r}_1]/2-\mathbf{R})\Phi_{Ps}(\mathbf{r}_0,\mathbf{r}_1)$ and integrated over all coordinates. Then a least-squares fit over $R\in[10,25]a_0$ to $B\sin(kR+\delta_0)/k$ was used to extract the phase shift.

A useful diagnostic check of basis quality was to compare the magnitude of the electron-nucleus and positron-nucleus correlation functions over the radial values of interest. They generally agreed to better than 0.1%

Once the amplitudes and phase shifts have been obtained, it was also possible to compute the annihilation parameter for pick-off annihilation, namely, $^1Z_{eff}$. This parameter is derived from experiment from the identity [37]

$$\lambda_p = \lambda_{o\text{-}Ps} + 0.804 n\, {}^1Z_{eff}. \tag{4}$$

In this equation, λ_p is the decay rate directly measured from experiment, $\lambda_{o\text{-}Ps}$ is the decay rate of orthopositronium ($\sim 7.21\times10^6$ s^{-1}), and n is the gas density in amagat units.

For a system consisting of orthopositronium interacting with a closed-shell system, the annihilation parameter can be written as

$${}^1Z_{eff} = \frac{1}{4}\int d^3r\, d^3x\, \rho(\mathbf{r})|\Psi(\mathbf{r},\mathbf{x})|^2, \tag{5}$$

where $\rho(\mathbf{r})$ is the electron density of the closed-shell target and $\Psi(\mathbf{r},\mathbf{x})$ is the Ps-scattering wave function (with $\mathbf{x}$ as the electron coordinate). The factor of $\frac{1}{4}$ reflects the fact that only electrons in a spin-singlet state with the positron contribute to the decay process (assuming all annihilation events are 2γ decays.) This expression is simpler than that used by other authors [8] since the present scattering wave function has been constructed so that the overlap integral between the core wave function and scattering wave function is effectively zero. In the plane-wave Born approximation, $^1Z_{eff}$ reduces to $N/4$, where N is the number of closed-shell electrons.

The existing FCSVM program used for the calculation automatically computes Eq. (5) every time a calculation is performed. Therefore $^1Z_{eff}$ was simply determined by converting the program output from bound-state normalization to continuum normalization. In effect, this amounted to dividing the output of the FCSVM program by B^2k^2. The validity of this procedure was easily verified by doing a calculation with the interaction potential between the target and Ps projectile set to zero. Such a calculation is equivalent to a plane-wave Born approximation (in the $L=0$ partial wave) and at low energies should give $^1Z_{eff}=N/4$. The tests on He, Ne, and Ar all gave values of the threshold $^1Z_{eff}$ within 0.5% of the expected limit of $N/4$.

A. The FCSVM Hamiltonian

The FCSVM has been used to describe the interaction of the projectile with the atom or ion [26]. The FCSVM replaces the full Hamiltonian for the N_e electrons and a positron, by a model Hamiltonian with the core electrons removed, viz.,

$$H = -\frac{1}{2}\nabla_0^2 - \frac{1}{2}\nabla_1^2 - V_{dir}(\mathbf{r}_0) + V_{dir}(\mathbf{r}_1) + V_{p1}(\mathbf{r}_0) + V_{p1}(\mathbf{r}_1)$$
$$+ V_{exc}(\mathbf{r}_1) - \frac{1}{r_{01}} + V_{p2}(\mathbf{r}_1,\mathbf{r}_0) + \lambda\hat{P}. \tag{6}$$

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

$$\lambda \hat{P} = \sum_{i=1} \lambda |\phi_i\rangle\langle\phi_i| \tag{7}$$

is an orthogonalizing pseudopotential that acts to produce wave functions orthogonal to the occupied core orbitals provided λ is a large positive number [38,39]. It (λ) was set to 5×10^4 hartree for the present calculations.

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

$$V_{p1}(r) = -\frac{\alpha_d g^2(r)}{2r^4}. \tag{8}$$

The factor α_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

$$g^2(r) = 1 - \exp(-r^6/\rho^6), \tag{9}$$

where ρ is an adjustable parameter. The two-body polarization potential V_{p2} is defined as

$$V_{p2}(\mathbf{r}_0, \mathbf{r}_1) = \frac{\alpha_d}{r_0^3 r_1^3}(\mathbf{r}_0 \cdot \mathbf{r}_1) g(r_0) g(r_1). \tag{10}$$

Inclusion of the two-body potential ensures that the polarization interaction reduces to a Van der Waals–type interaction when the Ps is at large distances from the nucleus.

The choice of the cutoff parameter is the chief source of uncertainty in the calculations since it can be tuned to the electron-atom interaction or the positron-atom interaction. For the Li^+, Na^+, and K^+ systems ρ was chosen so that the binding energies and spectra of neutral Li, Na, and K agreed with experiment [26,40,41]. These values of ρ are denoted as ρ_- to signify the fact that they are tuned to the e^--ion interaction. Little is known about e^+-ion interactions since there have hardly been any calculations of positron scattering from positive ions. Therefore the only core-polarization calculations for Li^+, Na^+, and K^+ were performed with $\rho = \rho_-$. The values of ρ_- and α_d for these systems are listed in Table I.

Two sources of information can be used to tune the values of ρ for He, Ne, and Ar. In the case of the electrons, ρ can be determined by solving the Schrödinger equation for the Hamiltonian

$$H = -\frac{1}{2}\nabla_1^2 + V_{p1}(\mathbf{r}_1) + V_{dir}(\mathbf{r}_1) + V_{exc}(\mathbf{r}_1) + \lambda \hat{P}. \tag{11}$$

Then ρ_- was tuned to give phase shifts in reasonable agreement with high-quality *ab initio* calculations [42–47], which are, in turn, in good agreement with momentum-transfer cross sections derived from swarm experiments [48–51]. For all practical purposes, this method of determining ρ_- contains the same physical content as tuning ρ_- to the binding energies of Li, Na, and K. However, it is also possible to tune ρ to the results of positron-atom scattering calculations. In the case of He, close to exact phase shifts have been computed by Van Reeth and Humberston [52]. For neon and argon, recourse is made to polarized-orbital (PO) phase shifts [53,54] since these appear to be the best calculations, and the available cross-section measurements do not permit a precise determination of the threshold cross sections. However, the temperature dependence of the annihilation parameter Z_{eff} is sensitive to the energy dependence of the positron-atom scattering cross section. A comparison of the temperature dependence predicted by the PO calculations has been shown to be broadly consistent with the experimental data for Ne and Ar [55]. The values of ρ derived from the e^+-atom scattering lengths are denoted as ρ_+. Values of α_d, ρ_-, and ρ_+ for He, Ne, and Ar are given in Table I. It is noticeable that the values of ρ_+ are all much smaller than those of ρ_-. The smaller value of ρ_+ indicates that the strength of the positron-atom polarization potential is stronger than the strength of the electron-atom polarization potential.

