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Semiempirical diabatic potential for low-energy positron-atom elastic scattering

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Cross sections and annihilation rates for the elastic scattering of positrons off hydrogen and helium atoms are calculated in an approximation in which nonadiabatic distortions of the targets are treated with a model potential. The wave functions of the targets are calculated in a bicentric spheroidal coordinate system by modifying a computer code written for self-consistent-field calculations on diatomic molecules. Virtual positronium and correct long-range polarization of the targets are accounted for explicitly in the wave function by proper choice of basis functions. The wave function for each target is calculated on a grid of positron-nucleus distances, which generates a scattering potential for the positron. This is solved by applying partial-wave analysis and numerical integration. The calculated results for cross sections and annihilation rates for both systems are reasonably accurate, and suggest that the method can be extended to larger targets.

I. INTRODUCTION

There have been several recent reviews of the theoretical aspects of positron-atom and positron-molecule scattering by Drachman,[1] Schrader and Svetic,[2] Ghosh, *et al.*,[3] and McEachran.[4] According to these reviews, the interactions that characterize elastic low-energy positron-atom collisions are traditionally divided into two categories: (i) static and (ii) polarization (adiabatic and nonadiabatic) or correlation. The effective one-body scattering potential is then a sum of terms corresponding to these categories:

$$V_{\mathrm{sc}}(\mathbf{r}_p)=V_{\mathrm{st}}(\mathbf{r}_p)+V_{\mathrm{pol}}(\mathbf{r}_p)\ , \tag{1}$$

where $\mathbf{r}_p$ is the spatial coordinate of the projectile positron. The static potential $V_{\mathrm{st}}(\mathbf{r}_p)$ is simply the average of the electrostatic e^+-atom interactions over the ground-state eigenfunctions Ψ_e of the unperturbed target. If Ψ_e can be written as a single determinant of spin orbitals $\psi_i^{(0)}$,

$$\Psi_e=\frac{1}{\sqrt{N!}}\det|\,\psi_1^{(0)}\psi_2^{(0)}\cdots\psi_N^{(0)}\,|\ , \tag{2}$$

then the static potential can be expressed in terms of these spin orbitals:

$$V_{\mathrm{st}}(\mathbf{r}_p)=\frac{Z}{r_p}-\sum_{i=1}^{N}J_i^{(0)}(\mathbf{r}_p) \tag{3}$$

where Z is the nuclear charge, and $J_i^{(0)}(\mathbf{r}_p)$ is the zeroth-order Coulomb integral

$$J_i^{(0)}(\mathbf{r}_p)=\int\frac{|\,\psi_i^{(0)}(\mathbf{r}_e,\sigma_e)\,|^2}{|\,\mathbf{r}_e-\mathbf{r}_p\,|}d\mathbf{r}_e d\sigma_e\ , \tag{4}$$

where σ_e is the spin coordinate. In the case of e^--atom scattering, there is a third term, the exchange potential, on the right-hand side of Eq. (1), and the signs of the Coulomb interactions in Eq. (3) are reversed.

As far as scattering is concerned, the major type of correlation between the positron and the atomic electrons is polarization. The incident positron polarizes the electrons and the induced multipole moments attract the positron. The induced potential, the so-called polarization potential, $V_{\mathrm{pol}}(\mathbf{r}_p)$, is nonlocal but its leading long-range part is simple: $-\alpha_d/2r_p^4$, where α_d is the static dipole polarizability of the atom. The next most important long-range term, which is due to the static quadrupole polarization and the nonadiabatic and second-order corrections to the static dipole contribution, is of the order of r_p^{-6} (Refs. 5–11). The short-range behavior is, in general, not known and has significant diabatic components.[5,12,13] Its determination, even approximately for simple atoms, requires a major computational effort.

Consequently, many workers have used semiempirical potentials for modeling the polarization effects at short range. One of the simplest and most popular is the asymptotic form multiplied by a short-range cutoff function containing parameters.[14–25] The simplicity of this scheme provides the chief advantage of the prescription; however, it also has a major drawback—the form is sometimes not flexible enough to describe accurately the complicated nature of $V_{\mathrm{pol}}(\mathbf{r}_p)$ at short range, and the results thus generated are sometimes inaccurate.[14]

An alternative approximation can be obtained by the use of polarized-orbital methods, first prescribed by Temkin.[26] A review of these approximation schemes has been given by Drachman and Temkin.[27] In general, a polarized orbital computation consists of two stages: (i) the calculation of the perturbed bound-state electronic spin orbitals ψ_i and (ii) the computation of the wave function of the incident particle. This technique accounts for the distortion of the target by the positron fixed at a given position in space, but it does not provide a good representation of the nonadiabatic effects; the positron kinetic energy operator is usually omitted in the first stage of polarized orbital calculations. Consequently, the calculated phase shifts tend to be too high.[13,28] An empirical remedy is to suppress the monopole contribution to the adiabatic $V_{\mathrm{pol}}(\mathbf{r}_p)$ (Refs. 28 and 29). The results are surprisingly good, but the underlying reasons for this are not entirely clear. It has been shown quantitatively by Wang *et al.*[5] that the monopole parts of the adiabatic and the diabatic terms fall off exponentially. Thus they have little or no long-range effects, and they have opposite signs and therefore tend to cancel each other. The tactic of suppressing the adiabatic monopole thus approximately corrects for the nonadiabatic effect at intermediate range. At short range the diabatic behavior is less well understood. Attempts to account for the diabatic effects in polarized orbital calculations by including both the monopole part of the polarization potential and the positron kinetic energy operator have proven to be less than satisfactory.[13] Following their encouraging results of the adiabatically polarized orbital method with monopole suppression when applied to e^+—noble-gas elastic scattering,[29] McEachran and co-workers have recently reformulated their polarized orbital scheme in terms of a polarized density.[30] This newer approach can be applied to e^+- and e^--molecule scattering and can be carried out variationally.

Evaluation of the complete wave function can provide information besides phase shifts and cross sections, such as the annihilation rate and the angular correlation of the two γ rays produced during annihilation.[27] The accuracy of calculated annihilation rates depends on the quality of the wave function at short-range which is primarily affected by e^--e^+ correlation.[31,32] The most direct approach to light-particle correlations is the Hylleraas method[33] which treats the correlational effects by introducing explicitly the interacting-pair coordinates into the wave function. The very elaborate many-term Hylleraas-type integrals discourage general application to one-positron, many-electron systems. Only a few variational Hylleraas-type calculations for elastic low-energy positron scattering by hydrogen[34,35] and by helium[36,37] have been carried out. Amusia *et al.*[38] have applied the random phase approximation with exchange, derived from many-body theory, to e^+-He elastic scattering by taking into account the formation of virtual positronium (Ps). The correction to the correlation effects is expressed through the self-energy part[39] with the use of a diagrammatic technique.

A recent self-consistent-field approach based on the variational principle has been tested for e^+-H elastic scattering by Horbatsch and co-workers.[40] Their calculated *s*-wave phase shifts are of good quality although the corresponding annihilation parameters are underestimated as compared to the accurate results.[40(a)]

As proposed by Massey and Mohr,[41] the close-coupling approximation (CCA) is a general approach that gives a clear picture of all physical terms. Basically, the trial wave function is expanded in terms of eigenstates of bound subsystems, giving rise to so-called virtual excitations and virtual Ps formation. The unknown expansion coefficients are determined as solutions of a set of coupled integrodifferential equations whose number depends on the size of the expansion. In fact, the CCA is a configurational interaction method which is widely used as an indirect means for treatment of e^--e^- correlation in bound states of purely electronic systems. A large number of short-range correlation terms may be required[42,43] in order to obtain accurate results. The poor results obtained by using a six-state close coupling calculation[44] on e^+-H elastic scattering suggest that the method may be inconvenient for more complicated one-positron, many-electron systems.

