

## Simple but accurate calculations on the elastic scattering of electrons and positrons from neon and argon

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The method for constructing model polarization potentials for electron- and positron-atom systems, previously presented for targets containing up to two electrons, is extended to neon and argon targets. The empirical character of the method is reduced to the determination of a single effective radius for each target, so that electron scattering calculations can be carried out by reference to positron scattering data, or vice versa. In this work, electron data are used to fix the value of the effective radius of each target, which is then used in positron scattering calculations. For electron scattering, exchange is approximated by a local effective potential with two adjustable parameters. The calculated elastic total and differential cross sections are nevertheless in excellent agreement with recent experimental values and are as accurate as the results from much more elaborate calculations.

### I. INTRODUCTION

Low-energy electron scattering in neon and argon gases has received intense attention for more than six decades since the pioneering work of Ramsauer and Townsend,<sup>1</sup> and there have been numerous advances in both experiment and theory, especially in the last few years. Great efforts have been devoted to lower the minimum energy for both transmission and crossed-beam experiments.<sup>2</sup> Since the total cross section increases rapidly as the incident electron energy goes to zero, precise measurements in the sub-electron-volt region are essential to obtain an accurate scattering length, even with the aid of the modified effective range theory (MERT).<sup>3,4</sup> The scattering length has theoretical as well as practical importance.

In the thermal energy region, electron-swarm experiments, either dc or ac (microwave) methods, have dominated experiments for many years and still have a little advantage over beam experiments in terms of convenience and the lower energy limit (e.g.,  $E_{\min}=3$  meV for neon<sup>5</sup> and  $E_{\min}=14$  meV for argon.<sup>6,7</sup>) They have, however, several disadvantages. In particular, they are not direct measurements; thus the accuracy of the final results, usually momentum-transfer cross sections, depends on the method of data analysis. An alternative method, electron-cyclotron-resonance (ECR) spectroscopy,<sup>8</sup> also suffers from a lengthy data analysis, although this method is free from averaging over an energy interval and gives continuous momentum-transfer cross sections (e.g.,  $E=10$  meV to 1 eV for neon and argon<sup>8</sup>).

For example, total cross sections have been measured down to 80 meV for argon<sup>9</sup> using a linearized Ramsauer technique and 20 meV for molecular hydrogen,<sup>10</sup> 25 meV for neon,<sup>11</sup> and 80 meV for argon<sup>12</sup> using a time-of-flight (TOF) technique. Measurements thus cover the Ramsauer-Townsend minimum for argon at 0.34 eV, and they show fairly good agreement among them and with the values<sup>4</sup> obtained from MERT using swarm data.<sup>6,7</sup> Crossed-beam experiments, on the other hand, offer a

direct observation of differential cross sections which can be easily decomposed into the partial-wave phase shifts, thus providing a more detailed comparison with theoretical results. These experiments, however, become extremely difficult as incident energies decrease since they require very intense and well-resolved beams. Only recently has this method been used to measure the differential cross sections which cover the Ramsauer-Townsend minimum for argon, krypton, and xenon.<sup>13</sup>

Positron scattering is becoming increasingly active and important (see recent reviews by Charlton,<sup>14</sup> Raith,<sup>15</sup> and Kauppila and Stein<sup>16,17</sup>). There are rather large differences among data for low-energy elastic scattering. For instance, the data for neon and argon below the positronium formation threshold from several research groups differ by about 30%, while recent direct measurements on those targets for electron scattering agree within 3% for neon<sup>18</sup> and 5% for argon. Only a few positron differential cross-section measurements have been reported to date. The first measurement was made by Coleman and McNutt<sup>19</sup> for positron-argon scattering in the energy range 2–9 eV with angular range 20°–60° using a TOF method. The first crossed-beam measurements have been made recently by Kauppila and co-workers for helium and argon in the energy range 4–20 eV at 90°,<sup>20</sup> and good agreement with theoretical values has been reported. They have recently presented their elastic differential cross section measurements for  $e^{\pm}$ -Ar at energies of 100 and 200 eV from 30° to 135°.<sup>21</sup>

Theoretical studies for low-energy electron scattering from neon and argon have also advanced significantly during the last decade. Among many theoretical approaches the  $R$ -matrix (RMM), polarized-orbital (POM), and optical potential methods (OPM) have gained popularity and yield quite satisfactory results, judging from the comparison with experimental values. The most recent calculations of low-energy electron scattering have been carried out by Fon and Berrington<sup>22</sup> (RMM) and by Dasgupta and Bhatia<sup>23</sup> (POM) for neon, and by Bell *et al.*<sup>24</sup> (RMM), by Dasgupta and Bhatia<sup>25</sup> (POM), and by Amu-

sia *et al.*<sup>26</sup> (OPM) for argon. Some of these methods are essentially free from *ad hoc* adjustments, although in other cases fitting, renormalization, etc., have been made to obtain better agreement with experimental data, especially at very low energy. Another approach known as the model potential or pseudopotential method (MPM) has been widely used because of its simplicity and applicability to large atoms and molecules, where the exchange (see, e.g., Refs. 27 and 28) and polarization effects (see, e.g., Ref. 29) are modeled by simple functions with adjustable parameters.

For purposes of performing calculations, a positron is taken to be a distinguishable electron with positive charge. Thus existing computational methods for electronic systems can be readily applied to positronic systems (see recent reviews by Drachman,<sup>30</sup> McEachran,<sup>31</sup> and Ghosh *et al.*<sup>32</sup>), except that one may want to make allowance for positronium formation. For neutral atomic targets, the static and polarization potentials are additive for electrons but tend to cancel for positrons. Thus positrons are much more sensitive probes of such targets, and accurate determination of polarization effects is important to obtain accurate phase shifts for positron scattering. Moreover, the polarization potential for positronic systems is not exactly the same as that for electronic systems. Therefore a simple transformation of computer codes from electronic systems does not guarantee good results for positronic systems. Most recent calculations were carried out by Câmpeanu and Dubau<sup>33</sup> using a close-coupling method (CCM), by Schrader<sup>34</sup> (MPM) and by McEachran *et al.*<sup>35</sup> (POM) for neon, and by Datta *et al.*,<sup>36</sup> by Schrader<sup>34</sup> (MPM), and by McEachran *et al.* (POM) for argon.

In the preceding paper<sup>29</sup> we proposed empirical relationships among the effective target radii which enable one to relate model polarization potentials for electronic systems to those of corresponding positronic systems, in cases where the target atom contains one or two bound electrons. In the present work we extend this idea to larger targets. This is an important feature of our approach. Most authors are interested in either electrons or positrons but not both, while the few who consider both projectiles in model potential calculations typically parametrize independently or assume effective target radii to be the same for each. They are not the same, however, due to differences in the projectile-target potentials. In our approach, we rationalize the difference by appealing to exclusion and angular-momentum effects in pairwise interactions.

Since there is no previous model potential calculation which accounts satisfactorily for electron scattering at very low energy due to errors in the local exchange potential, a local exchange potential which has the correct behavior at all energy ranges studied is devised and is described in the next section. The last part of Sec. II is devoted to the deduction of effective target radii by considering pair interactions developed earlier.<sup>29</sup> In Sec. III our results for  $e^\pm$ -Ne and -Ar scattering are given and compared to recent experimental and other theoretical results.