TABLE I. Parameters defining of the polarization potential. The dipole polarizability α_d is given in terms of a_0^3 while the cutoff parameter ρ is given for both electron (ρ_-) and positron (ρ_+) scaling. The parameter ρ_{av} is the average of the electron and positron parameters.

System	α_d	ρ_-	ρ_+	ρ_{av}
H (triplet channel)	4.5	5.05	2.05	3.55
He	1.383	2.40	1.50	1.95
Ne	2.67	2.10	1.50	1.80
Ar	11.1	2.45	1.70	2.08
Li^+	0.1925	1.40		
Na^+	0.99	1.48		
K^+	5.47	2.10		

Besides tuning the calculations to the electron or positron data, calculations have also been done with the ρ set for the arithmetic mean of these two values, i.e., for $\rho_{av} = (\rho_- + \rho_+)/2$. In order to make a definite statement for atomic targets, the calculation with ρ_{av} is chosen as the best estimate, and the calculations with ρ_- and ρ_+ are regarded as giving reasonable upper and lower limits on the possible variations of the phase shifts.

III. Ps SCATTERING FROM He

The Ps-He system is the most intensively studied of all the Ps-atom scattering systems and there have been four different estimates of the threshold cross section from positron-lifetime experiments [3–6]. The only beam experiment was at energies too high to be of relevance to the present work [7]. A compilation of the threshold cross sections from these experiments is given in Table II.

On the theoretical side, the situation is best described as confused. The first calculations were performed in the static-exchange approximation [8] The static-exchange approximation allows for direct and exchange scattering between the atomic target and the projectile, but does not allow for any distortion of the Ps or He atoms. The first estimate of the scattering length, $2.17a_0$ was the result of a poorly con-

TABLE II. The scattering length and effective range (in terms of a_0) for Ps-He scattering. Also tabulated are the results of some Ps-H calculations in the electron spin-triplet channel. The threshold cross section σ (in terms of πa_0^2) is also tabulated for all calculations and for a number of experiments.

Method	A	r_0	σ
Ps-He calculations			
Static exchange [8]	2.17		18.8
(Updated) static exchange [9]	1.882	0.94	11.9
Static exchange [10]	1.80		13.0
Static exchange and Van de Waals [11]	1.61		10.4
Kohn variational model static exchange [17]	1.72		11.9
Kohn variational model exchange [17]	1.39		7.73
R-matrix static-exchange [16]	1.91		14.58
R-matrix 22 Ps states [16]	1.82		13.19
T-matrix model static exchange [14]	1.03		4.24
T-matrix three Ps states model exchange [13]	0.91		3.34
T-matrix static exchange [2]	1.93		14.90
T-matrix three Ps states [2]	1.92		14.75
T-matrix two Ps and three He states [2]	1.360		7.40
Present FCSVM $\alpha_d=0$	1.840	0.619	13.54
Present FCSVM $\rho=\rho_-$	1.625	0.916	10.56
Present FCSVM $\rho=\rho_{av}$	1.568	0.914	9.83
Present FCSVM $\rho=\rho_+$	1.482	0.894	8.79
Ps-He experiments			
Skalsey *et al.* [3]			2.6 ± 0.5
Canter *et al.* [4]			8.4 ± 0.9
Coleman *et al.* [6]			9.0
Nagasihma *et al.* [5]			13 ± 4
Ps-H calculations (triplet)			
R-matrix 22 Ps states [62]	2.45	1.32	24.01
Present FCSVM $\alpha_d=0$	2.44	1.30	23.81
Present FCSVM $\rho=\rho_-$	2.31	1.29	21.34
Present FCSVM $\rho=\rho_{av}$	2.19	1.35	19.18
Present FCSVM $\rho=\rho_+$	1.88	1.27	14.14
Ab initio SVM [36]	2.22	1.29	19.71

verged calculation [8], an improved calculation subsequently gave an estimate of $1.882a_0$, [9,17,18]. A later Kohn-variational calculation included the influence of Ps distortion, but used a model exchange interaction to simplify the calculation [17]. The resulting scattering length was $1.39a_0$. The calculations of Barker and Bransden were notable in that they included an adiabatic Van der Waals potential into their calculations [10,11]. Their estimate of the static-exchange scattering length was $1.80a_0$ which was reduced to $1.61a_0$ [11] upon inclusion of the Van der Waals potential. It should be noted that all of these earlier calculations used a relatively simple model for the He ground state (it was represented by a single Slater-type orbital). There was a long hiatus before the modern generation of calculations was started by three groups.

Blackwood *et al.* used the *R*-matrix method to calculate Ps-He cross sections from 0 to 40 eV in a variety of approximations [16]. In the first instance their calculation in the static-exchange approximation gave a scattering length of $1.91a_0$. This scattering length is significantly different from the earlier values. One possible explanation would be the different structure of the helium wave function: Blackwood *et al.* used a Hartree-Fock wave function instead of a single Slater-type orbital. In their largest calculation, Blackwood *et al.* allowed for the distortion of the Ps projectile by using a channel space of 22 coupled pseudostates. Within its limitations (no distortion of the He target), the 22-state *R*-matrix calculation should be close to converged. The scattering length of this larger calculation was $1.82a_0$. One of the notable features of the *R*-matrix calculations was the small difference between the static-exchange and 22 state calculations.

Ghosh and co-workers used the momentum-space *T* matrix to determine the cross sections in a variety of small-dimension channel spaces [2,19]. Most significantly, they have performed a static-exchange calculation that gave a scattering length of $1.93a_0$, in good agreement with the *R*-matrix value (it is noted that they did their static-exchange calculation prior to the *R*-matrix calculation). When they allow for limited distortion of the Ps projectile, by doing a three-state calculation with the Ps$(1s)$, Ps$(2s)$, and Ps$(2p)$ states, the scattering length hardly changes. Once again this

result is consistent with the *R*-matrix calculation. They have also investigated the influence of He-target excitations by including the He $1s2s\,{}^1S^e$ and $1s2p\,{}^1P^o$ states in the channel space. The inclusion of these target excitations resulted in a dramatic drop in the scattering length, which effectively halved the threshold cross section. During this latter calculation, Ghosh and co-workers assumed that their target excited-state wave functions (taken from Winter and Lin [56]) are exact eigenstates. The extent to which this assumption can lead to systematic errors in high-precision calculations at low energies is currently unknown.