A diatomiclike model for e^+-He elastic collision has been carried out by Pai *et al.*[45] Their approach has no empirical input and is essentially statistical. The physical picture of their model is as follows: when the positron is close to or inside the target atom, its ability to polarize is reduced by its own dynamic motion. This polarization attenuation is modeled by reducing the charge of the positron. The calculation of the effective charge of e^+ as a function of r_p is performed by an energy width minimization principle. With the r_p-dependent positronic charge in hand, the effective e^+-atom potential can be calculated, and the scattering equation for positron is then solved.

In the present work, a diatomiclike model is also used, but with an empirical model potential replacing the positronic kinetic energy operator in calculating the polarized electronic orbitals. The resulting orbitals generate an effective scattering potential for the positron. We hope that this simple semiempirical method will be generally applicable to more complicated one-positron, many-electron systems without undue computation. The present method, described in Sec. II, is shown to give reasonably good results for e^+-H and e^+-He elastic scattering and annihilation rates.

Atomic units are used throughout this paper unless otherwise specified.

II. THEORY AND CALCULATIONS

A. Self-consistent-field equations

The self-consistent-field theory for one-positron, many-electron systems with approximate wave functions of the form

$$\Psi=\psi_p(\mathbf{x}_p)\mathscr{A}\prod_{\mu}\psi_\mu(\mathbf{x}_\mu,\mathbf{r}_p) \tag{5}$$

as derived by Schrader[46] ($\mathbf{x}$ denotes spatial and spin coordinates and $\mathscr{A}$ is the electron antisymmetrizer and normalizer) leads to differential equations for the electronic and positronic orbital functions defined by

$$\psi_\mu=\begin{cases}\phi_i\alpha & \text{for } \mu=2i-1\\ \phi_i\beta & \text{for } \mu=2i\ ,\end{cases}$$

$$\psi_p=\phi_p\alpha\ .$$

The electronic equation is

$$\left[-\frac{1}{2}\nabla_\mu^2-\frac{Z}{r_\mu}-\frac{1}{2}\nabla_p^2-\frac{1}{r_{\mu p}}+\sum_j(2J_j-K_j-\mathbf{B}_j\cdot\nabla_p)-\epsilon_i(r_p)\right]\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)=0\ , \tag{6}$$

and the positronic equation is

$$\left[-\frac{1}{2}\nabla_p^2+\frac{Z}{r_p}+V_{ee}(r_p)-E\right]\phi_p(\mathbf{r}_p)=0\ . \tag{7}$$

The term $\mathbf{B}_j$ appearing in Eq. (6) has an exchange character

$$\mathbf{B}_j\cdot\mathbf{F}(\mathbf{r}_\mu,\mathbf{r}_p)=\langle\phi_j(\mathbf{r}_\nu,\mathbf{r}_p)\,|\,\mathbf{F}(\mathbf{r}_\nu,\mathbf{r}_p)\rangle_\nu\cdot[-\boldsymbol{\nabla}_p\phi_j(\mathbf{r}_\mu,\mathbf{r}_p)]\ , \tag{8}$$

where **F** is an arbitrary vector function. The Coulomb (J_j) and exchange (K_j) integrals are familiar and are r_p dependent. The term V_{ee} in Eq. (7) is identifiable as the effective electronic energy of the one-positron, many-electron system concerned,

$$V_{ee}(r_p)=\sum_i\left\langle\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)\left|2\left[-\frac{1}{2}\nabla_\mu^2-\frac{Z}{r_\mu}-\frac{1}{2}\nabla_p^2-\frac{1}{r_{\mu p}}\right]\right.\right.$$
$$+\sum_j(2J_j-K_j-\mathbf{B}_j\cdot\boldsymbol{\nabla}_p)$$
$$\times\left|\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)\right\rangle_\mu\ . \tag{9}$$

Equation (6) does not depend upon the solution of Eq. (7), so the electronic orbitals ϕ_i and the potential V_{ee} can be calculated independently of ϕ_p. Thus Eq. (7) can also be applied to elastic scattering, even though it was originally formulated for bound states. For scattering systems, the total energy E is the sum of the energy of the incident positron and the ground-state energy of the isolated target E_0,

$$E=\frac{k^2}{2}+E_0\ , \tag{10}$$

where **k** is the wave vector of the positron. By substituting Eqs. (10) into (7) and writing

$$V_{ep}(r_p)=V_{ee}(r_p)-E_0\ , \tag{11}$$

we obtain the positronic equation in the form

$$\left[-\frac{1}{2}\nabla_p^2+\frac{Z}{r_p}+V_{ep}(r_p)-\frac{k^2}{2}\right]\phi_p(\mathbf{r}_p)=0\ . \tag{12}$$

In the present work, the dynamical positron operator, $-\frac{1}{2}\nabla_p^2-\sum_j\mathbf{B}_j\cdot\boldsymbol{\nabla}_p$ in Eqs. (6) and (9), which gives rise to the nonadiabatic effects, is replaced by an empirical model potential of the form of a screened Coulomb potential with a short-range cutoff function,

$$-\tfrac{1}{2}\nabla_p^2-\sum_j\mathbf{B}_j\cdot\boldsymbol{\nabla}_p\rightarrow V_{\mathrm{MP}}(\mathbf{r}_{\mu p},\mathbf{r}_p)$$
$$=(1-c\,e_n^ye^{-y})\frac{b\,e^{-ar_{\mu p}}}{r_{\mu p}}\ , \tag{13}$$

where e_n^y is the incomplete exponential:

$$e_n^y=\sum_{i=0}^{n}\frac{y^i}{i!},\quad y=\frac{r_p}{r_0}\ . \tag{14}$$

The parameters a, b, c, r_0, and n are disposable. Equations (6) and (9) can now be expressed as

$$\left[-\frac{1}{2}\nabla_\mu^2-\frac{Z}{r_\mu}-\frac{1}{r_{\mu p}}+V_{\mathrm{MP}}(\mathbf{r}_{\mu p},\mathbf{r}_p)\right.$$
$$\left.+\sum_j(2J_i-K_j)-\epsilon_i(r_p)\right]\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)=0 \tag{15}$$

and

$$V_{ee}(r_p)=\sum_i\left\langle\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)\left|2\left[-\frac{1}{2}\nabla_\mu^2-\frac{Z}{r_\mu}+V_{\mathrm{MP}}(\mathbf{r}_{\mu p},\mathbf{r}_p)\right]+\sum_j(2J_j-K_j)\right|\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)\right\rangle_\mu\ . \tag{16}$$

Equation (15) is very much simpler to solve than Eq. (6) because $\mathbf{r}_p$ appears in Eq. (15) only as a parameter. Equation (15) is solved for a given value of r_p by the Roothaan-Hall-Hartree-Fock technique: the electronic orbitals $\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)$ are expanded in terms of Slater-type orbitals (STO's) χ_{nlm} each of which is centered on either the atomic nucleus or the positron,

$$\phi_i(\mathbf{r}_\mu,\mathbf{r}_p)=\sum_{n,l,m}c_{i,nlm}\chi_{nlm}\ , \tag{17}$$

where $c_{i,nlm}$, the expansion coefficients for the ith occupied orbital, are functions of r_p. The electronic orbitals are then of diatomic symmetry, with the angular momentum quantization axis coincident with the positron position vector $\mathbf{r}_p$, and they are independent of the positronic function $\phi_p(\mathbf{r}_p)$. By repeating this calculation for different r_p values, V_{ep} is evaluated over an r_p grid, and Eq. (12) is then solved by numerical integration after resolution into its partial wave components.

These are the important features of the present framework: (a) the e^--e^+ correlation and virtual Ps formation are built into the electronic function by the proper choice of STO basis functions; (b) the model potential V_{MP} implicitly takes care of nonadiabatic and reduced mass effects of the e^--e^+ pair through parametrization; and (c) once $V_{ep}(r_p)$ is determined, it can be used in Eq. (12) for any reasonable value of k. The effective e^--e^+ potential $V_{ep}(r_p)$ is thus independent of the positron momentum, yet it includes the diabatic effect as well as the effect of virtual Ps formation.