Atomic units are used throughout in this paper unless otherwise stated.

## II. CALCULATIONS

### A. Scattering equations

The Schrödinger equation for the scattering wave function  $\phi_k$  for an incident particle with momentum  $k$  interacting with a neutral-closed-shell atom is

$$\left[ -\frac{1}{2}\nabla^2 + qV_s(r) - \delta_{q,-1}V_{ex}(r) + V_p(r) - \frac{k^2}{2} \right] \phi_k(\mathbf{r}) = 0, \quad (1)$$

where  $q$  is the charge of the incident particle,  $V_s$  is the static potential due to the nucleus and orbital electrons, and  $V_{ex}$  is the exchange potential. The Coulomb integrals in  $V_s$  are calculated from Hartree-Fock atomic wave functions tabulated by Clementi and Roetti.<sup>37</sup> The evaluation of  $V_{ex}$ , which is absent in positronic systems, is described in the next section. The effects of target polarization are included through a local effective potential  $V_p$  which has the functional form

$$V_p(r) = -\frac{\alpha_d}{2r^4} w\left(\frac{r}{\rho}\right). \quad (2)$$

$w$ , the cutoff function, is defined as

$$w(\xi) = (1 - e_n^\xi e^{-\xi})^m \quad (m=2, n=8). \quad (3)$$

Here,  $\alpha_d$  is the dipole polarizability of the target atom ( $2.663a_0^3$  for neon and  $11.08a_0^3$  for argon<sup>38</sup>), and  $e_n^\xi$  is the power series for the exponential function, truncated after the  $n$ th power of  $\xi$ .  $\rho$  is an adjustable parameter which is related to the effective target radius  $r_0$  by  $r_0 = 10.617\rho$  [see Eqs. (10) and (11) in Ref. 29 for details]. The method for determining  $r_0$  for neon and argon is given in Sec. II C.

Equation (1) is numerically integrated from the origin for each partial wave up to  $l=4$  using the subroutine DIFFSYS (Ref. 39) until the phase shift achieves convergence to five significant figures. Contributions from partial waves beyond  $l=4$  are taken into account by the effective range formula of O'Malley *et al.*<sup>40</sup> Total and differential elastic cross sections and momentum-transfer cross sections are then calculated.

### B. Exchange potential

The indistinguishability of electrons introduces a nonlocal term, the exchange potential, into the scattering equation. Although the equation can be solved with or without the contribution from polarization (called exchange-polarization and exchange-adiabatic approximations, respectively), it adds a considerable amount of computation time. Therefore a variety of local effective exchange potentials have been proposed to model the exchange effect by a simple free-electron-gas approximation since the original work of Slater.<sup>41</sup>

The general form of the local exchange potential in the free-electron-gas approximation may be expressed as

$$V_{ex}(r) = -\frac{2}{\pi} k_F(r) F(\eta), \quad (4)$$

where  $k_F$  is the Fermi-electron momentum of the target atom and  $F$  is the Fermi-electron distribution function defined as

$$k_F(r) = [3\pi^2 N(r)]^{1/3}, \quad (5)$$

$$F(\eta) = \frac{1}{2} + \frac{1-\eta^2}{4\eta} \ln \left| \frac{1+\eta}{1-\eta} \right|.$$

Here,  $N(r)$  is the electronic density of the target atom as calculated from Hartree-Fock atomic wave functions.<sup>37</sup>  $\eta$  is the momentum of the scattering electron normalized to the Fermi momentum, i.e.,  $\eta = K/k_F$ , and  $K$  is the momentum of the scattering electron, which differs from the initial momentum  $k$ .

Hara<sup>42</sup> initially estimated  $K$  from  $K^2 = k^2 + 2V_{\text{ion}} + k_F^2$ , where  $V_{\text{ion}}$  is the first ionization potential of the target. Morrison and Collins<sup>43</sup> found that much better results can be obtained by adjusting the value of  $V_{\text{ion}}$  in Hara's form. Riley and Truhlar<sup>27</sup> proposed the asymptotically adjusted form  $K^2 = k^2 + k_F^2$ . Noticing that the correct partial-wave phase shifts always lie between those calculated from Hara's form and the asymptotically adjusted form, they modified Hara's form as

$$K^2 = k^2 + 4V_{\text{ion}}/(2+k^2) + k_F^2,$$

which approaches Hara's form at low incident energies and the asymptotically adjusted form at high energies. Recently, Ghosh *et al.*<sup>44</sup> used this modified form for the electron-helium scattering calculations while imposing the orthogonality condition for the  $s$  scattering wave. Khan *et al.*<sup>45</sup> introduced a parameter  $\lambda$  as

$$K^2 = k^2 + 2V_{\text{ion}}/(1+\lambda k^2) + k_F^2,$$

where  $\lambda$  is set to be 30 in their electron-helium scattering calculations instead of imposing the orthogonality condition.

The modified form gives phase shifts which are moderately accurate at low energies and very accurate at high energies. It is, however, of great importance in our application to have an accurate scattering length, so we introduce an additional parameter  $\kappa$ :

$$K^2 = k^2 + \frac{2V_{\text{ion}}}{\kappa + \lambda k^2} + k_F^2. \quad (6)$$

$\kappa$  is then adjusted to reproduce the static-exchange scattering length ( $1.064a_0$  for neon<sup>23,46</sup> and  $1.50a_0$  for argon<sup>47</sup>), which turns out to be 2.65 for both neon and argon. Instead of imposing the orthogonality condition, we set  $\lambda = 6$ . This choice is made from comparisons of our calculated static-exchange phase shifts with the best available values.<sup>23,25,46-48</sup> Thus the local exchange potential used in this work is given by Eqs. (4)–(6) with  $\kappa = 2.65$  and  $\lambda = 6.0$  for both neon and argon. Although the orthogonality condition does not apply to the higher scattering waves, we use the same exchange potential for all partial waves.

### C. Effective target radius

In Ref. 29 we obtained several empirical relationships among the effective target radii  $r_0$  for positronic and elec-

tronic systems where the target contains one or two electrons. These enabled us to reduce the parametrization for a given target to a single effective radius which is the same for both incident particles. In order to extend our approach to more complicated targets, it is useful to introduce reduced effective radii  $\tilde{r}_0$  for each incident particle-target electron pair, and to consider a target radius to be the sum of pair contributions. To the symbol  $\tilde{r}_0$  we append a subscript to indicate the partial wave, a superscript to indicate the scattering particle (if the latter is an electron, the projectile-plus-target spin multiplicity is indicated), and parenthetical arguments to denote the target. Thus  $\tilde{r}_{0,s}^+(\text{H})$  is the reduced effective radius for  $s$ -wave positron scattering from a hydrogen atom,  $\tilde{r}_{0,d}^T(\text{H})$  is that for  $d$ -wave electron scattering from a hydrogen atom with overall triplet spin,  $\tilde{r}_{0,p}^D(\text{He})$  is that for  $p$ -wave electron scattering from helium (necessarily a doublet), and so forth. For the hydrogen target there is only one core electron, so there is no distinction between a reduced effective radius such as  $\tilde{r}_{0,p}^S(\text{H})$  and the corresponding effective radius of the whole target,  $r_{0,p}^S(\text{H})$ . But for helium  $r_{0,i}^X(\text{He}) = 2\tilde{r}_{0,i}^X(\text{He})$  for  $i = s, p, d, \dots$ , and  $X = +$  or  $D$ . For neon, we have

$$r_{0,i}^X(\text{Ne}) = 2\tilde{r}_{0,i}^X(\text{Ne}, 1s) + 2\tilde{r}_{0,i}^X(\text{Ne}, 2s) + 6\tilde{r}_{0,i}^X(\text{Ne}, 2p), \quad (7)$$

and similarly for argon.