Adhikari and co-workers also used the moment-space *T*-matrix method to solve the equations of motion for Ps-He scattering. There seem to be significant problems with their calculations. In the first instance their static-exchange scattering length of $1.03a_0$ [14] was almost a factor of 2 different from any value previously computed. In the second, they find that inclusion of Ps channels leads to a further decrease in the scattering length, with a value of $0.91a_0$ being achieved by the largest calculation [13]. These results are completely different from those of Ghosh and co-workers using exactly the same method to solve the Schrödinger equation. The problem with the calculations of Adhikari and co-workers seems to arise from the fact that they used a model exchange interaction of dubious validity. Due to computational difficulties associated with the evaluation of the Ps-He exchange interaction, Adhikari and Biswas replaced the exact exchange matrix element by a simplified approximation with an adjustable parameter. The adjustable parameter in their model exchange interaction was fixed by reference to e^--He scattering. However, rather than tuning the free parameter to the e^--He scattering length in the static-exchange approximation, in [14] they tune the parameter so as to reproduce the exact phase shifts of the e^--He system [14]. In [12], the free parameter is tuned so as to reproduce the cross section obtained by Skalsey *et al.* [3]. In effect they are also using their model exchange interaction to incorporate the influence of the core-polarization potential and to compensate for a channel space of limited size. Questions about the overall validity of the model exchange calculations of Adhikari and co-workers have been raised previously [16,20,36].

The present FCSVM calculations of Ps-He scattering were based on an inner-wave basis with dimension $K=240$. The final basis ($M=469$) was obtained when the asymptotic basis functions were included and all linearly dependent terms eliminated. The same ECG basis was used for all calculations of the Ps-He system. The first calculation was done with $\alpha_d=0$. This calculation allows for direct and exchange scattering of the electron and positron with the He atom, permits the distortion of the Ps projectile, but does not allow for any distortion of the He atom during the scattering event. The physical content of the $\alpha_d=0$ FCSVM calculations and the 22-state *R*-matrix calculation are similar. Therefore, it is to be expected that these two calculations would be in agreement, and this is indeed found to be the case. The present SVM scattering length of $1.84a_0$ could hardly be any closer to the *R*-matrix scattering length of $1.82a_0$ [16].

The scattering lengths were derived from the phase shifts by performing a least-squares fit of $k\cot(\delta)$, using effective-range theory (ERT). To be precise, the right-hand side of the expression

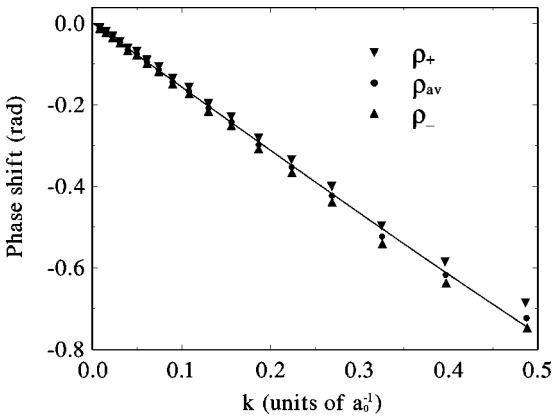

FIG. 1. The Ps-He *s*-wave phase shifts as a function of k (in units of a_0^{-1}). The phase shifts are shown with three model potentials, one with ρ tuned to electron-atom scattering, one to positron-atom scattering, and the middle points were computed with $\rho=\rho_{av}$. The solid curve shows the effective-range fit to the $\rho=\rho_{av}$ phase shifts.

$$k\cot\delta(k)=-\frac{1}{A}+\frac{1}{2}r_0k^2+O(k^4) \tag{12}$$

has been fitted to the values of $k\cot(\delta)$ extracted from the FCSVM calculation. The inclusion of the polarization interactions resulted in a modest reduction in the magnitude of the scattering length (values are listed in Table II). Depending on whether ρ_-, ρ_+, or ρ_{av} is chosen, one ends up with scattering lengths that range from $1.63a_0$ to $1.48a_0$. The scattering length for the ρ_{av} calculation was $1.568a_0$ and the effective range was $0.91a_0$. The uncertainty in the value of the scattering length derived from the fit is of the order of 1%. Extracting the effective range from the data was problematic since it was small and the uncertainty here was about $\pm 30\%$. The effective-range fit to the phase shifts for the ρ_{av} curve is shown in Fig. 1.

The modest reduction in the scattering length following inclusion of the core-polarization potentials is in agreement with the earlier calculations by Barker and Bransden [10,11] and an assertion by Blackwood *et al.* [16]. Barker and Brandsden found that inclusion of an adiabatic Van der Waals potential reduced the scattering length by $0.20a_0$, an estimate that is compatible with the present results. The assertion by Blackwood *et al.* [16] was not made on the basis of any quantitative information, rather it was based on criteria best described as subjective. Nevertheless, the present results are certainly supportive of their view. The inclusion of the two-body polarization potential had a big influence upon the calculations and drastically reduced the impact of the polarization potentials. The omission of the two-body polarization interaction results in a scattering length of $A\approx 1.0a_0$ for $\rho=\rho_{av}$.

The calculation with $\rho=\rho_{av}$ gave a threshold cross section of $9.83\pi a_0^2$. This cross section strongly favors the older experiments that give larger values for the threshold cross

section, namely, $(8.4\pm0.9)a_0^2$ [4], $9.0a_0^2$ [6], and $(13\pm4)\pi a_0^2$ [5]. The present FCSVM is more or less compatible with all of these measurements. A recent smaller estimate of the cross section, $(2.6\pm0.5)\pi a_0^2$, at about 1 eV energy [3] by Skalsey *et al.* is effectively excluded since the present phase shifts give a cross section of about $8.4\pi a_0^2$ at this energy. There will of course be some uncertainty in the threshold cross section related to the fact that ρ is not known precisely. Using $\rho=\rho_-$ $(2.40a_0)$ results in a threshold cross section of $10.6\pi a_0^2$, while using $\rho=\rho_+$ $(1.50a_0)$ gave a threshold cross section of $8.8\pi a_0^2$. Although, there is a 20% scatter in the threshold cross section, the results are still incompatible with the cross section of Skalsey *et al.* [3], irrespective of whether ρ_-, ρ_+, or ρ_{av} was used.