B. Method of parametrization

We can calibrate our model potential by applying it to positronium and a proton very far removed. Now r_p is very large, so Eq. (15) becomes

$$\left[-\frac{1}{2}\nabla_e^2-\frac{1}{r_{ep}}+\frac{b\,e^{-ar_{ep}}}{r_{ep}}-\tilde{E}\right]\tilde{\phi}_{\mathrm{Ps}}(\mathbf{r}_{ep})=0\ . \tag{18}$$

Substituting the ground-state wave function for Ps

$$\tilde{\phi}_{\mathrm{Ps}}(\mathbf{r}_{ep})=\frac{1}{\sqrt{8\pi}}e^{-0.5r_{ep}}\ , \tag{19}$$

and the ground-state energy $\widetilde{E}=-\frac{1}{4}$, premultiplying by $\widetilde{\phi}_{\text{Ps}}$, and integrating gives a simple relationship between the parameters a and b,

$$b=\frac{(1+a)^2}{4} . \tag{20}$$

This relationship is used throughout our calculations in order to make our model "true" to positronium.

The parameter r_0 is chosen to be proportional to the expectation value of the radius of the valence orbital $\langle r \rangle$ of the isolated target: in this work, we have found from trial calculations that $r_0=2\langle r \rangle$ gives good results. Similarly, trial calculations show that a suitable choice for n is 3–6 and that for a is 1–3. Values of 5 for n and 1 for a are used throughout this work although several other sets of values were used in test calculations.

Of the five parameters a, b, n, r_0, and c, the first three are taken to be universal; i.e., independent of target. The fourth one depends on target size. Once these four are chosen, the last parameter c is then empirically determined. That is, it is adjusted such that the calculated V_{ep} leads to known scattering lengths a_s for the system under consideration. These are $-2.1036a_0$ for e^+-H (Ref. 35) and $-0.472a_0$ for e^+-He [Ref. 36(a)].

C. Basis sets for the electronic orbitals

Normalized Slater-type orbitals, STO's, used for expressing the electronic orbitals [Eq. (17)] are given by

$$\chi_{nlm}(\zeta,r)=\frac{(2\zeta)^{n+1/2}}{\sqrt{(2n)!}}r^{n-1}e^{-\zeta r}Y_{lm}(\vartheta,\varphi) , \tag{21}$$

where $Y_{lm}(\vartheta,\varphi)$ are the normalized spherical harmonics. In selecting basis functions, the concept of even-tempered basis sets[47] is employed.

The sizes of the basis sets and the values of the orbital exponents ζ are determined as follows. When $r_p=0$, the e^+-H system, for example, becomes something like He$^+$; on the other hand, as $r_p \to \infty$, the system becomes H perturbed by a distant unit charge. Thus, the basis functions used should be sufficiently flexible to reflect these structures. Similar remarks hold for the helium target.

The basis functions centered on the positron include the 1s Ps function, Eq. (19), as well as properly chosen p-type STO's. The ground state of Ps is of s symmetry, so these additional p-type STO's have no effect on the calculated $\widetilde{E}$ [Eq. (18)] nor the condition given by Eq. (20).

Table I lists the basis functions used for e^+-H/He elastic scattering.

D. Method of calculation

The SCF diatomic program BISON[48] was modified to solve the electronic Schrödinger equation (15). The positron is treated as a hypothetical proton, so that r_p is identified as the internuclear distance of a hypothetical diatomic molecule. The r_p dependence of the electronic orbitals ϕ_i is obtained by repeating the calculation for different r_p values. The matrix elements of $-1/r_{\mu p}$ are equivalent to those of $-1/r_b$ coded in BISON. The calculation of the matrix elements of the model potential,

$$\langle \chi_{nlm} \mid V_{\text{MP}} \mid \chi_{n'l'm'} \rangle$$

$$=b(1-c\, e_n^{r_p/r_0} e^{-r_p/r_0})\left\langle \chi_{nlm} \left| \frac{e^{-ar_b}}{r_b} \right| \chi_{n'l'm'} \right\rangle , \tag{22}$$

is very straightforward, being quite similar to those of the nuclear attraction integrals coded in BISON.

A grid size of $0.1a_0$ when $r_p \le 7a_0$ for e^+-H and $r_p \le 5a_0$ for e^+-He is used. For r_p values greater than these ranges, a larger grid size of $0.5a_0$ is used for both systems, out to $r_p=20a_0$ for e^+-H and $r_p=10a_0$ for e^+-He. The dipole polarizabilities α_d of H and He are obtained from the slopes of plots of $V_{ep}(r_p)+Z/r_p$ vs $1/2r_p^4$ near the ends of these ranges (15–$20a_0$ for e^+-H and 8–10 for e^+-He). The results are $4.51a_0^3$ for H and $1.334a_0^3$ for He, which are essentially in exact agreement with accurately known values for these parameters. Beyond $r_p=20a_0$ for e^+-H and $10a_0$ for e^+-He, $V_{ep}(r_p)$ is not calculated by running BISON but instead is set equal to its asymptotic form,

$$V_{ep}(r_p) \underset{r_p\to\infty}{\longrightarrow} -\frac{Z}{r_p}-\frac{\alpha_d}{2r_p^4} . \tag{23}$$

With $V_{ep}(r_p)$ thus in hand, Eq. (12) is then solved by the partial wave method[49] for $l \le 4$ to extract phase shifts δ_l. The asymptotic solution for the partial waves $\phi_{p,l}$ have the general form of

$$\phi_{p,l}(k,r_p) \underset{r_p\to\infty}{\longrightarrow} kA_l(k)[j_l(kr_p)\cos\delta_l-\eta_l(kr_p)\sin\delta_l] , \tag{24}$$

where $j_l(x)$ and $\eta_l(x)$ are the spherical Bessel and Neu-

TABLE I. The basis functions used for e^+-H and e^+-He elastic scattering.

Target	No. of STO's n	Type of STO's	Orbital exponents ζ_j $\zeta_{i+1}=\alpha\beta^i$; $i=0,1,\ldots,n-1$
H	6	1s on H	$\alpha=1.0$, $\beta=1.5$
	5	2p on H	$\alpha=1.0$, $\beta=1.5$
	1	1s on e^+	$\zeta=0.5$
	4	2p on e^+	$\alpha=0.5$, $\beta=1.6$
He	6	1s on He	$\alpha=0.9445$, $\beta=1.55$
	4	2p on He	$\alpha=0.8$, $\beta=1.5$
	1	1s on e^+	$\zeta=0.5$
	4	2p on e^+	$\alpha=1.0$, $\beta=1.5$

man functions, respectively, and the constants $A_l(k)$ are subject to the normalization condition

$$A_l(k)=\frac{[4\pi(2l+1)]^{1/2}}{k} \tag{25}$$

which corresponds to one positron per unit volume.

The total elastic cross sections $\sigma_{\text{el}}(k)$ are calculated from the equation

$$\sigma_{\text{el}}(k)=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \ . \tag{26}$$

In addition, partial-wave phase shifts with $4<l\leq 10$ are calculated by the formula

$$\delta_l=\frac{\alpha_d\pi k^2}{(2l-1)(2l+1)(2l+3)} \tag{27}$$

derived by O'Malley *et al.*[50] Contributions to the sum in Eq. (26) for $l>10$ are ignored.