In order to reduce the number of these parameters, we use the relationships among them reported in Ref. 29, which are given in Eqs. (8) below:

$$\tilde{r}_{0,s}^S(\text{H}) = \tilde{r}_{0,s}^+(\text{H}), \quad (8a)$$

$$\tilde{r}_{0,s}^T(\text{H}) = 2\tilde{r}_{0,s}^+(\text{H}). \quad (8b)$$

These show the effect of exclusion—incident particles which are not excluded from the target region (electrons in singlet scattering and positrons) encounter what appears to be a smaller target than those which are. For  $s$ -wave electron scattering from helium there is always a partial exclusion effect, which is discussed in Ref. 29. This gives rise to the relationship

$$\tilde{r}_{0,s}^D(\text{He}) = \frac{5}{3}\tilde{r}_{0,s}^+(\text{He}). \quad (8c)$$

We found that positrons do not encounter an "enlargement" of the target due to angular momentum,

$$\tilde{r}_{0,i}^+(T) = \tilde{r}_{0,i}^+(T), \quad i = p, d, \dots, \quad T = \text{H and He}, \quad (8d)$$

but incident electrons do:

$$\tilde{r}_{0,i}^X(T) = \frac{3}{2}\tilde{r}_{0,i}^+(T), \quad i = p, d, \dots,$$

$$X = S, D, \text{ and } T, \quad T = \text{H and He}. \quad (8e)$$

These relationships enabled us to deduce the reduced effective radii for all partial waves, spin states, and incident particles from a single reduced effective radius for each target. The choice of the particular reduced effective radius in which to express the others is arbitrary. We chose to express all the others in terms of  $\tilde{r}_{0,s}^+$  for each target, which were determined in Ref. 29 by fitting our calculat-

ed positron scattering lengths to well-established values. We found that the values

$$\tilde{r}_{0,s}^+(H) = 1.926, \quad \tilde{r}_{0,s}^+(He) = 0.712 \quad (9)$$

gave excellent elastic cross sections for both electron and positron scattering.

To extend our approach to the targets neon and argon, we must generalize the basic relations given by Eqs. (8) somewhat. For electron  $s$ -wave scattering, the same partial exclusion effect found for helium [Eq. (8c)] must apply to any  $ns$  target electron,

$$\tilde{r}_{0,s}^D(T, ns) = \frac{5}{3} \tilde{r}_{0,s}^+(T, ns), \quad (8c')$$

and we assume the same angular-momentum effect as well:

$$\tilde{r}_{0,i}^D(T, nl) = \frac{3}{2} \tilde{r}_{0,s}^+(T, ns), \quad i \neq s \text{ and } i \neq l. \quad (8e')$$

The restriction  $i \neq l$  above is necessary because there are exclusion effects for an  $l$ -wave electron scattering from an  $nl$  target electron. For  $l = s$ , these are considered in Ref.

29 and embodied in Eq. (8c'). We now apply the same reasoning for the  $l = p$  case.

Target  $p$  electrons come in groups of six. A scattering  $p$  electron gives a total of seven  $p$  electrons from which 21 pairs can be distinguished. They are of three types:

- (i) One pair with both electrons having identical spins and angular momenta (necessarily an overall triplet);
- (ii) four pairs with different spins but same angular momenta (half singlet and half triplet);
- (iii) sixteen pairs with different spins and angular momenta (no exclusion effect).

We assume that the interactions between bound and scattering  $p$  electrons are described by the same basic relationships [Eqs. (8a) and (8b)] for those between  $s$  electrons, i.e.,

$$\tilde{r}_{0,p}^T(T, np) = 2\tilde{r}_{0,p}^S(T, np) \quad (8a')$$

$$= 2\tilde{r}_{0,p}^+(T, np). \quad (8b')$$

The effective pair radius for  $p$ -wave electron scattering from a filled  $p$  subshell is now given by

TABLE I. Calculated partial-wave phase shifts and total  $\sigma_{el}$  and momentum-transfer cross sections  $\sigma_m$  for electrons elastically scattered from neon. The entry for  $k=0$  under  $s$  wave is the scattering length. All phase shifts are in radians and are normalized to be between  $-\pi/2$  and  $\pi/2$ .

$k$ (a.u.)	$E$ (eV)	$s$ wave	$p$ wave	$d$ wave	$f$ wave	$g$ wave	$\sigma_{el}$ ( $\pi a_0^2$ )	$\sigma_m$ ( $\pi a_0^2$ )
0.0000	0.000	0.2397	0.0000	0.0000	0.0000	0.0000	0.2298	0.2298
0.1000	0.136	-0.0460	0.0032	0.0008	0.0003	0.0001	0.8588	0.9716
0.2000	0.544	-0.1207	0.0046	0.0032	0.0011	0.0005	1.4634	1.5648
0.2711	1.000	-0.1838	-0.0003	0.0061	0.0020	0.0009	1.8312	1.8208
0.3000	1.225	-0.2111	-0.0041	0.0076	0.0024	0.0011	1.9694	1.8938
0.3834	2.000	-0.2939	-0.0211	0.0130	0.0039	0.0018	2.3476	2.0472
0.4000	2.177	-0.3110	-0.0254	0.0144	0.0043	0.0019	2.4206	2.0720
0.4696	3.000	-0.3845	-0.0471	0.0209	0.0060	0.0027	2.7182	2.1679
0.5000	3.401	-0.4174	-0.0581	0.0243	0.0068	0.0030	2.8461	2.2109
0.5422	4.000	-0.4639	-0.0747	0.0295	0.0081	0.0036	3.0196	2.2735
0.6000	4.898	-0.5286	-0.0998	0.0378	0.0100	0.0044	3.2475	2.3666
0.6062	5.000	-0.5355	-0.1027	0.0388	0.0102	0.0045	3.2705	2.3763
0.6641	6.000	-0.6013	-0.1302	0.0485	0.0125	0.0054	3.4810	2.4789
0.7000	6.667	-0.6423	-0.1481	0.0552	0.0140	0.0060	3.6025	2.5466
0.7173	7.000	-0.6620	-0.1568	0.0586	0.0148	0.0063	3.6564	2.5789
0.7668	8.000	-0.7185	-0.1827	0.0689	0.0172	0.0072	3.8023	2.6745
0.8000	8.708	-0.7564	-0.2003	0.0763	0.0190	0.0079	3.8890	2.7385
0.8133	9.000	-0.7715	-0.2075	0.0793	0.0197	0.0082	3.9215	2.7642
0.8573	10.000	-0.8213	-0.2314	0.0897	0.0222	0.0091	4.0187	2.8472
0.9000	11.021	-0.8692	-0.2547	0.1004	0.0248	0.0101	4.0983	2.9248
1.0000	13.606	-0.9797	-0.3096	0.1267	0.0317	0.0127	4.2286	3.0866
1.0500	15.000	-1.0336	-0.3369	0.1406	0.0354	0.0141	4.2652	3.1536
1.1000	16.463	-1.0867	-0.3638	0.1547	0.0394	0.0157	4.2852	3.2105
1.2000	19.592	-1.1898	-0.4167	0.1834	0.0479	0.0190	4.2794	3.2896
1.2124	20.000	-1.2024	-0.4232	0.1870	0.0490	0.0194	4.2750	3.2964
1.4849	30.000	-1.4613	-0.5571	0.2655	0.0750	0.0304	4.0323	3.2820
1.5000	30.613	-1.4748	-0.5640	0.2698	0.0766	0.0311	4.0131	3.2735
1.9170	50.000	1.3294	-0.7392	0.3838	0.1191	0.0509	3.4170	2.8577
2.0000	54.423	1.2696	-0.7704	0.4056	0.1275	0.0561	3.3007	2.7518
2.1857	65.000	1.1432	-0.8360	0.4537	0.1460	0.0660	3.0536	2.5090
2.3789	76.997	1.1022	-0.8990	0.5020	0.1651	0.0761	2.8216	2.2579