The semiempirical nature of the core-polarization potential naturally raises questions about its accuracy. Fortunately, reference to calculations of the binding energies of e^+-He $(^3S^e)$ $(\equiv$Ps-He$^+)$ [57,58] and e^+-Li $(\equiv$Ps-Li$^+)$ [26,40] scattering shed light on this issue. These systems can be characterized as positronium interacting with a residual ion, and they are analogs of the Ps-atom scattering systems. Both systems have only a few particles, and therefore comparisons between the *ab initio* SVM and the semiempirical FCSVM binding energies can be used to test the overall validity of the FCSVM-model Hamiltonian. The FCSVM binding energy for e^+-He$(^3S^e)$ scattering was 0.000 586 3 hartree [58], about 1% smaller than the close-to-exact SVM binding energy of 0.000 592 4 hartree [58]. The FCSVM binding energy was computed with a polarization cutoff parameter derived from an analysis of the He$(1s\,nl)^3L$ energy spectrum. In the language of the present paper, the e^+-He$(^3S^e)$ calculation was done with $\rho=\rho_-$. The inclusion of the polarization potential was important in obtaining a correct estimate of the binding energy as its omission from the calculation gave a binding energy of 0.000 493 1 hartree [57]. The FCSVM binding energy for e^+-Li scattering of 0.002 477 hartree [40] is about 0.2% smaller than the latest estimate of the SVM binding energy of 0.002 473 hartree [59]. The SVM binding energy is not converged, and it is likely that the converged SVM binding energy will be slightly larger than the FCSVM binding energy. These two comparisons suggest that the FCSVM model Hamiltonian with $\rho=\rho_-$ probably slightly underestimates the strength of the polarization potential.

We have also applied the present method using a semiempirical Van der Waals–type potential to the calculation of Ps-H scattering in the channel with the two electrons in a triplet state (the triplet channel was chosen since it more closely resembles the physics of Ps-He scattering than the singlet channel). The collision is treated in a fixed-core model, with the hydrogen target represented by the $1s$ ground state. The scattering length for triplet Ps-H scattering [21,36] has been computed in a purely *ab initio* calculation giving $2.22a_0$ and therefore can be used as an additional test of the procedure used to construct the core-polarization potentials. The polarizability of hydrogen is $4.5a_0^3$ and ρ_- and ρ_+ were tuned to the scattering lengths for positron-hydrogen scattering $(-2.10a_0$ [60]) and triplet electron-hydrogen scattering $(1.77a_0$ [61]). The scattering lengths of the ρ_+, ρ_-, and ρ_{av} calculations and a calculation with $\alpha_d=0$ are also listed in Table II. The *ab initio* scattering length of $2.22a_0$ lies in the range bounded by the ρ_- and ρ_+ scattering lengths and the ρ_{av} scattering length of $2.19a_0$ is within 2% of the *ab initio* scattering length. It is also worth noting that the $\alpha_d=0$ scattering length is almost the same as the scattering length from the 22-state *R*-matrix calculation by Campbell *et al.* [62]. This further suggests that the present calculations are numerically reliable.

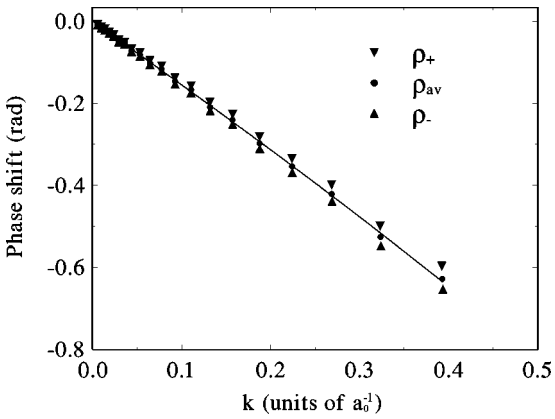

FIG. 2. The Ps-Ne s-wave phase shifts as a function of k (in units of a_0^{-1}). The phase shifts are shown for three model potentials, the lower points were computed with $\rho=\rho_-$, the upper points with $\rho=\rho_+$, and the middle set were computed with $\rho=\rho_{av}$. The solid curve shows the effective-range fit to the $\rho=\rho_{av}$ phase shifts.

We believe that a consensus about the precise value of the threshold Ps-He cross section is beginning to emerge. On the theoretical side, calculations by a number of different groups are giving the same scattering lengths provided the physical content of the models are the same. For example, the present FCSVM calculations with $\alpha_d=0$ upon Ps-He and Ps-H (triplet) scatterings with $\alpha_d=0$ agree with the 22-state *R*-matrix calculations. In addition, the present calculation with its threshold cross section of $9.83\pi a_0^2$ is consistent with three experiments and is also consistent with the expectations expressed by Blackwood *et al.*

We note now that Adhikari *et al.* noted a relation between the size of the pick-off annihilation parameter $^1Z_{eff}$ and the scattering length. A discussion of the implications of this result is postponed to a later section.

IV. Ps SCATTERING FROM Ar AND Ne

The only published account of Ps scattering from the heavier rare gases at threshold is that by Adhikari and Biswas who used the momentum space *T*-matrix technique to solve the static-(model) exchange equations for Ps scattering from neon and argon [14]. The present calculations of these systems use a basis set formed in essentially the same way as described above for He. The basis for neon had $K=250$ and $M=484$. The basis for argon had $K=260$ and $M=496$.

The phase shifts for different calculations on neon and argon are displayed in Figs. 2 and 3, respectively. Once again, phase shifts were shown for polarization potentials

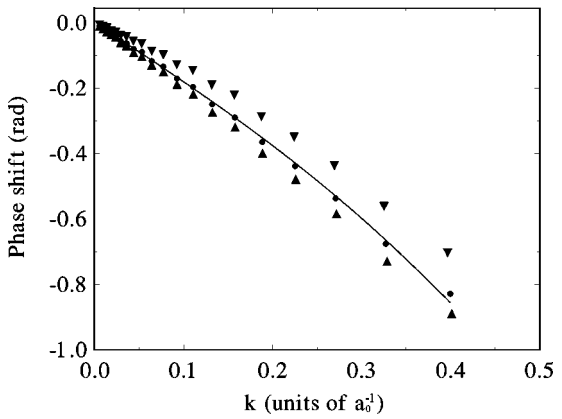

FIG. 3. The Ps-Ar s-wave phase shifts as a function of k (in units of a_0^{-1}). The phase shifts are shown for three model potentials, the lower points were computed with $\rho=\rho_-$, the upper points with $\rho=\rho_+$, and the middle set were computed with $\rho=\rho_{av}$. The solid curve shows the effective-range fit to the $\rho=\rho_-$ phase shifts.

using all three values of ρ. The ERT fits displayed in the figures were done for the calculations with $\rho=\rho_{av}$. The values of A and r_0 derived from the fits are given in Table III.