The annihilation parameter $Z_{\text{eff}}(k)$ for e^+-H/He elastic scattering is

$$\begin{aligned} Z_{\text{eff}}(k) &= \sum_{l=0}^{\infty} Z_{\text{eff}}^{(l)}(k) \\ &= n_e \sum_{l=0}^{\infty} \int |\phi_{p,l}(k,\mathbf{r})|^2 |\phi_e(\mathbf{r},\mathbf{r})|^2 d\mathbf{r} \ , \end{aligned} \tag{28}$$

where n_e is the number of electrons in the target. The contributions to $Z_{\text{eff}}(k)$ from partial waves with $l>4$ are small and are neglected.

In terms of scattering length a_s,

$$a_s=-\lim_{k\to 0}\frac{\tan\delta_0}{k} \ , \tag{29}$$

the zero energy partial cross section for the s wave is

$$\sigma_0(0)=\lim_{k\to 0}\frac{4\pi\sin^2\delta_0}{k^2}=4\pi a_s^2 \ , \tag{30}$$

while those for higher partial waves vanish.

Table II lists the parameter defining the potential V_{MP}, Eq. (13).

TABLE II. Parameters used in the model potential, Eq. (13).

	Parameters				
Target	a	b	c	r_0	n
H	1.0	1.0	0.8583	3.0	5
He	1.0	1.0	0.9881	1.854 546	5

III. RESULTS AND DISCUSSION

The target electron(s) is (are) always in a σ orbital as far as the present diatomiclike model is concerned. The total angular momentum of the system is thus carried by the positron. Term splittings due to angular momentum coupling do not result. Spin-spin coupling gives rise to multiplets, however. For e^+-H, the separation of the singlet and triplet terms for each L term (determined by the l value of the positron) is very small, presumably of the order of that for Ps [8.57×10^{-4} eV (Ref. 51)]. They are neglected. Only doublets occur for e^+-He elastic scattering.

The present model, as well as other approximation schemes (e.g., Refs. 13, 29, and 30), allows for only one type of distorted wave symmetry. In general, there are $l+1$ possible symmetries for the lth wave and each distorted wave should be constructed as a linear combination of those spherical harmonics that carry the total angular momentum and parity dependence of the total wave function.[34(b),52] For example, a full treatment of p-wave e^+-H scattering would entail the mixing of the (major) p-positron + s-electron configuration with the (minor) s-positron + π-electron configuration. We ignore these minor configurations in this work, although they probably become more important for higher incident energies than considered here.

A. Positron-hydrogen elastic scattering

Table III lists our calculated phase shifts for e^+-H elastic scattering. The lower partial-wave phase shifts and total cross sections are shown in Figs. 1–3. The most ac-

TABLE III. Phase shifts and cross sections for e^+-H elastic scattering.

k (a_0^{-1})	δ_0 (rad)	δ_1 (rad)	δ_2 (rad)	δ_3 (rad)	δ_4 (rad)	σ_{el} (πa_0^2)
0.00	−2.103 74[a]					17.7029
0.05	0.090 02	0.002 31	0.000 34	0.000 11	0.000 05	12.9575
0.10	0.146 60	0.009 04	0.001 36	0.000 45	0.000 20	8.6378
0.15	0.173 95	0.019 65	0.003 09	0.001 01	0.000 46	5.5415
0.20	0.179 39	0.033 28	0.005 62	0.001 81	0.000 82	3.5349
0.25	0.169 56	0.048 75	0.009 00	0.002 84	0.001 28	2.3095
0.30	0.149 63	0.064 64	0.013 32	0.004 15	0.001 84	1.5910
0.35	0.123 37	0.079 58	0.018 55	0.005 76	0.002 52	1.1804
0.40	0.093 54	0.092 42	0.024 60	0.007 71	0.003 32	0.9470
0.45	0.062 12	0.102 38	0.031 28	0.010 04	0.004 26	0.8109
0.50	0.030 47	0.109 10	0.038 32	0.012 77	0.005 35	0.7262
0.55	−0.000 44	0.112 57	0.045 39	0.015 89	0.006 62	0.6682
0.60	−0.030 02	0.113 05	0.052 17	0.019 36	0.008 09	0.6245
0.65	−0.057 90	0.110 96	0.058 36	0.023 11	0.009 76	0.5887
0.70	−0.083 90	0.106 78	0.063 72	0.027 04	0.011 64	0.5575

[a] Scattering length (a_0).

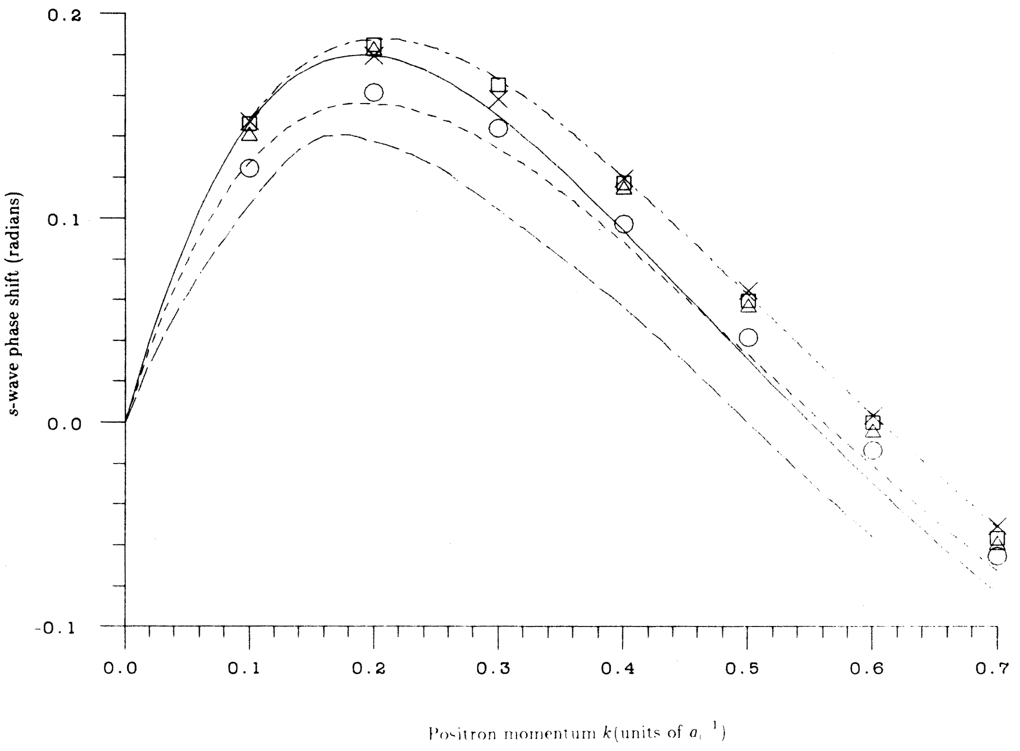

FIG. 1. Elastic s-wave phase shifts for e^+-H scattering. Legend: ——, present work (Table III); — — —, polarization and virtual positronium (Ref. 55); - - -, modified adiabatic [Ref. 28(b)]; —·—·—·, accurate [Ref. 34(a)]; □, Harris-Nesbet variational (Ref. 54); ×, T matrix (Ref. 53); △, close coupling with correlation (Ref. 42); ○, coupled SCF [Ref. 40(a)].