$$\begin{aligned} \tilde{r}_{0,p}^D(T,np) &= \frac{1}{21} \{ \tilde{r}_{0,p}^T(T,np) + 4[\frac{1}{2}\tilde{r}_{0,p}^T(T,np) \\ &\quad + \frac{1}{2}\tilde{r}_{0,p}^S(T,np)] \\ &\quad + 16\tilde{r}_{0,p}^S(T,np) \} \\ &= \frac{8}{7}\tilde{r}_{0,p}^+(T,np) = \frac{8}{7}\tilde{r}_{0,s}^+(T,ns). \end{aligned} \quad (10)$$

In order to get the last result, we extend Eq. (8d) by assuming that the absence of an angular-momentum effect for an incident positron applies to  $p$  target electrons as

well as  $s$ :

$$\tilde{r}_{0,i}^+(T,ni) = \tilde{r}_{0,s}^+(T,ns), \quad i, l = s, p, \dots \quad (8d')$$

In the same spirit, we assume that, in cases where exclusion plays no role, the angular momenta of incident and target electrons are interchangeable:

$$\tilde{r}_{0,s}^D(T,np) = \tilde{r}_{0,p}^D(T,ns). \quad (11)$$

Now we can write the electron effective radii in terms of

TABLE II. Comparison of partial-wave phase shifts (rad) for electron-neon collisions with recent theoretical and experimental studies at some selected energies. An asterisk indicates that interpolated values are listed.

$E$ (eV)	Ref.	$s$ wave	$p$ wave	$d$ wave	$f$ wave	$\sigma_{el}$ ( $\pi a_0^2$ )	$\sigma_m$ ( $\pi a_0^2$ )
0.136	PW <sup>a</sup>	-0.0460	0.0032	0.0008	0.0003	0.8588	0.9716
	DB <sup>b</sup>	-0.0400	0.0040	0.0008	0.0003	0.6600	0.7808
	MS <sup>c</sup>	-0.0507	0.0031	0.0007	0.0002	1.0408	1.1629
	OL <sup>d</sup>	-0.050	0.005			1.032	1.222
	GK <sup>e</sup>	-0.0428	0.0040	0.0008		0.7534	0.8844
	OC <sup>f</sup>	-0.0440	0.0036	0.0008		0.7910	0.9123
0.544	PW <sup>a</sup>	-0.1207	0.0046	0.0032	0.0011	1.4634	1.5648
	DB <sup>b</sup>	-0.1158	0.0086	0.0030	0.0012	1.3629	1.5462
	MS <sup>c</sup>	-0.1283	0.0055	0.0029	0.0009	1.6517	1.7818
	OL <sup>d</sup>	-0.131	0.007			1.727	1.897
	GK <sup>e</sup>	-0.1134	0.0099	0.0032		1.3161	1.5231
	OC <sup>f</sup>	-0.1180	0.0070	0.0030		1.4063	1.5589
5.0	PW <sup>a</sup>	-0.5355	-0.1027	0.0388	0.0102	3.2705	2.3763
	DB <sup>b</sup>	-0.5367	-0.0876	0.0354	0.0104	3.1755	2.4016
	MS <sup>c</sup>	-0.5440	-0.0974	0.0346	0.0090	3.2989	2.4305
	FB <sup>g</sup>	-0.514	-0.089			3.039	2.197
	OL <sup>*d</sup>	-0.553	-0.101	0.037		3.414	2.509
	RT <sup>h</sup>	-0.5220	-0.0911	0.0344	0.0070	3.0477	2.2652
	A <sup>i</sup>	-0.5182	-0.1065	0.0360	0.0099	3.1206	2.2059
	W <sup>*j</sup>	-0.530	-0.090	0.028		3.099	2.289
10.0	PW <sup>a</sup>	-0.8213	-0.2314	0.0897	0.0222	4.0187	2.8470
	DB <sup>b</sup>	-0.8130	-0.2255	0.0797	0.0214	3.8844	2.7142
	MS <sup>c</sup>	-0.8156	-0.2302	0.0848	0.0191	3.9497	2.7797
	TT <sup>k</sup>	-0.835	-0.272	0.081		4.361	2.919
	FB <sup>g</sup>	-0.811	-0.217			3.979	2.521
	OL <sup>*d</sup>	-0.824	-0.230	0.084		3.988	2.813
	RT <sup>h</sup>	-0.7868	-0.2203	0.0787	0.0190	3.6967	2.5730
	BNHS <sup>l</sup>	-0.8054	-0.2340	0.0873		3.95	2.77
	A <sup>i</sup>	-0.7981	-0.2335	0.0874	0.0197	3.8929	2.7190
20.0	PW <sup>a</sup>	-1.2024	-0.4232	0.1870	0.0490	4.2750	3.2964
	DB <sup>b</sup>	-1.1787	-0.4341	0.1773	0.0447	4.2432	3.1945
	MS <sup>c</sup>	-1.1753	-0.4277	0.2013	0.0424	4.3114	3.3544
	RT <sup>h</sup>	-1.1479	-0.4133	0.1909	0.0347	4.1052	3.1810
	BNHS <sup>l</sup>	-1.1630	-0.4294	0.2056	0.0407	4.33	3.37
	A <sup>i</sup>	-1.1633	-0.4294	0.2100	0.0396	4.3426	3.3998

<sup>a</sup>PW: Present work.

<sup>b</sup>DB: POM, Ref. 23.

<sup>c</sup>MS: POM, Ref. 56.

<sup>d</sup>OL: MPM, Ref. 57.

<sup>e</sup>GK: ECR, Ref. 59.

<sup>f</sup>OC: dc swarm, Ref. 51.

<sup>g</sup>FB: RMM, Ref. 22.

<sup>h</sup>RT: crossed-beam, Ref. 18.

<sup>i</sup>A: crossed-beam, Ref. 61.

<sup>j</sup>W: crossed-beam, Ref. 60.

<sup>k</sup>TT: MPM, Ref. 58.

