Determination and applications of enhancement factors for positron and ortho-positronium annihilations

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Electron-positron annihilation rates calculated directly from the electron and positron densities are known to underestimate the true annihilation rate. A correction factor, known as the enhancement factor, allows for the local increase of the electron density around the positron caused by the attractive electron-positron interaction. Enhancement factors are given for positrons annihilating with the $1s$ electron in H, He$^+$, He, Li^{2+}, and Li$^+$. The enhancement factor for a free positron annihilating with He$^+$ and He is found to be close to that of ortho-positronium (i.e., Ps in its triplet state) annihilating with these atoms. The enhancement factor for Ps-He scattering is used in conjunction with the known annihilation rate for pickoff annihilation to derive a scattering length of $1.47a_0$ for Ps-He scattering. Further, enhancement factors for e^+-Ne and e^+-Ar annihilation are used in conjunction with the pickoff annihilation rate to estimate scattering lengths of $1.46a_0$ for Ps-Ne scattering and $1.75a_0$ for Ps-Ar scattering.

I. INTRODUCTION

When positrons interact with electronic systems strong short-range correlations act to increase the electron-positron annihilation rate. This effect is well known in condensed matter systems [1,2], positron-atom or positron-ion scattering systems [3–7], and positron-atom bound states [8,9]. The effect is due to the attractive nature of the electron-positron interaction which leads to a localization of the positron in the vicinity of the electron. These strong correlations greatly complicate the theoretical analysis. Indeed, in the case of positronium- (Ps-) atom scattering, there are few calculations of the pick-off annihilation parameter despite it being one of the standard parameters extracted from positron annihilation experiments in the gas phase [10] (pickoff annihilation describes the annihilation of the positron with an electron that is not part of the Ps atom). The only calculations of pickoff annihilation reported so far neglect the strong correlations between the positron and annihilating electron [11–15]. This is not surprising since scattering calculations allowing without restriction for the interactions between the internal constituents of the two composite objects are notoriously difficult.

Methods exist for the calculation of the annihilation rate in atomic systems for both bound and continuum positrons. The 2γ annihilation rate for bound systems is proportional to the probability of finding an electron and a positron at the same position in a spin-singlet state according to

$$\Gamma = 4\pi r_e^2 c \left\langle \Psi \left| \sum_i O_{ip}^S \delta(\mathbf{r}_i - \mathbf{r}_p) \right| \Psi \right\rangle$$
$$= 2.018\,788 \times 10^{11} \sum_i \langle \delta(\mathbf{r}_i - \mathbf{r}_p) \rangle_S \qquad (1)$$

[16–18], where the sum is over the electron coordinates, the δ-function expectation is evaluated in a_0^3, and Γ is given numerically in s^{-1}. The operator O_{ip}^S is a spin projection operator to select spin-singlet states for the ip electron-positron

pairs in the wave function Ψ which is antisymmetrized in the electron coordinates. In the scattering domain, one writes the annihilation parameter Z_{eff} as

$$Z_{\text{eff}} = 4 \left\langle \Psi \left| \sum_i O_{ip}^S \delta(\mathbf{r}_i - \mathbf{r}_p) \right| \Psi \right\rangle \qquad (2)$$

where the wave function for the positron is normalized according to plane-wave boundary conditions.

The matrix element of the wave function $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{r}_{N+1})$ [with $(N+1)$ referring to the positron coordinate] for $O_{1,(N+1)}^S \delta(\mathbf{r}_1 - \mathbf{r}_{N+1})$ is

$$\langle \Psi | O_{1,(N+1)}^S \delta(\mathbf{r}_1 - \mathbf{r}_{N+1}) | \Psi \rangle = 4 \langle O_{1,(N+1)}^S \rangle$$
$$\times \int d^3\tau |\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}_1)|^2, \qquad (3)$$

where the $d^3\tau$ represents an integration over all electron coordinates [9]. The factor $4\langle O_{1,(N+1)}^S \rangle$ reduces to 1 for a closed-shell target.