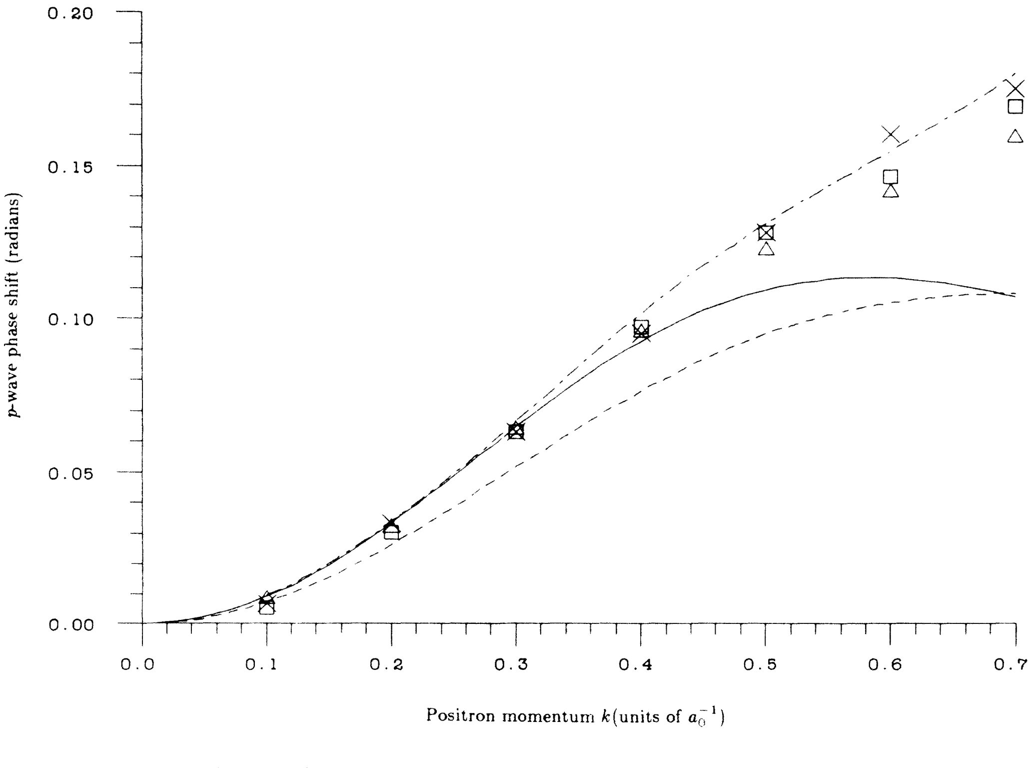

FIG. 2. Elastic p-wave phase shifts for e^+-H scattering. Legend: ——, present work (Table III); — — —, modified adiabatic [Ref. 28(b)]; —·—·—·, accurate [Ref. 34(b)]; □, Harris-Nesbet variational (Ref. 54); ×, T matrix (Ref. 53); △, close-coupling with correlation (Ref. 43).

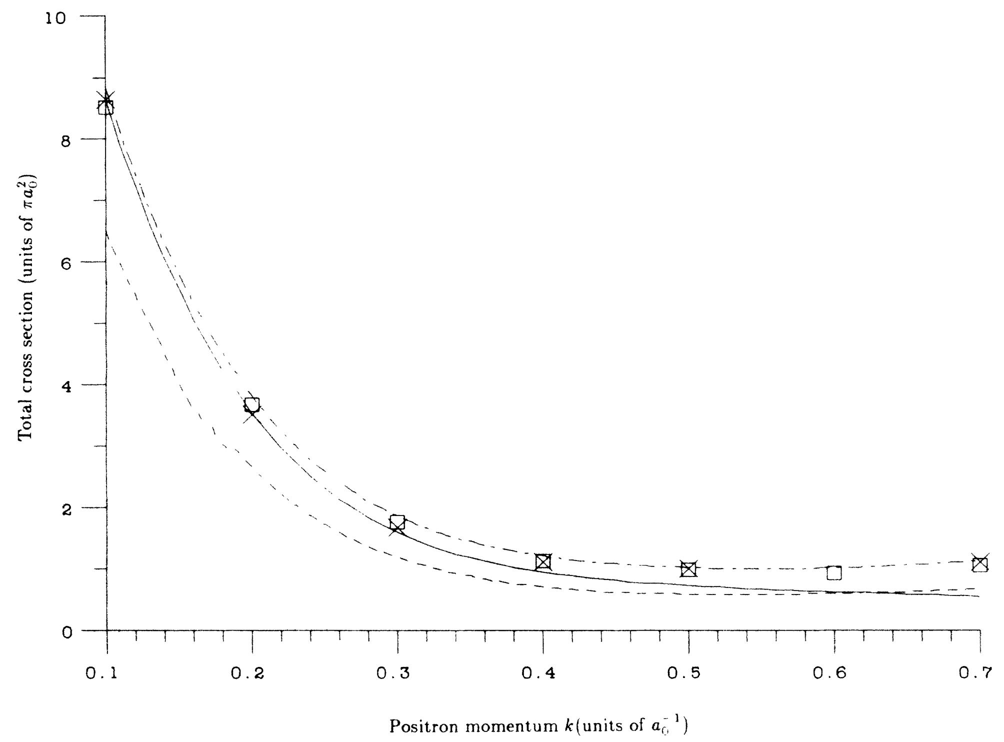

FIG. 3. Total cross section for elastic e^+-H scattering. Legend: ——, present work (Table III); — — —, modified adiabatic [Ref. 28(b)]; —·—·—·, accurate [Ref. 34(c)]; □, Harris-Nesbet variational (Ref. 54); ×, T matrix (Ref. 53).

curate calculation of the total cross section[34] shows a very shallow minimum, as do other *ab initio* calculations.[53–55] Its absence in the present work and in other semiempirical work[14(a)] is mainly due to the underestimation of the p- and d-wave phase shifts for $k > 0.4a_0^{-1}$. Overall, the present results are satisfactory compared to the best values.

Numerical values of $Z_{\rm eff}$ are given in Table IV. The quality of our s-wave contribution is as good as the coupled SCF results of Horbatsch, Darewych, and McEachran.[40(a)] It is worthwhile to note that the $Z_{\rm eff}$ of Chan and Fraser,[42] calculated by using the two-state CCA with 26 correlation terms, are inferior to our results, while the reverse is true for δ_0 and δ_1. It should be mentioned that the error in $Z_{\rm eff}$ is of first order in the error of the wave function whereas the errors in phase shifts are of second order. In Fig. 4, our total $Z_{\rm eff}$ values are shown as well as the results of other calculations. Our results are encouraging in view of the simple theoretical framework of the model.

TABLE IV. The annihilation parameters $Z_{\rm eff}^{(l)}$ for e^+-H elastic scattering.

$k(a_0^{-1})$	$Z_{\rm eff}^{(0)}$	$Z_{\rm eff}^{(1)}$	$Z_{\rm eff}^{(2)}$	$Z_{\rm eff}^{(3)}$	$Z_{\rm eff}^{(4)}$	$Z_{\rm eff}$[a]
0.00	8.5919					8.592
0.05	8.0533	0.0409	0.0001	0.0000	0.0000	8.096
0.10	7.0562	0.1610	0.0017	0.0000	0.0000	7.219
0.15	6.0305	0.3499	0.0083	0.0001	0.0000	6.389
0.20	5.1319	0.5588	0.0245	0.0008	0.0000	5.716
0.25	4.3899	0.8520	0.0551	0.0026	0.0001	5.300
0.30	3.7903	1.1120	0.1034	0.0070	0.0004	5.013
0.35	3.3083	1.3452	0.1707	0.0155	0.0011	4.841
0.40	2.9200	1.5355	0.2555	0.0298	0.0028	4.744
0.45	2.6057	1.6758	0.3540	0.0516	0.0060	4.693
0.50	2.3494	1.7671	0.4607	0.0816	0.0116	4.670
0.55	2.1390	1.8155	0.5694	0.1203	0.0202	4.664
0.60	1.9646	1.8298	0.6740	0.1670	0.0327	4.668
0.65	1.8189	1.8189	0.7694	0.2205	0.0495	4.677
0.70	1.6958	1.7909	0.8521	0.2787	0.0711	4.689

[a] $Z_{\rm eff} = \sum_{l=0}^{l=4} Z_{\rm eff}^{(l)}$.