<sup>l</sup>BNHS: crossed-beam, Ref. 62.

positronic parameters. For neon, substitution into Eq. (7) (with  $X=D$  and  $i=s,p,\dots$ ) with Eqs. (8'), (10), and (11) gives

$$r_{0,s}^D(\text{Ne}) = \frac{10}{3} \bar{r}_{0,s}^+(\text{Ne}, 1s) + \frac{37}{3} \bar{r}_{0,s}^+(\text{Ne}, 2s), \quad (12)$$

$$r_{0,p}^D(\text{Ne}) = 3\bar{r}_{0,s}^+(\text{Ne}, 1s) + \frac{69}{7} \bar{r}_{0,s}^+(\text{Ne}, 2s), \quad (13)$$

$$r_{0,i}^D(\text{Ne}) = 3\bar{r}_{0,s}^+(\text{Ne}, 1s) + 12\bar{r}_{0,s}^+(\text{Ne}, 2s), \quad i=d,f,\dots, \quad (14)$$

and for argon,

$$r_{0,s}^D(\text{Ar}) = \frac{10}{3} \bar{r}_{0,s}^+(\text{Ar}, 1s) + \frac{37}{3} \bar{r}_{0,s}^+(\text{Ar}, 2s) + \frac{37}{3} \bar{r}_{0,s}^+(\text{Ar}, 3s), \quad (15)$$

$$r_{0,p}^D(\text{Ar}) = 3\bar{r}_{0,s}^+(\text{Ar}, 1s) + \frac{69}{7} \bar{r}_{0,s}^+(\text{Ar}, 2s) + \frac{69}{7} \bar{r}_{0,s}^+(\text{Ar}, 3s), \quad (16)$$

$$r_{0,i}^D(\text{Ar}) = 3\bar{r}_{0,s}^+(\text{Ar}, 1s) + 12\bar{r}_{0,s}^+(\text{Ar}, 2s) + 12\bar{r}_{0,s}^+(\text{Ar}, 3s), \quad i=d,f,\dots. \quad (17)$$

Now we turn to finding values of the positron parameters. We fix the parameters  $\bar{r}_{0,s}^+(T, ns)$  for inner  $ns$  target electrons by assuming that this distance is the same func-

tion of  $Z_{\text{eff}}$ , the nuclear charge  $Z$  as screened by any inner electrons. We take this function to be a constant times a power of  $Z_{\text{eff}}$ . From Eqs. (9) we can deduce this power:

$$\frac{\bar{r}_{0,s}^+(\text{H})}{\bar{r}_{0,s}^+(\text{He})} = \left[ \frac{Z(\text{H})}{Z(\text{He})} \right]^\gamma = \left[ \frac{1}{2} \right]^{-1.4357}. \quad (18)$$

$\gamma$  is now taken to be a universal parameter. Thus,

$$\bar{r}_{0,s}^+(\text{Ne}, 1s) = 10^\gamma \bar{r}_{0,s}^+(\text{H}) = 0.07, \quad (19)$$

$$\bar{r}_{0,s}^+(\text{Ar}, 1s) = 18^\gamma \bar{r}_{0,s}^+(\text{H}) = 0.03, \quad (20)$$

$$\bar{r}_{0,s}^+(\text{Ar}, 2s) = \left[ \frac{Z(\text{Ar})-2}{Z(\text{Ne})-2} \right]^\gamma \bar{r}_{0,s}^+(\text{Ne}, 2s). \quad (21)$$

All effective target radii for neon are now expressed [Eqs. (12)–(14)] in terms of one parameter,  $\bar{r}_{0,s}^+(\text{Ne}, 2s)$ . We could evaluate this by reproducing the experimentally determined positron scattering length for neon  $[(-0.53 \pm 0.15)a_0]$ .<sup>49</sup> We use, however, the electron scattering length as a reference value since it is much more accurate (although less sensitive to the polarization potential).

Recently reported values of the electron-scattering

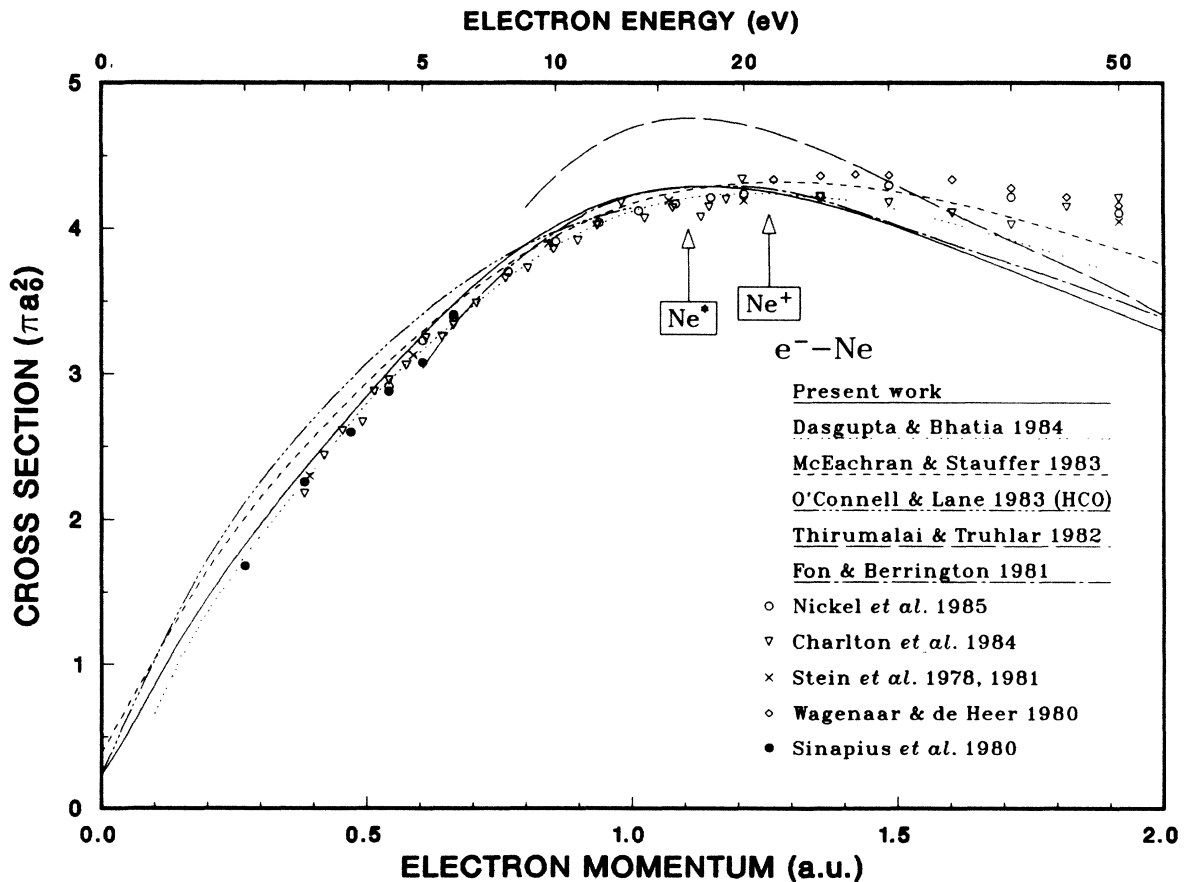


FIG. 1. Total cross sections of electrons elastically scattered from neon. Our results and other recent theoretical values are shown with lines, and recent experimental values with symbols. Note that the calculations shown here include only elastic scattering, while measurements include contributions from other open channels. The first excitation and ionization thresholds are indicated.