These expressions simplify in those cases where the wave functions are written in simple product form, e.g., as $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)\Phi(\mathbf{r}_{N+1})$ when the long-range form of the wave function can be written as a positron+atomic fragment. In these cases one writes

$$\Gamma = \pi r_0^2 c N_e \int d^3\tau |\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 |\Phi(\mathbf{r}_1)|^2 \qquad (4)$$

$$= \pi r_0^2 c \int d^3 r \, \rho_{\text{atom}}(\mathbf{r}) \rho_{e^+}(\mathbf{r}) \qquad (5)$$

for the bound-state *spin-averaged* annihilation rate and

$$Z_{\text{eff}} = N_e \int d^3\tau |\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2 |\Phi(\mathbf{r}_1)|^2 \qquad (6)$$

$$= \int d^3r \, \rho_{\text{atom}}(\mathbf{r}) \rho_{e^+}(\mathbf{r}) \qquad (7)$$

for the collisional annihilation rate. The electron density $\rho_{\text{atom}}(\mathbf{r})$ is normalized to N_e while $\rho_{e^+}(\mathbf{r})$ is normalized to unity for Eq. (5) and to scattering boundary conditions for Eq. (7).

For Ps-atom scattering states or bound systems with Ps-A^+ boundary conditions, one defines the pickoff annihilation rate as the annihilation rate of the positron in the Ps cluster with all the electrons except that in the Ps cluster. For Ps-He scattering and the PsLi$^+$ ground state, this can be done by forcing the Ps species to be in a triplet state and then the only 2γ annihilations that can occur are those with the electrons in the He or Li$^+$ subsystem. A simplified calculation in the case of a closed-shell target is

$$\Gamma = \pi r_0^2 c N_e \int d^3\tau |\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})|^2 |\Phi_{\text{Ps}}(\mathbf{r}_N,\mathbf{r}_1)|^2 \qquad (8)$$

$$= \pi r_0^2 c \int d^3r_1 d^3r_N \, \rho_{\text{atom}}(\mathbf{r}_1) |\Phi_{\text{Ps}}(\mathbf{r}_N,\mathbf{r}_1)|^2, \qquad (9)$$

where the positron $\mathbf{r}_1$ does not annihilate with the electron $\mathbf{r}_N$, forming part of the Ps cluster $\Phi_{\text{Ps}}(\mathbf{r}_N,\mathbf{r}_1)$. The pickoff annihilation rate for a scattering state in the simplified model is then

$$_1Z_{\text{eff}} = \frac{N_e}{4} \int d^3\tau |\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1})|^2 |\Phi_{\text{Ps}}(\mathbf{r}_N,\mathbf{r}_1)|^2 \qquad (10)$$

$$= \frac{1}{4} \int d^3r_1 \, d^3r_N \, \rho_{\text{atom}}(\mathbf{r}) |\Phi_{\text{Ps}}(\mathbf{r}_N,\mathbf{r}_1)|^2, \qquad (11)$$

where $\Phi_{\text{Ps}}(\mathbf{r}_N,\mathbf{r}_1)$ is the Ps scattering wave function.

Using simple model potential calculations, Mitroy and Ivanov [6] studied the energy dependence of Z_{eff} for hydrogen, the noble gases, and some metals. One of the major outcomes of this work was the demonstration that a model potential tuned to give the correct phase shifts also gave the energy dependence of Z_{eff} correctly over a surprisingly large energy range. This idea was further reinforced by the investigation of e^+ scattering from positive hydrogenic ions [7]. Once again, a simple central field calculation tuned to give the correct phase shifts also reproduced the energy dependence of $Z_{\text{eff}}(k)$. The work on ions had an additional refinement; the enhancement factor was allowed to be ℓ dependent. In order to avoid multiplication of parameters in the initial effort on atoms [6] a single enhancement factor, tuned to the s-wave Z_{eff} at low energies, was used. This approximation was justified in the context of that work since the main interest was in near-threshold behavior which is dominated by s-wave scattering. These ideas have also been expressed in the calculations of atomic hydrogen by Gribakin and Ludlow [19] which employed a variant of many-body perturbation theory (MBPT). Their estimate of the enhance-

ment factor was made by examining the relative contribution that correlation corrections make to the annihilation vertex. They showed s-wave and p-wave enhancement factors that also did not change much with energy. There has been one attempt to apply enhancement factors used in condensed matter physics to the single-atom environment with somewhat mixed results [20].