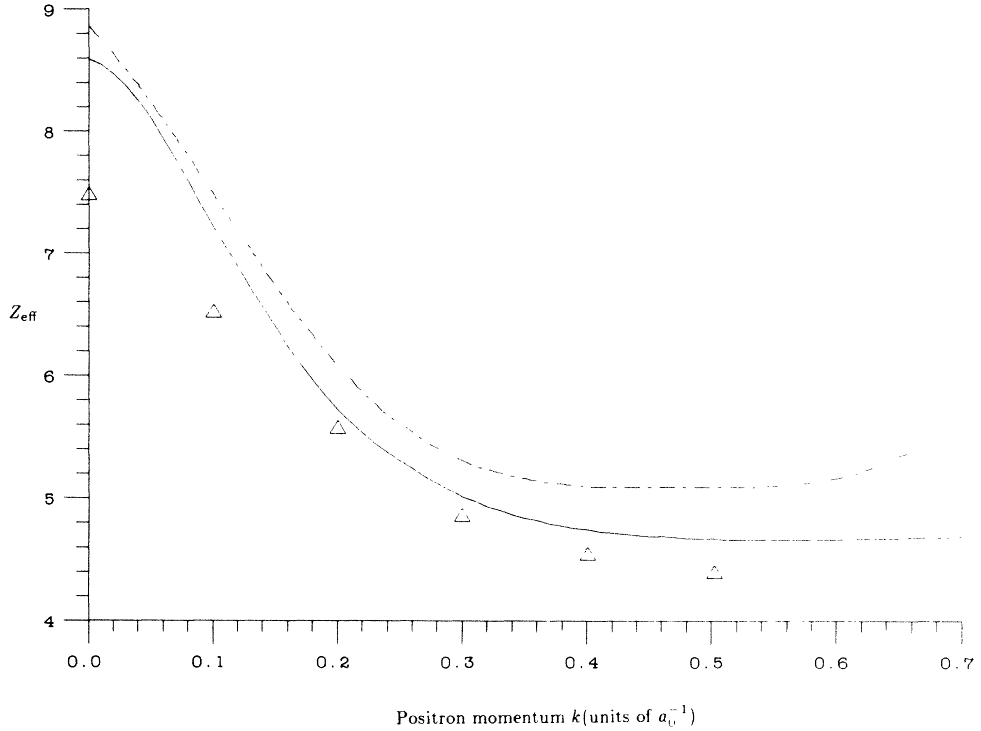

FIG. 4. Annihilation parameters Z_{eff} for elastic e^+-H scattering. Legend: ——, present work (Table IV); —·—·—·, accurate [Ref. 34(c)]; △, close-coupling with correlation (Refs. 42 and 43).

B. Positron-helium elastic scattering

Intuitively, it is expected that nonadiabatic effects are smaller for the heavier atom. For He, each electron has an average kinetic energy of 39.5 eV while that of the positron is less than the Ps formation threshold (17.8 eV). In the case of e^+-H, the mean kinetic energy of the atomic electron is 13.6 eV and that of the positron is less than the corresponding Ps formation threshold (6.8 eV). One can see that the positron moves somewhat slower relative to the target electron(s) for He than for H. The parametrized value of c for V_{MP} (Table II) is larger for the e^+-He system than for e^+-H. In view of the proposed functional form of the model potential, this indicates that the nonadiabatic correction required for the former is less than for the latter. Perhaps this semiclassical criterion for the adiabatic approximation is the key for the success of the polarized orbital calculations of McEachran *et al.*[29]

The calculated phase shifts and Z_{eff} are presented in Tables V and VI, respectively. The lower partial-wave phase shifts and total cross sections are shown in Figs. 5–7 along with other theoretical results[28,29,36–38,56,57] for comparison. For helium, high quality measurements of the total cross section have recently become available,[58–61] and these results are also shown. All the theoretical results shown reproduce the Ramsauer-Townsend minimum first observed by Stein and coworkers.[58] Our results are in good agreement with the accurate results (model H5) of Campeanu and Humberston.[36,37]

An indication of the importance of e^--e^- correlation is provided by the difference between the σ_{el} for model H5 (Ref. 37) and for model DB [Ref. 28(b)]. The former involves using an e^--e^- correlated target function while the latter does not. The effects are small but unmistakable. Since He is less polarizable than H, virtual Ps formation is expected to be less significant. Without virtual Ps formation, Amusia *et al.*[38] found that the cross-section minimum shifts to a lower k value and becomes deeper. For $k \geq 0.4a_0^{-1}$, the influence of virtual Ps on the elastic channel is insignificant. This is in conjunction with the poor s-wave phase shifts given by the close-coupling calculation of Ho *et al.*[56] and Wardle.[57] Inclusion of the Ps channel only is obviously inadequate. In contrast to the e^+-H case, it seems that virtual excitations are the dominant processes governing the e^+-He elastic collision.

Our values for Z_{eff} are given in Fig. 8. Other results are also presented for comparison. Test calculations show that for e^+-He, as for e^+-H, increasing the value of the parameter a for V_{MP} gives less accurate Z_{eff} values, but the resulting cross sections are slightly better. Overall the present results are satisfactory.

Z_{eff} values as calculated by the polarized orbital method[29] are amazingly good in spite of its use of first-order adiabatic polarized orbitals. It is rather surprising

TABLE V. Phase shifts and cross sections for e^+-He elastic scattering.

k (a_0^{-1})	δ_0 (rad)	δ_1 (rad)	δ_2 (rad)	δ_3 (rad)	δ_4 (rad)	$\sigma_{\rm el}$ (πa_0^2)
0.00	−0.471 99[a]					0.8911
0.05	0.020 09	0.000 65	0.000 10	0.000 03	0.000 02	0.6478
0.10	0.033 56	0.002 40	0.000 40	0.000 13	0.000 06	0.4576
0.15	0.041 35	0.005 01	0.000 88	0.000 30	0.000 13	0.3180
0.20	0.044 35	0.008 31	0.001 53	0.000 53	0.000 24	0.2187
0.25	0.043 32	0.012 16	0.002 31	0.000 82	0.000 42	0.1506
0.30	0.038 82	0.016 49	0.003 23	0.001 16	0.000 54	0.1061
0.35	0.031 37	0.021 18	0.004 29	0.001 53	0.000 73	0.0799
0.40	0.021 42	0.026 08	0.005 50	0.001 95	0.000 93	0.0672
0.45	0.009 44	0.031 00	0.006 91	0.002 39	0.001 19	0.0646
0.50	−0.004 13	0.035 73	0.008 53	0.002 87	0.001 40	0.0688
0.55	−0.018 89	0.040 06	0.010 37	0.003 42	0.001 64	0.0771
0.60	−0.034 47	0.043 86	0.012 40	0.004 05	0.001 92	0.0878
0.65	−0.050 59	0.047 00	0.014 58	0.004 78	0.002 19	0.0993
0.70	−0.067 00	0.049 43	0.016 85	0.005 61	0.002 48	0.1106
0.75	−0.083 51	0.051 12	0.019 17	0.006 54	0.002 83	0.1214
0.80	−0.099 97	0.052 06	0.021 49	0.007 56	0.003 23	0.1311
0.85	−0.116 25	0.052 27	0.023 77	0.008 66	0.003 68	0.1397
0.90	−0.132 23	0.051 78	0.025 96	0.009 83	0.004 18	0.1470
0.95	−0.147 66	0.050 64	0.028 04	0.011 06	0.004 74	0.1529
1.00	−0.163 08	0.048 92	0.029 95	0.012 33	0.005 33	0.1582
1.05	−0.177 86	0.046 67	0.031 68	0.013 64	0.005 97	0.1623
1.10	−0.192 17	0.043 95	0.033 20	0.014 95	0.006 65	0.1655

[a] Scattering length (a_0).

that there have been no published data for e^+-H scattering using the same method.