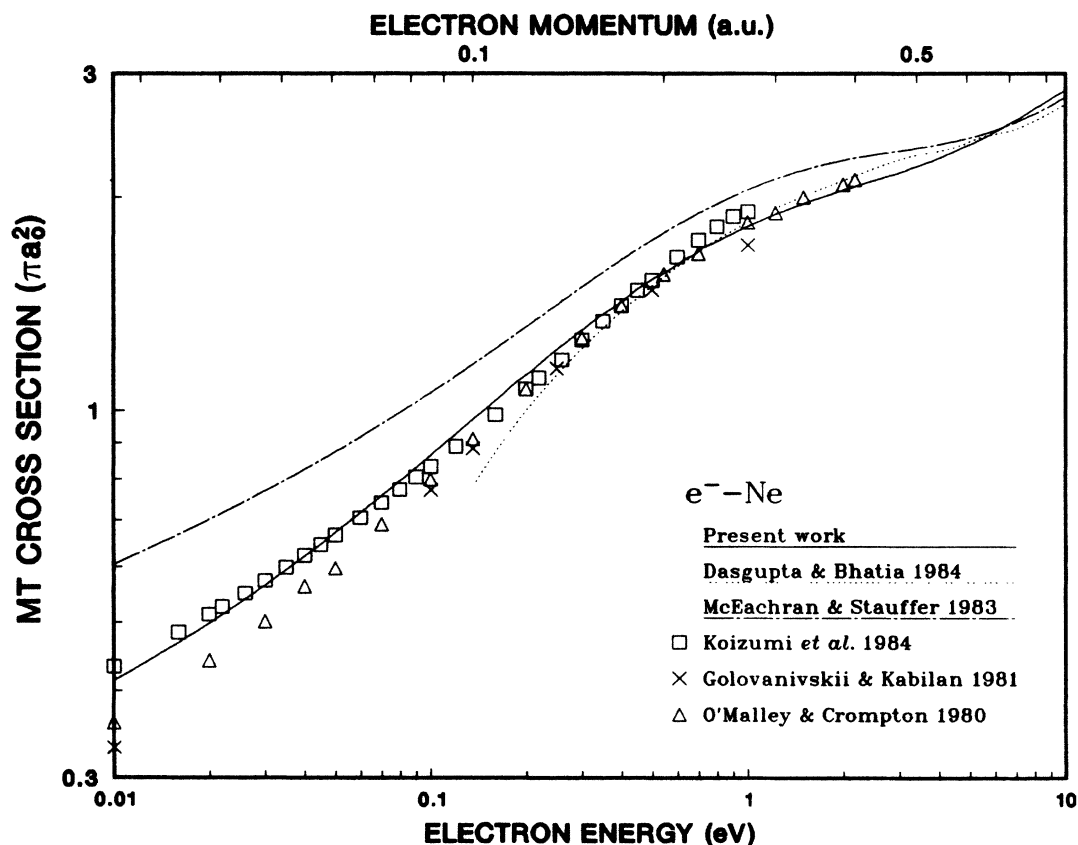


FIG. 2. Momentum-transfer (MT) cross sections of electrons scattered from neon compared with recent calculations and measurements.

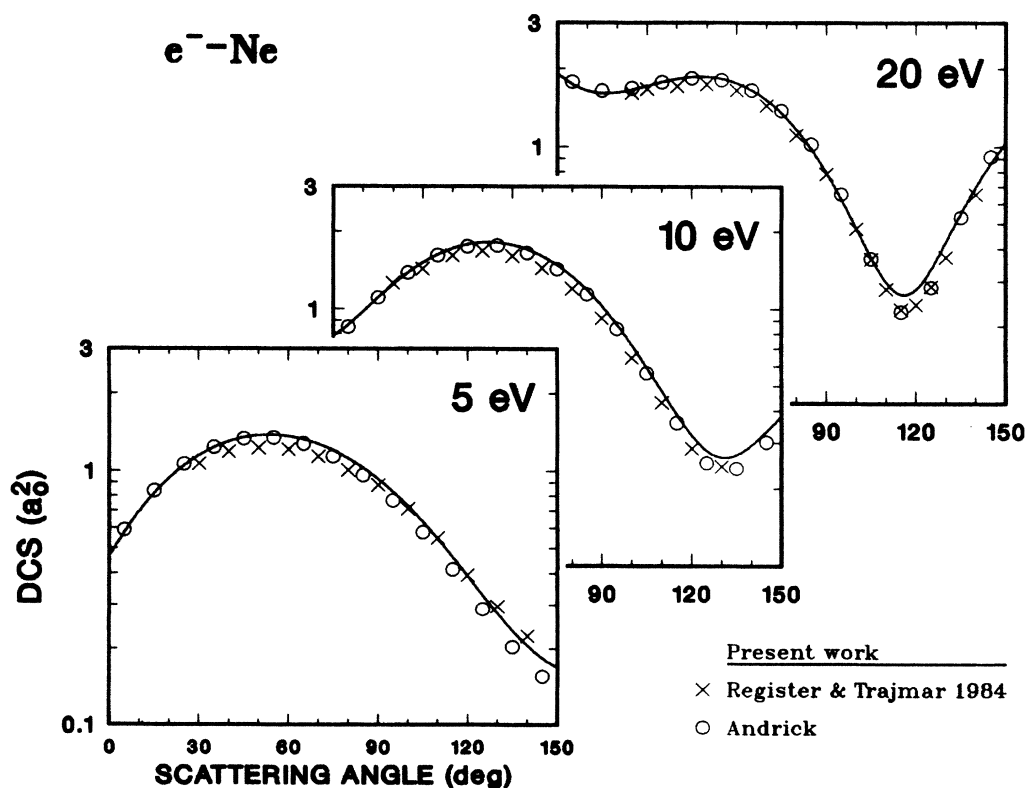


FIG. 3. Differential cross sections (DCS's) of electrons scattered from neon at incident energies 5, 10, and 20 eV compared with recent crossed-beam experiments.

length for neon as extrapolated from experimental data are  $0.24a_0$  by Koizumi *et al.*<sup>50</sup> from the MERT and EMERT (extended MERT<sup>51</sup>) analyses of their dc swarm data in the energy range 0.01–0.2 eV, by Sol *et al.*<sup>5</sup> from the MERT analysis of their ac swarm data in the energy range 0.003–0.5 eV, by Robertson<sup>52</sup> from the MERT analysis of his dc swarm data in the energy range 0.04–0.2 eV,  $0.204a_0$  by Golovanivskii and Kabilan<sup>8</sup> from the MERT analysis of their ECR data in the energy range 0.01–1 eV,  $0.214a_0$  by O'Malley and Crompton<sup>51</sup> from the EMERT analysis of Robertson's data<sup>52</sup> in the energy range 0.03–2 eV,  $0.22a_0$  by McDowell<sup>53</sup> from eleven-parameter fitting with experimental data, and  $0.30a_0$  by Salop and Nakano<sup>54</sup> from the MERT analysis of their scattering data in the energy range 0.37–1.65 eV. Choosing  $0.24a_0$  as our standard and finding the value of  $\tilde{r}_{0,s}^D(\text{Ne})$  which reproduces that in a calculation yield  $\tilde{r}_{0,s}^+(\text{Ne},2s)=0.144$ . Substituting this into Eqs. (12)–(14), we obtain the effective neon radii as

$$r_{0,s}^D(\text{Ne})=2.0, \quad r_{0,p}^D(\text{Ne})=1.65, \quad r_{0,i}^D(\text{Ne})=1.95 \\ (i=d,f,\dots). \quad (22)$$

We use these values in all subsequent calculations.