In the present work, enhancement factors for positrons and ortho-positronium annihilation with the $1s$ electrons in H, He$^+$, He, Li$^+$, and Li^{2+} are derived directly from *ab initio* calculations. The enhancement factors show regularities with respect to the binding energy of the annihilating electron and further (with the exception of H) the enhancement factors for ortho-positronium annihilation are only slightly different from those for free positron annihilation on the same atom. Finally, the enhancement factor derived for He, and earlier estimates of enhancement factors for Ne and Ar (derived from semiempirical analyses of positron scattering for these atoms) are used in conjunction with pickoff annihilation data to derive estimates of the Ps-He(Ne,Ar) scattering lengths.

II. EVALUATION OF THE ENHANCEMENT FACTOR

A number of different approaches have been used to determine the enhancement factors listed in Table I. In the first instance, the enhancement factor is defined as the ratio between Z_{eff} or Γ (depending on whether the system is a bound or scattering state) calculated in a simple model potential and close-to-exact values obtained from more sophisticated methods (note, the central field of the model potential is tuned to give the same scattering length as the more exact calculation), e.g.,

$$G_1 = \frac{Z_{\text{eff}}^{\text{exact}}}{Z_{\text{eff}}^{\text{model}}} \quad \text{or} \quad G_1 = \frac{\Gamma^{\text{exact}}}{\Gamma^{\text{model}}}. \qquad (12)$$

The estimates of $Z_{\text{eff}}^{\text{exact}}$ and Γ^{exact} are taken from a variety of sources.

In the second approach, all estimates are essentially derived from high-accuracy *ab initio* wave functions. The $Z_{\text{eff}}^{\text{density}}$ (Γ^{density}) annihilation rate is determined by first computing the positron densities $\rho_{e^+}(\mathbf{r})$ from the *ab initio* wave functions. This positron density is then used to compute the annihilation rate using Eq. (5), (7), (9) or (11) with ρ_{atom} being taken from the parent atom ground state, e.g.,

$$G_2 = \frac{Z_{\text{eff}}^{\text{exact}}}{Z_{\text{eff}}^{\text{density}}} \quad \text{or} \quad G_2 = \frac{\Gamma^{\text{exact}}}{\Gamma^{\text{density}}}. \qquad (13)$$

So the positron density in the denominator of Eq. (13) is calculated using the same wave function used in the evaluation of the numerator.

Method 1 for G_1 is model dependent since the overlap of the positron density with the annihilation electrons does depend to some extent on the shape of the potential. Method 2 gives probably the purest definition of the enhancement factor since almost no approximations are made in the calculation of the positron density and the G_2 enhancement factors are obtained from highly accurate variational wave func-

TABLE I. Enhancement factors for positrons annihilating with atomic electrons in H, He$^+$, He, Li$^+$, and Li^{2+}. The identification as (core) means the annihilation rate is that associated with the tightly bound atomic electron. All the enhancement factors relate to s-wave positrons or positronium annihilating with the parent atom. The references denote those instances where the enhancement factor has previously been computed or the source of the wave function used to evaluate G_2. The column labeled "Parameter" denotes whether G was derived from a bound-state calculation (Γ) or a scattering calculation of the direct (Z_{eff}) or pickoff ($_1Z_{\text{eff}}$) annihilation rate. It should be noted that the spin coupling of either of the Ps-H scattering states is not exactly the same as the PsH($2e^-T$) state which is unbound.

System	Parameter	G	Method
e^+H	Z_{eff}	6.03	G_1 [6]
e^+H	Z_{eff}	5.65	G_2 SVM [21]
e^+H	Z_{eff}	5.66	G_2 Kohn [22]
e^+H	Z_{eff}	≈ 5.9	MBPT [19]
PsH($2e^-T$) (core)	Γ_{1s}	8.40	G_2 SVM
e^+He$^+$	Z_{eff}	2.52	G_1 [7]
e^+He$^+$	Z_{eff}	2.55	G_2 Kohn [7]
PsHe$^+$($2e^-T$) (core)	Γ_{1s}	2.40	G_1 [23]
PsHe$^+$($2e^-T$) (core)	Γ_{1s}	2.28	G_2 SVM [23]
e$^+$He	Z_{eff}	2.92	G_1 [6]
e$^+$He	Z_{eff}	2.75	G_2 SVM
^{3}PsHe (core)	$_1Z_{\text{eff}}$	2.65	G_2 SVM
^{3}PsLi$^+$ (core)	Γ	1.96	G_1 [24]
^{3}PsLi$^+$ (core)	Γ	1.86	G_2 SVM [24]
e^+Li^{2+}	Z_{eff}	1.83	G_1 [7]
e^+Li^{2+}	Z_{eff}	1.89	G_2 Kohn [7]

tions. In effect, the only difference between Γ^{model} ($Z_{\text{eff}}^{\text{model}}$) and Γ^{density} ($Z_{\text{eff}}^{\text{density}}$) is that the positron density in the former is taken from a model potential calculation density while the latter use a positron density computed from a high-accuracy *ab initio* calculation.