The similar diatomiclike approach of Pai *et al.*[45] has the advantage that the method is nonphenomenological although the computational procedure is rather laborious. In view of the present work, it is expected that their results would have been improved if they had used a proper basis set. The size of their basis set used is too small to describe adequately the e^+-He system for the entire range of r_p, as explained above. In their work, only *s*-type STO's were imposed on the He target which is then not properly polarized. In addition, the orbital exponent of

TABLE VI. The annihilation parameters $Z_{\rm eff}^{(l)}$ for e^+-He elastic scattering.

k (a_0^{-1})	$Z_{\rm eff}^{0}$	$Z_{\rm eff}^{(1)}$	$Z_{\rm eff}^{(2)}$	$Z_{\rm eff}^{(3)}$	$Z_{\rm eff}^{(4)}$	$Z_{\rm eff}$[a]
0.00	3.7003					3.700
0.05	3.6473	0.0064	0.0000	0.0000	0.0000	3.654
0.10	3.5387	0.0273	0.0001	0.0000	0.0000	3.566
0.15	3.4045	0.0609	0.0004	0.0000	0.0000	3.466
0.20	3.2589	0.1066	0.0014	0.0000	0.0000	3.367
0.25	3.1099	0.1631	0.0033	0.0001	0.0000	3.276
0.30	2.9627	0.2287	0.0066	0.0002	0.0000	3.198
0.35	2.8206	0.3015	0.0117	0.0004	0.0000	3.314
0.40	2.6858	0.3792	0.0189	0.0008	0.0000	3.085
0.45	2.5598	0.4597	0.0288	0.0015	0.0001	3.050
0.50	2.4430	0.5407	0.0413	0.0027	0.0002	3.028
0.55	2.3354	0.6205	0.0567	0.0044	0.0003	3.017
0.60	2.2367	0.6975	0.0751	0.0068	0.0005	3.017
0.65	2.1461	0.7705	0.0961	0.0100	0.0009	3.024
0.70	2.0629	0.8385	0.1198	0.0141	0.0015	3.037
0.75	1.9866	0.9011	0.1457	0.0194	0.0023	3.055
0.80	1.9164	0.9581	0.1736	0.0257	0.0035	3.077
0.85	1.8517	1.0093	0.2030	0.0332	0.0050	3.102
0.90	1.7919	1.0548	0.2336	0.0419	0.0069	3.129
0.95	1.7365	1.0951	0.2649	0.0518	0.0093	3.158
1.00	1.6849	1.1303	0.2967	0.0629	0.0122	3.187
1.05	1.6369	1.1609	0.3285	0.0749	0.0156	3.217
1.10	1.5920	1.1872	0.3601	0.0880	0.0197	3.247

[a] $Z_{\rm eff}=\sum_{l=0}^{l=4} Z_{\rm eff}^{(l)}$

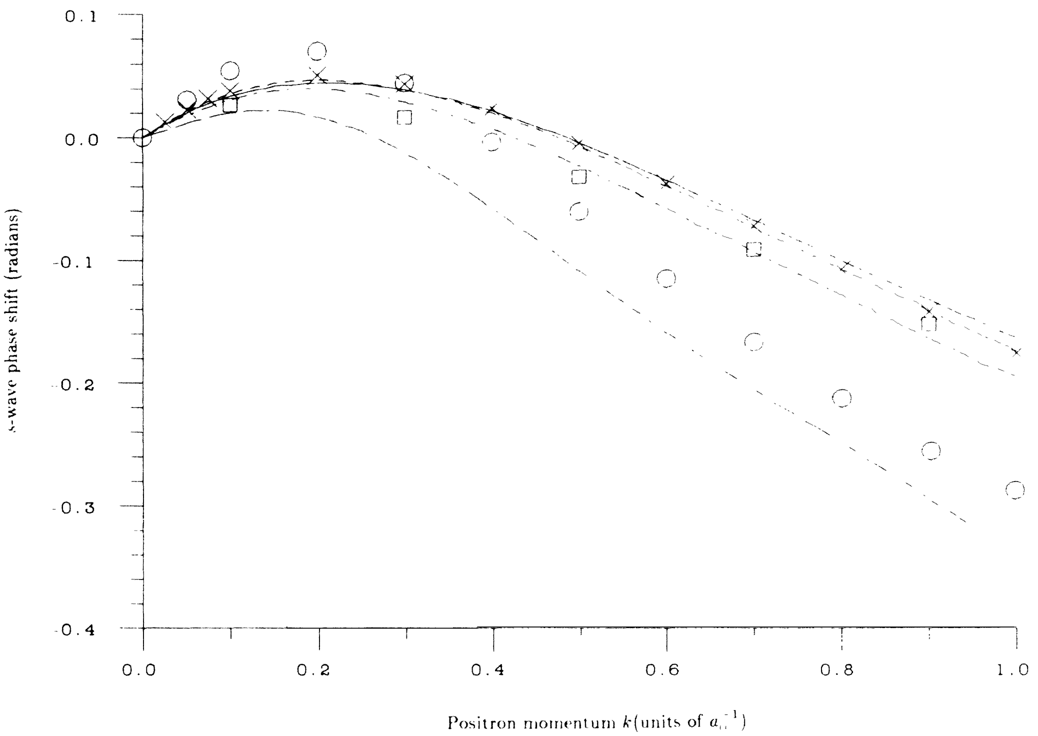

FIG. 5. Elastic s-wave phase shifts for e^+-He scattering. Legend: ——, present work (Table V); — — —, coupled static (Ref. 56, model HY2); - - -, modified adiabatic [Ref. 28(b)]; —·—·—·, accurate (Ref. 36); □, random phase with virtual positronium (Ref. 38); ×, polarized orbital [Ref. 29(a)]; ○, static plus virtual positronium (Ref. 57).

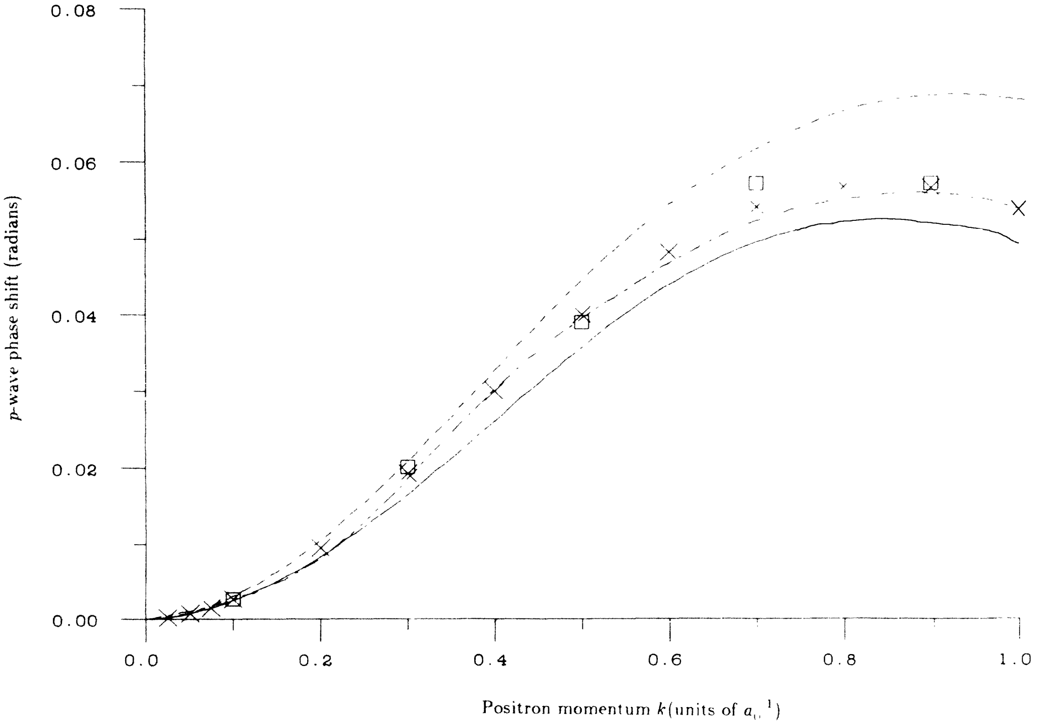

FIG. 6. Elastic p-wave phase shifts for e^+-He scattering. Legend: ——, present work (Table V); - - -, modified adiabatic [Ref. 28(b)]; —·—·—·, accurate (Ref. 37); □, random phase with virtual positronium (Ref. 38); ×, polarized orbital [Ref. 29(a)].