For neon, the $\alpha_d=0$ calculation gave a scattering length of $2.02a_0$, while the ρ_{av} calculation gave $1.55a_0$. The decrease in the scattering length is about twice as large as the decrease between the equivalent pair of calculations for helium. This is not surprising since the polarizability for neon, $2.67a_0^3$ is about twice as large as that for helium. The model potential T-matrix calculation in the static-exchange approximation by Adhikari and Biswas gave the smallest scattering length of $1.41a_0$. The static-exchange approximation does not have the variational flexibility of the FCSVM calculation and therefore should give a scattering length that is larger than any of the FCSVM values. Taking into consideration previous comments on helium, one concludes that the small static-exchange scattering length of Adhikari and Biswas is nothing more than an artifact of their model exchange potential.

TABLE III. The scattering length and effective range (in terms of a_0) and threshold cross section for Ps-Ne and Ps-Ar scattering. Although the value of A and r_0 are quoted to four significant digits, the inherent uncertainties associated with the ERT fits are larger than indicated by the quoted precision. The uncertainty in A is about $\pm 0.02a_0$ while the uncertainties in r_0 are about $\pm 30\%$.

System	A	r_0	σ
Ps-Ne calculations			
Present FCSVM $\alpha_d=0$	2.018	0.858	16.12
Present FCSVM $\rho=\rho_-$	1.616	1.430	10.45
Present FCSVM $\rho=\rho_{av}$	1.547	1.563	9.57
Present FCSVM $\rho=\rho_+$	1.460	1.510	8.53
T-matrix static model exchange [14]	1.41		7.95
Skalsey *et al.* [3]			6.5 ± 0.9
Coleman *et al.* [6]			9.0
Nagashima *et al.* [27]			11.4 ± 8.0
Ps-Ar calculations			
Present FCSVM $\alpha_d=0$	2.847	1.744	32.8
Present FCSVM $\rho=\rho_-$	1.984	2.382	15.75
Present FCSVM $\rho=\rho_{av}$	1.787	2.662	12.77
Present FCSVM $\rho=\rho_+$	1.301	4.541	6.77
T-matrix static model exchange [14]	1.65		10.9
Skalsey *et al.* [3]			7.4 ± 1.5
Coleman *et al.* [6]			9.0
Nagashima *et al.* [28]			17 ± 11

The argon atom has a dipole polarizability about four times larger than neon (seven times larger than helium) and therefore can be expected to have the largest degree of variation in the calculated scattering lengths. The values of the scattering length ranged from $1.98a_0$ (ρ_-) to $1.30a_0$ (ρ_+) with the best estimate being $1.79a_0$ (ρ_{av}). This leads to a factor of 2 variation in the threshold cross section. The polarizability of argon is sufficiently large so that the uncertainties in the definition of the core-polarization potential have a major impact on the predicted cross section. The one result that is unequivocal is that inclusion of the polarization potential does have a significant impact on the threshold cross section; the calculation with no polarization potential gave a threshold cross section of $32.8\pi a_0^2$, which is twice as large as any of the other cross sections.

The calculations for He, Ne, and Ar reveal an interesting trend. There is a tendency for the model Hamiltonian with $\alpha_d=0$ to give larger scattering lengths as the atomic size increases from helium to argon. However, the scattering lengths of the $\rho=\rho_{av}$ models are all roughly the same size. The increased Ps-atom exchange repulsion for the larger atoms was counterbalanced by the stronger Van der Waals attraction. This result is consistent with the experiment of Coleman *et al.* [6]. They found that the low-energy Ps-atom cross sections for He, Ne, and Ar could be characterized by the formula $\sigma=(9.0-0.5E)\pi a_0^2$ (with E in eV).

V. Ps SCATTERING FROM ALKALI IONS

Two calculations were performed for the three alkali systems. The initial calculation was performed without the core-polarization potential. As mentioned earlier in the discussion on Ps-He scattering, this calculation can be expected to underestimate the strength of the Van der Waals interaction between the Ps atom and residual ion core. In the primary calculation, the parameters of the polarization potential were set to the values quoted in Table I.

The method used to extract the phase shifts had to be modified for these charged systems. The polarization of the Ps-atom by the residual ion is quite strong, and therefore the use of $B\sin(kR+\delta)$ as a fitting function is not justified at distances with $R\in[10,25]a_0$. Instead the fit was done to an asymptotic function that included the polarization of the Ps atom due to the $-\alpha_d/(2R^4)$ field of the residual-ion superposition.

A. Ps-Li^+ scattering

The scattering calculation for the Ps-Li^+ system ($K=170$, $M=382$) was based upon an existing wave function

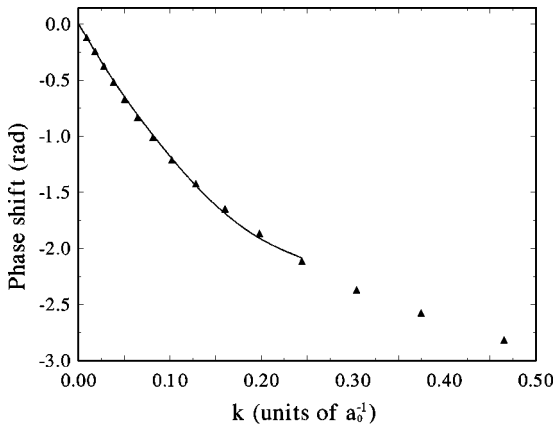

FIG. 4. The Ps-Li^+ s-wave phase shifts as a function of k (in units of a_0^{-1}). The solid line shows a fit to the ρ_- phase shifts using MERT.