Model potential calculations of the G_1 enhancement factors for s-wave positrons annihilating with H, He$^+$, Li^{2+}, and He during collisions have been previously computed [6,7].

A single-center Kohn variational method [7,22] was used to compute the wave functions used to determine G_2 for H, He$^+$, and Li^{2+}. The configuration-interaction (CI) Kohn calculations for these three systems were done at $k=0.3a_0^{-1}$, $0.75a_0^{-1}$, and $1.0a_0^{-1}$, respectively. The positron density from the large-basis CI Kohn calculation was multiplied by the electron density of the hydrogenic ground state and the resulting integral used to estimate G_2. There is a 2–3 % uncertainty in the values of G_2 extracted from the CI Kohn calculations since 10–20 % of the final value of Z_{eff} comes from a partial-wave extrapolation.

The values of G_2 for ^{3}PsLi$^+$ (where ^{3}Ps denotes triplet Ps) were obtained from a bound-state wave function. The annihilation rate for the triplet ^{3}PsLi$^+$ state is identified with the annihilation rate of the positron with the Li$^+$ core. The ^{3}PsLi$^+$ G_2 was obtained by evaluating the denominator of Eq. (13) [i.e., Eq. (10)] with the positron density determined

by the stochastic variational method (SVM) [8,9,24–26] and the electron density of the Hartree-Fock (HF) Li$^+$ ground state. The SVM expands the wave function in a linear combination of explicitly correlated Gaussians (ECGs). The extreme simplicity of the Hamiltonian matrix elements with an ECG basis makes it feasible to do extensive energy optimizations with a big basis and thus generate very accurate wave functions.

The mechanics of the G_2 calculation for the bound PsHe$^+$($2e^-T$) state are more complicated [17,23] as the two electrons are in a spin-triplet state (denoted $2e^-T$) while the total spin with the positron coupled can be doublet or quartet. The annihilation parameter used to define the enhancement factor is the annihilation rate for annihilation with the core $1s$ electron [17,23]. Once again, the PsHe$^+$($2e^-T$) wave function was taken from a SVM calculation [23].

The estimates of G_1 for the PsHe$^+$($2e^-T$) and ^{3}PsLi$^+$ states were obtained by comparison of the fixed-core stochastic variational method (FCSVM) [8,9,17,23].

The scattering version of the SVM was used to determine values of G_2 for the e^+H, e^+He, PsH($2e^-T$), and ^{3}PsHe systems. The relevant annihilation parameter for the e^+H and e^+He systems is Z_{eff}, that for ^{3}PsHe is $_1Z_{\text{eff}}$, while the annihilation rate with the H($1s$) electron is the relevant parameter for PsH($2e^-T$) [which has the same spin structure as PsHe$^+$($2e^-T$)]. In the scattering version of the SVM, an initial optimization of the energy is done with the ECG basis constrained to only include functions that are localized close to the scattering center [say $(10–20)a_0$] [11,21,27]. Then an additional set of ECGs designed to give a good representation of the wave function in the large-r asymptotic region are added to the basis. The basis is diagonalized and the phase shifts and annihilation rate determined by fitting the positive-energy pseudostates to a sinusoidal, $A \sin(kr+\delta)$ continuum function over the interval $15a_0 \leqslant r \leqslant 30a_0$. The scattering version of the SVM has been mainly applied to Ps scattering problems (since these are largely inaccessible by orthodox scattering calculations) but has been extensively validated and it has reproduced the scattering length and low-energy Z_{eff} for e^+-H scattering [21].