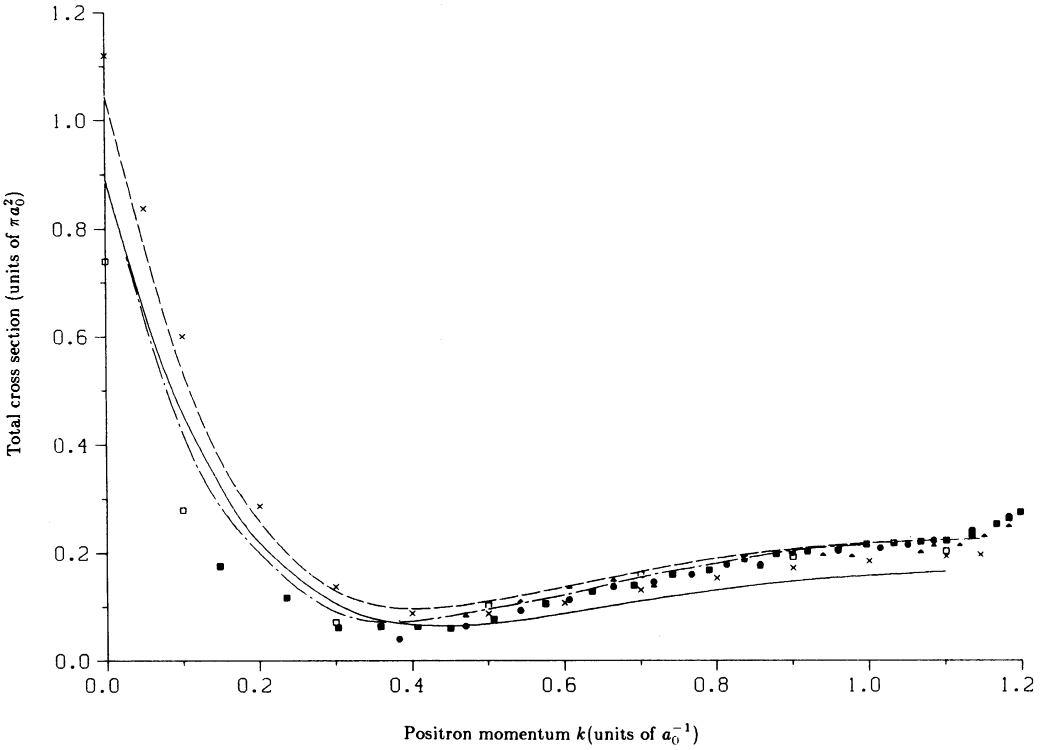

FIG. 7. Total cross section for elastic e^+-He scattering. Legend: ——, present work (Table V); — — —, modified adiabatic (Ref. 28); —·—·—·, accurate [Ref. 36(b)]; □, random phase with virtual positronium (Ref. 38); ×, polarized orbital [Ref. 29(a)]; ■, experiment (Ref. 58); ▲, experiment (Ref. 59); ●, experiment (Ref. 60).

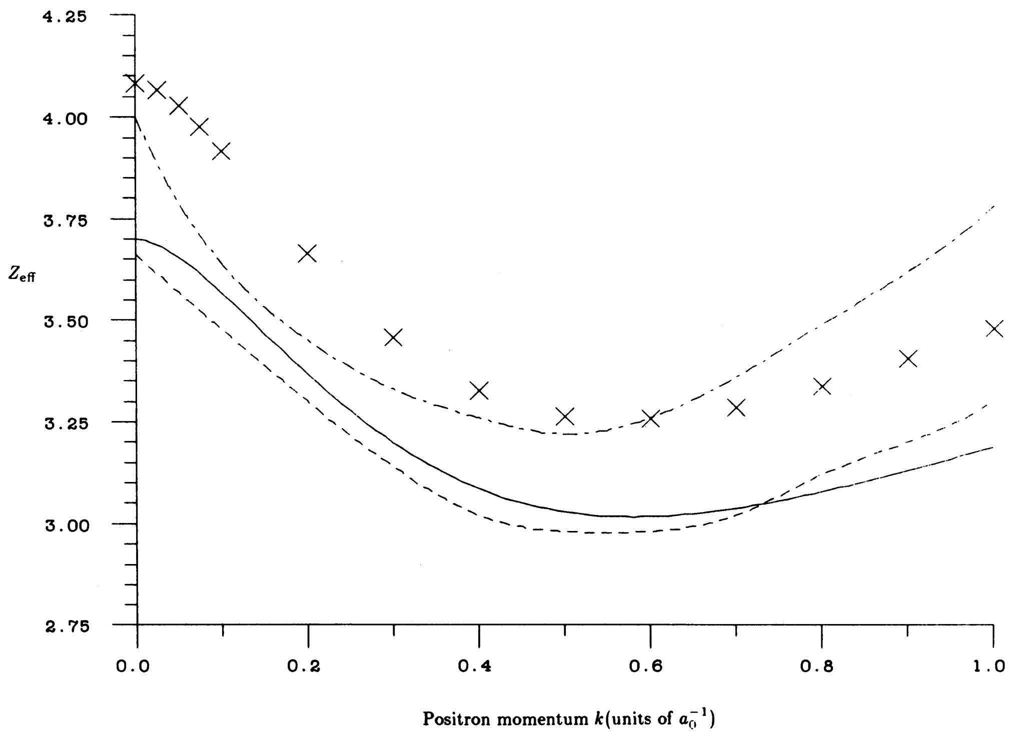

FIG. 8. Annihilation parameters Z_{eff} for elastic e^+-He scattering. Legend: ——, present work (Table VI); — — —, modified adiabatic [Ref. 28(b)]; —·—·—·, accurate [Ref. 37(b)]; ×, polarized orbital [Ref. 29(a)].

the 1*s* STO centered on the positron is other than (the positronium parameter) 0.5.

IV. CONCLUSION

The present results for both e^+-H and e^+-He scattering suggest that the model can be extended to other one-positron, many-electron atomic systems provided that their scattering lengths or some other properties are known. It may be even possible to correlate the parameter c for V_{MP} with known atomic properties (such as dipole polarizabilities, ionization potentials, etc.) by an empirical formula with the other parameters fixed as proposed in the present work. Certainly, this requires one or two more test systems for calibration. One convenient choice would be e^+-H$^-$. For this one-positron, two-electron atomic system, the parameter c would then be adjusted such that the $V_{ep}(r_p)$ in Eq. (12) gives the known binding energy of e^+ to H$^-$. Once the method is calibrated in this way, it can be applied to larger one-positron, many-electron systems such as e^+-noble-gas, e^+-halogen, etc., without knowledge of any scattering parameters.

Since Eq. (15) is uncoupled from Eq. (12), one may parametrize a proposed model potential for $V_{ep}(r_p)$ by applying Eq. (12) directly without going through Eq. (15). This procedure requires less computation and perhaps the results for scattering cross sections are more reliable. However, evaluation of the complete wave function can provide additional information such as the annihilation rates and the angular correlation of the two γ rays produced during annihilation.

One may reverse the computational sequence if a reliable V_{ep} is in hand. The desired $V_{ee}(r_p)$ can be determined by Eq. (11) easily. Then Eq. (15) may be used to calculate the closed-channel function by adjusting c for each r_p such that the desired $V_{ee}(r_p)$ is obtained.

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