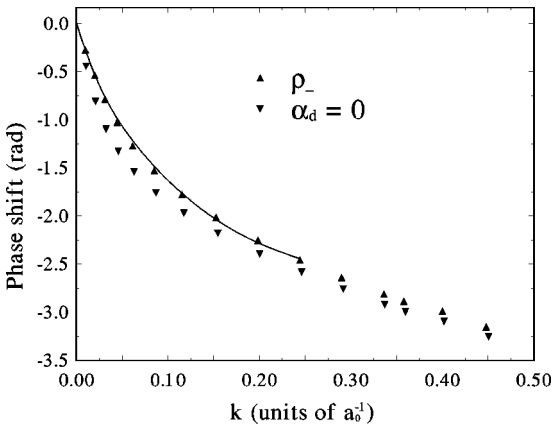

FIG. 5. The Ps-Na^+ s-wave phase shifts as a function of k (in units of a_0^{-1}). The solid line shows a fit to the ρ_- phase shifts using MERT.

for the Ps-Li^+ ground state [26,40]. The phase shifts with the core-polarization potential are shown in Fig. 4. Phase shifts without the polarization potential were not plotted since they were very close to the polarization phase shifts and to include them in the figure would make it more difficult to interpret.

The potential for a Ps atom scattered in the field of a positive charge has a long-range polarization potential. Therefore a modified form of the effective-range theory [50,51,63] (MERT) should be used in the phase-shift analysis. The MERT expansion for a P atom scattered in the field of a positive charge is

$$k\cot\delta(k) = -\frac{1}{A} + \frac{\alpha_d \pi k}{3A^2} + \frac{2\alpha_d k^2}{3A}\ln\frac{\alpha_d k^2}{16} + Bk^2 + Ck^3 + O(k^4), \tag{13}$$

where $\alpha_d = 72a_0^3$ is the effective polarizability of the Ps atom in the field and A is the scattering length. A fit from $k=0$ to $k=0.2a_0^{-1}$ gave $A=12.936$, $B=7.748$, and $C=-27.361$ and these values were used in creating the solid line in Fig. 4. The range over which the fit was valid was relatively small, being confined to the $k\in[0,0.2]a_0^{-1}$ interval. This appears to be a consequence of the large polarizability associated with this system. The scattering length should be regarded as having an uncertainty of $\pm 3\%$. The fluctuations of the phase shifts and the large contributions made by the long-range terms in Eq. (13) contributed to the relatively large uncertainty. The scattering length of the $\alpha_d=0$ calculation was $A=13.85a_0$. This is consistent with bound-state calculations of the e^+-Li system, which predict that omission of the core-polarization potential leads to a smaller binding energy [26,40].

B. Ps-Na^+ scattering

The basis set for the Ps-Na^+ system was based on an existing wave function for positronic sodium [26,40] and the dimensions were $K=250$ and $M=460$. The phase shifts for the calculations with and without polarization potential are shown in Fig. 5.

The values of A, B, and C obtained from the fit to Eq. (13) were 28.471, 6.6068, and -7.525, respectively. The e^+-Na system is very weakly bound with a binding energy of 0.000 473 hartree [26,40], so a large scattering length is expected. Once again the range over which the MERT fit was valid was restricted to a relatively small range. The uncertainty in the scattering length was about $\pm 1a_0$. The scattering length for the $\alpha_d=0$ calculation was $45.6a_0$ with an uncertainty of $\pm 2a_0$.

C. Ps-K^+ scattering

The basis dimension for K^+ contained $K=220$ inner basis functions, which was increased to $M=430$ after the 240 outer basis functions were added to the basis. Attempts to demonstrate the existence of an electronically stable state of the e^+-K system have not been successful and it is thought that this system does not support a bound state [26,64,65]. This results in the k dependence of the Ps-K^+ phase shifts is

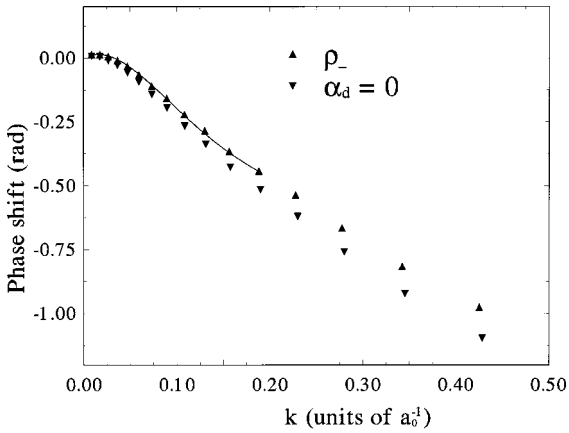

FIG. 6. The Ps-K^+ s-wave phase shifts as a function of k (in units of a_0^{-1}). The solid line shows a fit to the ρ_- phase shifts using MERT.

TABLE IV. The scattering lengths (in terms of a_0) for Ps-Li^+, Ps-Na^+, and Ps-K^+ scatterings.

System	Present FCSVM ($\alpha_d=0$)	Present FCSVM ($\rho=\rho_-$)	Estimation using ERT from binding energy	Model potential
Ps-Li^+	13.8	12.9	10.05	12.3
Ps-Na^+	45.6	28.5	23.0	27.5
Ps-K^+	−1.36	−1.93		

shown in Fig. 6 being completely different from Ps-Li^+ and Ps-Na^+ phase shifts. The cotangent form of the effective-range function is limited in its application here since the phase shift has a zero close to threshold. Therefore the tangent form of the effective-range function, namely,

$$\tan\delta(k) = -Ak - \frac{\alpha_d \pi k^2}{3} - \frac{2\alpha_d k^3}{3}\ln\frac{\alpha_d k^2}{16} + Bk^3 + Ck^4 \tag{14}$$

has been used in the fit to the FCSVM phase shifts. The MERT parameters were $A=-1.9301$, $B=240.93$, and $C=-289.62$. The uncertainty in the scattering length as a result of the fit was about $\pm 0.2a_0$. The small size of the scattering length provides very strong evidence that the e^+-K complex does not support a bound state. The omission of the polarization potential results in the magnitude of the scattering length decreasing further with a value of $-1.3601a_0$ being obtained. The uncertainty associated with the fit was $\pm 0.1a_0$ with the validity of the fit restricted to points with $k<0.15a_0^{-1}$.

D. Model-potential estimations of the scattering length

Two of the alkali systems, Li and Na, are known to bind a positron in configurations best described as Ps-Li^+ and Ps-Na^+ systems. Therefore, the known binding energies can be used in an ERT analysis or a model-potential analysis to deduce the scattering length.