The enhancement factors for e^+ and Ps scattering were obtained without going through the tedium of taking the calculation to completion. Only the short-range inner basis was included in the calculation. Positron annihilation is a short-range interaction, and the dynamical interactions that govern this process are incorporated in the energy optimized inner basis. The longer-range outer basis used for the large-r region merely serves to give the overall normalization of the wave function. Since the G_2 enhancement factor is a ratio with the positron density in the denominator derived from the wave function also used to determine the numerator, its value does not depend on the overall normalization of the wave function. The G_2 enhancement factors obtained via this approach were reasonably stable with respect to increasing basis size. For example, G_2 for e^+He varied from 2.63 to 2.75 when the basis set was increased in size from 350 to 800 ECGS. Similarly, the total variation in G_2 for ^{3}PsHe scattering ranged from 2.51 to 2.69 for basis sets ranging in size from 900 to 1300 ECGs. Large ECG basis sets of di-

mensions 450 and 800 were used in the final determination of G_2 for the e^+H and PsH($2e^-$ T) systems. The comparison of the SVM $G_2=5.65$ for e^+H scattering with that of the CI Kohn $G_2=5.66$ could hardly be any better and indicates that the scattering version of the SVM is reliable.

One feature of Table I is that model-dependent enhancement factors G_1 are only 5–10 % different from enhancement factors G_2 from the *ab initio* calculations. The model potentials so far adopted [6,7,23] do a reasonable job of estimating the overlap of the positron density with the atomic electrons. The model potential G_1 is smaller than G_2 for the e^+H, e^+He, PsLi$^+$, and PsHe$^+$ systems, while being slightly larger than G_2 for the e^+He$^+$ and e^+Li^{2+} systems.

It is also apparent from Table I that the enhancement factors G_1 and G_2 tend to increase as the ionization energy of the annihilation electron(s) decrease(s). This has been noticed in previous work [4,6]. The final notable feature of Table I is that the enhancement factors for Ps and e^+ annihilating with He$^+$ are close to each other as are the enhancement factors for ^{3}Ps and e^+ interacting with He. However, the enhancement factors for Ps and e^+ annihilating with H are different. The difference between He$^+$, He, and H is that the electrons are more tightly bound to He$^+$ and He. An interesting conjecture is that the enhancement factors for Ps or free e^+ annihilating with atomic electrons could be the same when the atomic electrons are tightly bound.

III. ESTIMATION OF THE Ps-He, Ps-Ne, AND Ps-Ar SCATTERING LENGTHS

In this section estimates are made of the scattering lengths for Ps scattering from He, Ne, and Ar. The experimental determination of the scattering length for Ps-atom scattering is very difficult and there is considerable variation between estimates obtained by different techniques (see tabulations in Ref. [11]). However, the pickoff annihilation rate $_1Z_{\text{eff}}$ is relatively straightforward to measure precisely in gas phase experiments [10].

The low-energy interaction between Ps and the rare gases is largely repulsive and the available calculations of the scattering lengths and give positive values [11,12]. This repulsive interaction inhibits the overlap of the positron with the target electrons and generally results in small $_1Z_{\text{eff}}$ values. Increasing the strength of the attractive polarization interactions does increase the pickoff annihilation rate as the positron is able to penetrate further in the target electron cloud. In the case of Ps-He scattering, calculations giving scattering lengths of $1.625a_0$, $1.568a_0$, and $1.482a_0$ gave $_1Z_{\text{eff}}$ of 0.0344, 0.0378, and 0.0451, respectively [11].

Values of the enhancement factor extracted from calculations are used to tune FCSVM calculations of Ps-atom scattering to the experimental $_1Z_{\text{eff}}$ in order to derive estimates of the scattering length. The tuning is achieved by adjusting the parameter that governs the short-range behavior of a model polarization potential (this potential incorporates both one-body and two-body effects and the parameter is denoted ρ in Ref. [11]).

A. The Ps-He scattering length

Consider the case of Ps-He scattering where 2.65 is estimated for the enhancement factor. This enhancement factor is then applied to the calculation of $_1Z_{\text{eff}}$ in the FCSVM model of Ps-He scattering [11]. The polarization potential is then tuned until the FCSVM model reproduces the experimental $_1Z_{\text{eff}}$ of 0.125±0.002 [10]. The equation used is