Now Eq. (21) gives  $\tilde{r}_{0,s}^+(\text{Ar},2s)=0.05$ , and we have all the effective target radii for argon [Eqs. (15)–(17)] ex-

pressed in terms of a single parameter,  $\tilde{r}_{0,s}^+(\text{Ar},3s)$ . We again use the electron-scattering length rather than the less-well-established positron-scattering length. Recent values for the electron-scattering length as determined from experimental data are  $(-1.45 \pm 0.02)a_0$  by Ferch *et al.*<sup>12</sup> from the EMERT analysis of their TOF data in the energy range 0.08–0.5 eV,  $-1.49a_0$  by Buckman and Lohmann<sup>55</sup> from the EMERT analysis of their TOF data in the energy range 0.012–0.5 eV, by Haddad and O'Malley<sup>4</sup> from the EMERT analysis of Robertson's dc swarm data<sup>6,7</sup> in the energy range 0.014–4 eV,  $-1.55a_0$  by Golovanivskii and Kabilan<sup>8</sup> from the MERT analysis of their ECR data in the energy range 0.01–1 eV, and  $-1.63a_0$  by Gus'kov *et al.*<sup>11</sup> from the MERT analysis of their scattering data in the energy range 0.025–1 eV. We have chosen the most recent value of  $-1.45a_0$  as a reference value which, in turn, gives  $\tilde{r}_{0,s}^+(\text{Ar},3s)=0.149$ . Substituting this value into Eqs. (15)–(17), we obtain effective argon radii,

$$r_{0,s}^D(\text{Ar})=2.6, \quad r_{0,p}^D(\text{Ar})=2.1, \quad r_{0,i}^D(\text{Ar})=2.6 \\ (i=d,f,\dots). \quad (23)$$

which are used in the remainder of this work.

For positron scattering, Eq. (8d') reduces the parameterization for neon [Eq. (7) with  $X = +$ ] and argon to

TABLE III. Calculated partial-wave phase shifts and total  $\sigma_{\text{el}}$  and momentum-transfer cross sections  $\sigma_m$  for positrons elastically scattered from neon. The entry for  $k=0$  under  $s$  wave is the scattering length. All phase shifts are in rad and are normalized to be between  $-\pi/2$  and  $\pi/2$ .

$k$ (a.u.)	$E$ (eV)	$s$ wave	$p$ wave	$d$ wave	$f$ wave	$g$ wave	$\sigma_{\text{el}} (\pi a_0^2)$	$\sigma_m (\pi a_0^2)$
0.0000	0.000	-0.7283	0.0000	0.0000	0.0000	0.0000	2.1220	2.1220
0.1000	0.136	0.0449	0.0050	0.0008	0.0003	0.0001	0.8366	0.6513
0.2000	0.544	0.0436	0.0177	0.0032	0.0010	0.0005	0.2903	0.1109
0.2711	1.000	0.0241	0.0293	0.0058	0.0019	0.0009	0.1836	0.0644
0.3000	1.225	0.0131	0.0343	0.0071	0.0024	0.0011	0.1786	0.0892
0.3834	2.000	-0.0258	0.0487	0.0115	0.0039	0.0018	0.2338	0.2313
0.4000	2.177	-0.0345	0.0514	0.0125	0.0042	0.0019	0.2520	0.2659
0.4696	3.000	-0.0737	0.0619	0.0170	0.0059	0.0027	0.3389	0.4123
0.5000	3.401	-0.0919	0.0659	0.0191	0.0066	0.0030	0.3790	0.4736
0.5422	4.000	-0.1179	0.0707	0.0221	0.0078	0.0036	0.4333	0.5518
0.6000	4.898	-0.1546	0.0756	0.0265	0.0095	0.0043	0.5031	0.6436
0.6062	5.000	-0.1587	0.0761	0.0270	0.0097	0.0044	0.5103	0.6525
0.6641	6.000	-0.1964	0.0789	0.0315	0.0116	0.0053	0.5718	0.7235
0.7000	6.667	-0.2200	0.0797	0.0343	0.0129	0.0059	0.6057	0.7583
0.7173	7.000	-0.2315	0.0798	0.0357	0.0135	0.0062	0.6212	0.7730
0.7668	8.000	-0.2644	0.0790	0.0396	0.0153	0.0071	0.6610	0.8064
0.8000	8.708	-0.2864	0.0776	0.0421	0.0166	0.0077	0.6847	0.8229
0.8133	9.000	-0.2952	0.0769	0.0431	0.0172	0.0080	0.6933	0.8280
0.8573	10.000	-0.3244	0.0738	0.0464	0.0189	0.0088	0.7201	0.8417
0.9000	11.021	-0.3526	0.0698	0.0494	0.0207	0.0097	0.7428	0.8492
1.000	13.606	-0.4180	0.0567	0.0557	0.0249	0.0120	0.7857	0.8507
1.0500	15.000	-0.4503	0.0484	0.0584	0.0271	0.0131	0.8026	0.8451
1.1000	16.463	-0.4822	0.0391	0.0607	0.0293	0.0143	0.8170	0.8367
1.2000	19.592	-0.5449	0.0177	0.0641	0.0336	0.0169	0.8399	0.8142
1.2124	20.000	-0.5526	0.0148	0.0644	0.0342	0.0172	0.8423	0.8111
1.4849	30.000	-0.7135	-0.0582	0.0635	0.0447	0.0245	0.8747	0.7335
1.5000	30.613	-0.7220	-0.0627	0.0630	0.0451	0.0250	0.8757	0.7291
1.9170	50.000	-0.9382	-0.1936	0.0332	0.0530	0.0356	0.8812	0.6142
2.0000	54.423	-0.9769	-0.2204	0.0239	0.0529	0.0374	0.8789	0.5933



$$r_{0,i}^+(\text{Ne}) = 2\bar{r}_{0,s}^+(\text{Ne}, 1s) + 8\bar{r}_{0,s}^+(\text{Ne}, 2s), \quad (24)$$

$$r_{0,i}^+(\text{Ar}) = 2\bar{r}_{0,s}^+(\text{Ar}, 1s) + 8\bar{r}_{0,s}^+(\text{Ar}, 2s) + 8\bar{r}_{0,s}^+(\text{Ar}, 3s),$$

$$i = s, p, d, \dots$$

All the reduced effective radii above have been evaluated, so we find

$$r_{0,i}^+(\text{Ne}) = 1.3, \quad (25)$$

$$r_{0,i}^+(\text{Ar}) = 1.7, \quad (26)$$

which are used in the remainder of this work.