It is known from effective-range theory that in case of a weak binding, the binding energy and scattering length are related as

$$A \approx 1/\sqrt{2\mu E}, \tag{15}$$

where μ is the system reduced mass. The scattering lengths derived from the e^+-Li and e^+-Na binding energies are listed in Table IV. The discrepancies of the order of 10–30 % are not surprising since there is a strong polarization potential between the Ps atom and the residual ion, which is not taken into consideration in Eq. (15).

Therefore a model potential approach has been adopted to this problem. The interaction between the Ps atom and the residual ion is approximated by the Hamiltonian

$$H = -\frac{1}{4}\nabla_R^2 - \frac{\alpha_d(\mathrm{Ps})}{2R^4}[1-\exp(-R^6/w^6)], \tag{16}$$

where the polarizability of Ps is $36a_0^3$ and w is a cutoff parameter. The Schrödinger equation was solved for the ground state of the Ps-Li^+ and Ps-Na^+ systems and the parameter ρ was tuned to reproduce the FCSVM binding energies [26,40].

Once ρ was set, the Schrodinger equation was solved at positive energies and the scattering lengths derived from an analysis of the phase shifts using Eq. (13). As can be seen from Table IV, the model-potential estimates of the scattering length are within 5% of the present FCSVM calculations. Therefore, a simple model-potential analysis can be used to accurately deduce the scattering length from the binding energy.

VI. $^1Z_{eff}$ FOR RARE GASES

There have been a number of experiments measuring the value of $^1Z_{eff}$ for rare gases. Rather than quote every single experimental measurement in Table V, the values given in [66] are taken as an evaluated summary of existing work.

Figure 7 shows the values of $^1Z_{eff}(k)$ as a function of momentum for the different models of Ps-He scattering. One feature of Fig. 7 is the small fluctuations of the order of 1% in $^1Z_{eff}$. In order to present the results in a concise form, a least-squares fit to the calculated values using the function

$$^1Z_{eff}(k) = {}^1Z_{eff}^{(0)} + {}^1Z_{eff}^{(1)}k^2 \tag{17}$$

has been performed. The values of this fit are tabulated in Table V for helium, neon, and argon. The parameters in Table V give an adequate description of the present $^1Z_{eff}(k)$ in the $k\in[0,0.5]a_0^{-1}$ interval. The variation in the helium $^1Z_{eff}^{(0)}$ using the three different choices for ρ, span a range of $\pm 15\%$. A similar degree of variation with ρ occurs for the neon $^1Z_{eff}^{(0)}$. The larger degree of variation in the argon $^1Z_{eff}^{(0)}$ with ρ was expected due to the larger polarizability of argon. Table V also gives the results of earlier calculations of $^1Z_{eff}^{(0)}$ by other authors. It is noted that there have been no previous calculations of $^1Z_{eff}^{(0)}$ reported for neon and argon.

The most noticeable result from Table V is the tendency for the values of $^1Z_{eff}^{(0)}$ derived from the $\rho=\rho_{av}$ Hamiltonian to underestimate the experiment by a factor of 2.5–3. However, such a discrepancy is not surprising. All of the present FCSVM calculations of $^1Z_{eff}(k)$ were performed with scattering wave functions that have inert atomic cores. Although the present calculations have used polarization potentials to overcome this limitation in the scattering Hamiltonian, no consideration was given to short-range electron-positron correlations during the evaluation of $^1Z_{eff}^{(0)}$. Such correlations are known to increase electron-positron contact densities and therefore increase the annihilation rate [58,64,67–69]. The

TABLE V. The parameters $^1Z_{eff}^{(0)}$ and $^1Z_{eff}^{(1)}$ describing pick-off annihilation for three Ps-rare-gas collisions. Although the parameters are quoted to three significant digits, the inherent uncertainties associated with the present fits are larger than the quoted precision. The uncertainty in $^1Z_{eff}^{(0)}$ is about $\pm 2\%$ while the uncertainty in $^1Z_{eff}^{(1)}$ is about $\pm 20\%$.

Method	$^1Z_{eff}^{(0)}$	$^1Z_{eff}^{(1)}$
Ps-He collision		
Static exchange [8]	0.0177	
(Updated) static exchange [9]	0.033	
Static exchange [10]	0.0347	
Static exchange and Van de Waals [10]	0.0445	
Kohn variational model static exchange [17]	0.042	
Kohn variational model exchange [17]	0.098	
T-matrix model static exchange [14]	~ 0.11	~ 1.4
Present FCSVM $\alpha_d=0$	0.0287	0.0044
Present FCSVM $\rho=\rho_-$	0.0344	-0.0114
Present FCSVM $\rho=\rho_{av}$	0.0378	-0.0152
Present FCSVM $\rho=\rho_+$	0.0451	-0.0218
Experiment [66]	0.125 ± 0.002	
Ps-Ne collision		
Present FCSVM $\alpha_d=0$	0.0533	0.0100
Present FCSVM $\rho=\rho_-$	0.0810	-0.0573
Present FCSVM $\rho=\rho_{av}$	0.0922	-0.0717
Present FCSVM $\rho=\rho_+$	0.111	-0.0950
Experiment [66]	0.235 ± 0.008	
Ps-Ar collision		
Present FCSVM $\alpha_d=0$	0.0340	0.0084
Present FCSVM $\rho=\rho_-$	0.0743	-0.112
Present FCSVM $\rho=\rho_{av}$	0.0964	-0.168
Present FCSVM $\rho=\rho_+$	0.158	-0.384
Experiment [66]	0.314 ± 0.003	

Ps-He^+ ground state (electrons coupled to spin-triplet state) can serve as an example to illustrate this point. The ground state of the Ps-He^+ system system has been computed to very high accuracy in the FCSVM model and also in an *ab initio* SVM calculation [58]. The FCSVM annihilation rate of the positron with the $1s$ core electron was a factor of 2.5 smaller than the *ab initio* SVM annihilation rate.

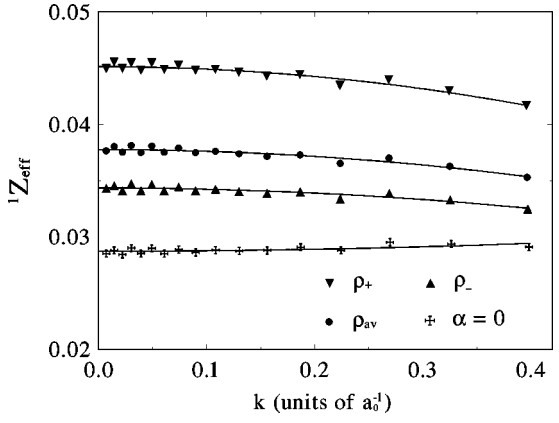

FIG. 7. The s-wave annihilation parameter, $^1Z_{eff}(k)$, for Ps-He scattering as a function of k (in units of a_0^{-1}). Results are shown for four model potentials, one with $\alpha_d=0$, and the others with ρ set to ρ_-, ρ_+, and ρ_{av}. The curves show the least-squares fit to $^1Z_{eff}$ using Eq. (17).