$$_1Z_{\text{eff}}(\text{FCSVM}) \times 2.65 = 0.125. \tag{14}$$

The resultant scattering length of the FCSVM model when Eq. (14) was satisfied was $1.47a_0$ ($\rho=1.40a_0$). The experimental $_1Z_{\text{eff}}$ is taken at thermal energies, i.e., $k \approx 0.06a_0^{-1}$, and the FCSVM calculations show that the s-wave $_1Z_{\text{eff}}$ varies slowly with energy. At thermal energies the contribution from the p wave should also be very small. The present estimate of the scattering length is not exact since there is some uncertainty in G_2 and the overlap of the SVM and FCSVM positron densities with the He($1s^2$) ground state will be slightly different. Accordingly a 10% variation in the G_2 used in Eq. (14) is permitted, giving a maximum possible G of 2.92 and a minimum possible G of 2.39. The scattering lengths obtained with these enhancement factors were $1.52a_0$ (2.92) and $1.42a_0$ (2.39). So, transferring the SVM enhancement factor to the FCSVM calculation and tuning to the experimental $_1Z_{\text{eff}}$ gives a Ps-He scattering length of $(1.47\pm0.05)a_0$.

These Ps-He scattering lengths can be compared to those obtained from the original FCSVM calculation. Three different core-polarization potentials were used. They were determined by tuning a short-range cutoff parameter to either the e^--He and e^+-He scattering length (the third potential used an average cutoff parameter). With three different specifications of the polarization, Mitroy and Ivanov obtained three different scattering lengths which can be summarized as $\approx(1.57\pm0.09)a_0$. The lowest estimate of Mitroy and Ivanov, $1.48a_0$ [11], is close to the present middle estimate of $1.47a_0$.

The middle estimate of $1.47a_0$ is only 5% larger than the scattering length of $(1.405\pm0.001)a_0$ obtained from a quantum Monte Carlo (QMC) calculation [28]. The uncertainty quoted by the QMC calculation is the statistical uncertainty and does not include any estimate of the error arising from the definition of the nodal surfaces.

When all this information is taken together one sees that a consistent picture of threshold Ps-He scattering is finally starting to emerge. The present G-factor analysis, the earlier FCSVM calculations [11], the QMC calculation [28], and the experimental $_1Z_{\text{eff}}$ [10] are all consistent at the 10% level. They give threshold cross sections that range between $7.8\pi a_0^2$ and $10.3\pi a_0^2$. These are compatible with the larger estimates of the Ps-He cross section, namely, $(8.4\pm0.9)\pi a_0^2$ [29], $9.0a_0^2$ [30], and $(13\pm4)\pi a_0^2$ [31] that were derived from angular correlation of annihilation radiation (ACAR) measurements. The more recent estimate of the low-energy cross section derived from the Doppler-broadening spectra, namely, $(3.8\pm0.8)\pi a_0^2$ [32], lies outside the range of these theoretical determinations.

B. The Ps-Ne and Ps-Ar scattering lengths

A similar analysis can be done for neon and argon, which are the noble gases with reasonably large ionization potentials. The analysis in this case is more speculative since a

direct calculation of the SVM enhancement factor for Ps-Ne and Ps-Ar scattering has not been made. The enhancement factors were determined by recourse to low-energy positron-neon and positron-argon scattering data. Additional uncertainties exist since the low-energy positron-neon and positron-argon cross sections are not known as precisely [6,33,34] as the positron-helium cross section. The values of $G=2.26$ (Ne) and $G=3.02$ (Ar) [6] were fixed by tuning the phase shifts to polarized orbital calculations [33,34] and then normalizing to the experimental Z_{eff} [35–37].

In these cases, the one- and two-body polarization potentials of the FCSVM scattering calculation [11] are then tuned until $_1Z_{eff}$(FCSVM)$\times 2.26=0.235\pm0.008$ in the case of neon and $_1Z_{eff}$(FCSVM)$\times 3.02=0.314\pm0.003$ for argon. A variation of $\pm25\%$ in G was permitted. The derived scattering length for Ps-Ne scattering was $1.46^{+0.12}_{-0.16}a_0$ ($\rho=1.65a_0$) while that for Ps-Ar scattering was $1.75^{+0.18}_{-0.27}a_0$ ($\rho=2.05a_0$). The relatively tight bounds (e.g., 10% and 12%, respectively) on the scattering lengths arise because $_1Z_{eff}(k=0)$ varies relatively quickly as a parametric function of scattering length. So a large change in $_1Z_{eff}(k=0)$ leads to a small change in the scattering length. In terms of zero-energy elastic cross sections, the present scattering lengths for Ne convert to $8.5^{+1.5}_{-1.7}\pi a_0^2$ while those for Ar are $12.2^{+2.7}_{-3.4}\pi a_0^2$. These scattering lengths are compatible with those predicted by the FCSVM scattering calculations [11]. Allowing for reasonable variations in the form of the polarization potential resulted in scattering lengths of $1.55^{+0.07}_{-0.09}a_0$ for Ps-Ne scattering and $1.79^{+0.20}_{-0.39}a_0$ for Ps-Ar scattering.