Another interesting trend is the tendency for $^1Z_{eff}^{(0)}$ to increase as the attractive Van der Waals interaction between the Ps projectile and atom increases in strength. Adhikari and co-workers have previously noted the same tendency [15] for Ps-He scattering although they investigated the relation between the size of the scattering length and $^1Z_{eff}^{(0)}$. A more attractive interaction leads to a smaller value of A and a larger threshold $^1Z_{eff}$. There is a simple qualitative explanation for this phenomenon. The Ps projectile is able to penetrate deeper into the electron-charge cloud as the scattering length decreases, and thus it is to be expected that $^1Z_{eff}$ should increase. Relations between the scattering length and the annihilation parameter Z_{eff} have also been noted in analyses of positron-atom annihilation dynamics [67,70]. As a further illustration of this effect, a further FCSVM calculation of Ps-He scattering was undertaken with an artificially small value of ρ, namely, $0.95a_0$. This calculation gave a scattering length of $1.05a_0$ and a $^1Z_{eff}^{(0)}$ of 0.105. Thus, the present results are consistent with the purely descriptive aspects of [15].

However, Adhikari *et al.* [15] also use the $^1Z_{eff}$-A correlation to make an inference that does not seem justified.

Briefly, they make the inference that the apparently good agreement between their calculated Ps-He $^1Z_{eff}$ of 0.11 and the experimental value of 0.125 ± 0.002 [66] provides additional support for a Ps-He scattering length of about $\approx 1a_0$. This conclusion does not take into consideration the possible impact that short-range electron-positron correlations can have in enhancing the annihilation rate.

Figure 7 and the tabulations of $^1Z_{eff}^{(1)}$ also reveal an interesting trend in the momentum dependence of $^1Z_{eff}(k)$. There is a tendency for $^1Z_{eff}(k)$ to decrease more rapidly with energy as the scattering length increases and the threshold value $^1Z_{eff}^{(0)}$ increases. This trend is present for helium, neon, and argon. The calculation of Adhikari and co-workers gave an *s*-wave curve for $^1Z_{eff}(k)$ that increased more rapidly with energy. Using Fig. 2 of [15] as a guide it is estimated that this calculation had $^1Z_{eff}^{(1)} = 1.4$, a value at variance with all of the present Ps-He calculations. The reasons for this difference are unknown.

The temperature dependence and thus the energy dependence of $^1Z_{eff}$ has also been the subject of experimental investigation. Some older experiments have reported that $^1Z_{eff}$ is practically independent of temperature for He [71], Ne [72], and Ar [72]. However, a recent experiment by Skalsey and co-workers [73] came to a different conclusion: the annihilation rate for He, Ne, and Ar increased by 5%, 5%, and 12% when the temperature was increased from 295 to 600 K. The momentum dependence of the present $^1Z_{eff}(k)$ generally shows a tendency to decrease slowly with energy. The present calculations suggest that if $^1Z_{eff}$ is increasing with temperature, then it is most likely due to processes that are absent from the present calculation. To be specific, Vallery *et al.* [73] have suggested that the *p* wave could be responsible. However, another possibility would be short-range electron-positron correlations between the positron and target electrons having an impact on the effective range.

VII. CONCLUSION

The fixed-core SVM has been used to investigate positronium scattering from a number of rare gas atoms and atomic ions. Two sets of calculations have been done. The first set does not include the Van der Waals interaction between the Ps projectile and the atom. These calculculations are fully *ab initio* and probably give a close-to-exact description of the scattering between Ps and the undisturbed target atom (or ion). The inclusion of target excitations is more problematic and a semiempirical Van der Waals–type interaction was incorporated into the calculation by adding one- and two-body core-polarization potentials to the fixed-core Hamiltonian. The parameters of these semiempirical polarization potentials were derived from experimental data, close to exact calculations, and in a few instances from some polarized orbital calculations.

One of the salient features of the present calculations was the fact that the scattering lengths for He, Ne, and Ar were all rather similar. The $\rho = \rho_{av}$ models gave scattering lengths that varied between $1.5a_0$ and 1.8 a_0. This result is consistent with the experiment by the Coleman *et al.* [6].

The Ps-He system is the most intensively studied of these systems, however, the different calculations and experiments have given conflicting results [2,20]. We believe the present calculation goes a long way to resolving the existing confusion. The present threshold cross section of $9.8\pi a_0^2$ is compatible with the three older experiments [4–6]. The agreement of the no-core-polarization calculation with the *R*-matrix calculation validates the approach used to extract the phase shifts. The main source of uncertainty with the present calculations relates to the definition of core-polarization potentials. Comparison of FCSVM binding energies for e^+-Li and e^+-He($^3S^e$) systems with completely *ab initio* SVM binding energies does suggest the reliability of the present approach. However, it is obvious that a fully *ab initio* and demonstratably converged calculation of the Ps-He scattering length would be very desirable.

The results on Ps-alkali ion systems mainly have implications for descriptions of e^+-alkali-atom scattering. The present phase shifts can be used to validate calculations of e^+-alkali scattering performed with more traditional methods.

Besides reporting phase shifts and scattering lengths, the annihilation parameter $^1Z_{eff}$ was given for Ps-He, Ps-Ne, and Ps-Ar scatterings. Since no consideration was given to short-range electron-positron correlations in the evaluation of the annihilation matrix element, it is not unusual that the present values underestimate the experimental values [66] by a factor of 2.5–3.

One of the most pleasing features of the present calculations was the ease with which they were done. Calculations of Ps-atom(ion) scattering are notoriously difficult and tedious since both the projectile and target are composite objects with their own internal structures. The present calculations were done on a 6-year-old work station and were completed over a very short amount of time. The computationally most expensive part of the calculation was the generation of the inner basis for the larger systems, e.g., this took about a week to complete for the Ps-Ar system. Once the inner basis was made, individual calculations involving a complete diagonalization took about 1 h or less to complete. The ability to compute phase shifts for Ps-atom scattering relatively quickly represents a major advance in the treatment of Ps-atom collisions.

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