The present estimates of the threshold cross section are generally closer to the ACAR-derived cross sections of Coleman *et al.* ($9.0\pi a_0^2$ for Ne and $9.0\pi a_0^2$ for Ar) [30] and Nagashima *et al.* [$(11.4\pm8.0)\pi a_0^2$ for Ne and $(17\pm11)\pi a_0^2$ for Ar] [31] than to the most recent Doppler-derived cross section estimates of Skalsey *et al.* [$(7.3\pm0.2)\pi a_0^2$ for Ne and $(7.5\pm1.1)\pi a_0^2$ for Ar] [32].

Time-of-flight experiments of positron-neon and positron-argon scattering to measure the elastic cross section in the 0.1–1.0 eV energy range would be valuable in reducing the uncertainties and improving the precision of this cross-experiment exercise.

Although FCSVM descriptions of the scattering and experimental $_1Z_{eff}$ data exist for the Ps-Kr and Ps-Xe systems [10,12], application of the present technique is problematic. There are larger uncertainties in the positron-atom scattering and annihilation data [11], the larger polarizabilities of Kr and Xe increase the uncertainties in the FCSVM core-polarization potentials, and there are reasons to believe that the $_1Z_{eff}$ measurements could be affected by the spin-orbit quenching of ortho-Ps [38].

IV. CONCLUSION

Enhancement factors have been determined for positrons annihilating with H, He$^+$, He, Li^{2+}, and Li$^+$. The enhancement factors for a free positron or in a Ps atom are generally quite close for He$^+$ and He. Further, since the available evidence suggests that the enhancement factor for a given atom depends weakly on energy, this suggests that the enhancement factor depends more on the structure of the target electrons and less on the environment in which the positron moves. This is a useful result since it suggests that it may be possible to cross-correlate positron scattering and annihilation data with Ps scattering and pickoff annihilation data. However, it must be stressed that the evidence to support this conjecture is more indicative than conclusive.

The enhancement factors have been utilized to estimate the scattering lengths for Ps-He, Ps-Ne, and Ps-Ar scattering. The scattering length for Ps-He should be reasonably accurate since the enhancement factor is taken directly from an *ab initio* calculation. Those for Ps-Ne and Ps-Ar scattering are more speculative, since they were based on the conjecture that the enhancement factors for e^+-Ne (Ar) annihilation are the same as that for Ps-Ne (Ar) pickoff annihilation, and in addition there is greater uncertainty in the low-energy e^+-Ne (Ar) cross section which is used to fix the enhancement factor. The scattering lengths obtained by the present procedure are compatible with those obtained from the earlier FCSVM scattering calculation [11]. Comparisons with the available experimental data suggest that estimates of the low-energy cross section using the Doppler-broadening technique (e.g., Ref. [32,39]) tend to underestimate the threshold cross section.

One of the motivations concerns the possibility of utilizing calculations of positron-atom or positron-ion scattering to determine enhancement factors that can then be used in the condensed matter environment. The enhancement factors to a first-order approximation can be taken as simple multiplicative constants with different values used for the valence and core electrons [40]. While the determination of the enhancement factors for the valence electrons of simple metals is reasonably well understood [40–42], the same cannot be said for the core electrons. Indeed, one of the outstanding problems concerning the application of positron annihilation spectroscopies is the determination of enhancement factors for the core electrons [20,41,42]. One possible way forward would be to use single-atom calculations to determine enhancement factors which could then be applied to the condensed matter domain. Most previous determinations of the enhancement factor [4,6,20,24,43] are based on approximate formula for the electron-positron localization or use approximate wave functions. The set of G_2 values given in Table I represents a comprehensive set of enhancement factors directly calculated from high-quality *ab initio* wave functions. Of the factors presented here, only those for He and Li$^+$ are likely to be applied to the condensed matter environment, but the present set of calculations on these small systems are a necessary starting point.

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