### III. RESULTS AND DISCUSSIONS

#### A. Electron-neon

Our results for the partial-wave phase shifts ( $l \leq 4$ ) in the energy range 0–77 eV are listed in Table I along with the elastic total ( $\sigma_{el}$ ) and momentum-transfer ( $\sigma_m$ ) cross sections. Comparisons with recent POM (Refs. 23 and 56), RMM (Ref. 22), and MPM (Refs. 57 and 58) calculations, and dc swarm,<sup>51</sup> ECR,<sup>59</sup> and crossed-beam<sup>18,60,61,62</sup> experiments at some selected energies are shown in Table II. Our  $s$ -wave results lie between those from POM calculations with exchange-adiabatic<sup>56</sup> and with exchange-polarization approximations,<sup>23</sup> and within 5% of those from experiments in the whole energy range

studied. Our  $p$ -wave results are very close to the  $p$ -wave results of McEachran and Stauffer and are in almost perfect agreement with Andrick's crossed-beam results,<sup>61</sup> except around its crossover point ( $\sim 1$  eV). Although of less importance than the higher partial waves, our  $d$ - and  $f$ -wave results are in excellent agreement with the best theoretical and experimental data available.

Our total elastic cross sections are compared with recent theoretical<sup>22,23,56–58</sup> and experimental<sup>63–68</sup> values in Fig. 1, where only direct measurements of the total cross sections are included. Our results show excellent agreement with experimental values up to the excitation threshold (16.67 eV), beyond which agreement between our elastic calculations and experimental measurements should not be expected. Our results in the sub-eV region are compared to the momentum-transfer cross sections from two POM calculations,<sup>23,56</sup> and dc swarm<sup>50,51</sup> and ECR (Ref. 8) measurements in Fig. 2. Although good low-energy behavior is to be expected from our parameter-fitting procedure, in which the scattering length is chosen as a reference value, our calculations are surprisingly accurate, and reproduce perfectly the measurements of Koizumi *et al.* up to 0.5 eV and of O'Malley and Crompton thereafter. MPM calculations of O'Connell and Lane produce accurate elastic cross sections with model polarization and exchange potentials which are connected at the crossover point, although this method does not seem to be applicable to positronic systems.

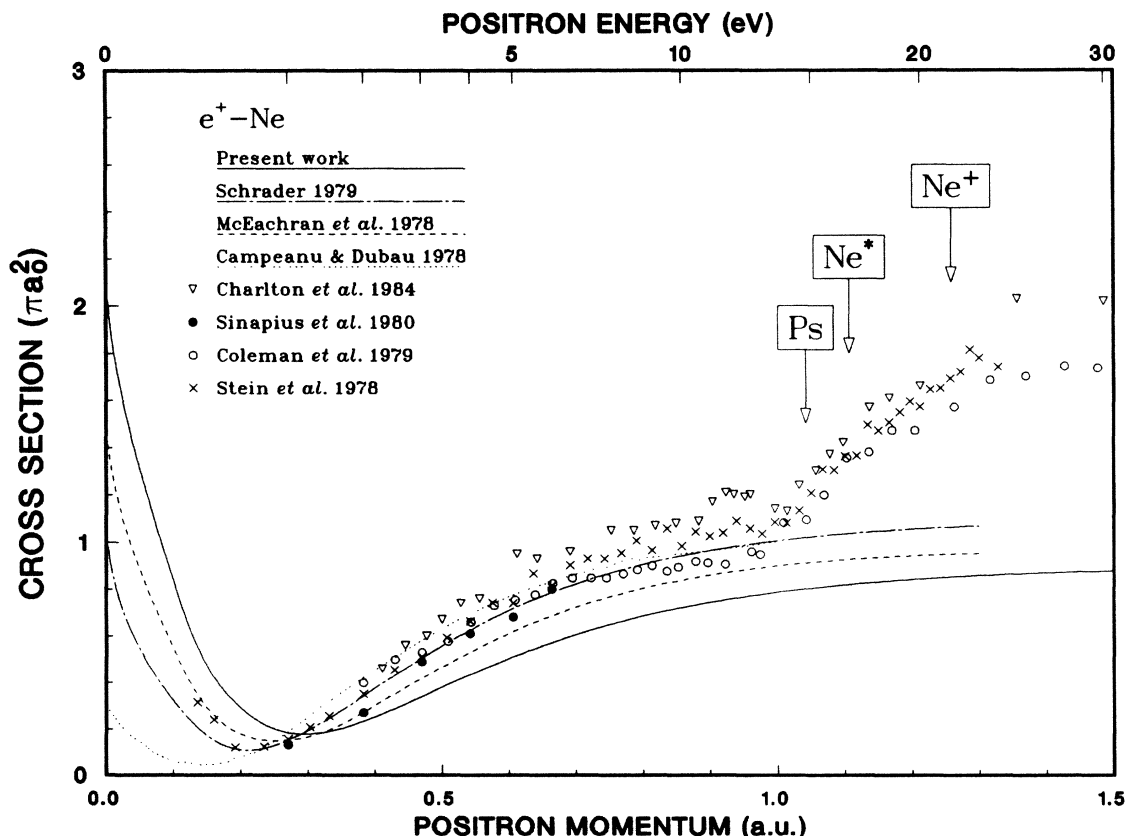


FIG. 4. Total cross sections of positrons elastically scattered from neon. The positronium formation, target first excitation, and target first ionization thresholds are indicated.

Our elastic differential cross sections are shown in Fig. 3 for the incident electron energies of 5, 10, and 20 eV. Our results are at most 10% higher than those of Register and Trajmar,<sup>18</sup> and are in excellent agreement with the values of Andrick calculated from the partial waves listed in Table II. The critical point in the elastic differential cross section has been found to be  $(8.7 \times 10^{-6})a_0^2$  at  $k=2.3789$  ( $E=77$  eV) and  $\theta=98.1^\circ$ . Our present result agrees moderately with the observation of Register and Tramjar<sup>18</sup> ( $E=62.5$  eV and  $\theta=101.5^\circ$ ) and the RMM calculation of Fon *et al.* ( $E=64$  eV and  $\theta=103.6^\circ$ ).<sup>22</sup> The discrepancy may be due to the absence of inelastic channels in our method or to the influence in our local exchange potential for the higher partial waves for which the same parameters are used after the orthogonality condition is removed.

### B. Positron-neon

Our results for positron-neon elastic scattering are listed in Table III along with the elastic total and

momentum-transfer cross sections up to  $k=2$ . The elastic total cross sections are compared with recent MPM,<sup>34</sup> POM,<sup>35</sup> and CCM (Ref. 33) calculations and measurements<sup>64,65,68,69</sup> in Fig. 4. Compared to electron scattering, discrepancies are large, amounting to about 30% among experimental and theoretical values. Experimental problems include the difficulty in estimating small-angle forward scattering correctly, as has been discussed by Stein and Kauppila<sup>17</sup> and by Charlton.<sup>14</sup> Theoretical difficulties include the approximate cancellation of the static and polarization potentials, which leads to great sensitivity of calculated values to errors in these potentials.<sup>70</sup>

At first sight our results may seem disappointing. The calculated scattering length ( $-0.7283a_0$ ) is lower than the experimental value [ $(-0.53 \pm 0.15)a_0$ ] of Tsai *et al.*<sup>49</sup> and the theoretical values of Schrader ( $-0.542a_0$ ),<sup>34</sup> of McEachran ( $-0.61412a_0$ ),<sup>35</sup> and of Câmpeanu and Dubau ( $\sim -0.3a_0$ ),<sup>33</sup> and our total cross sections are smaller than the most experimental values shown in Fig. 4. However, if we had chosen the electron-scattering length of Salop and Nakano<sup>54</sup> ( $0.30a_0$ ) as our reference value in-

TABLE IV. Calculated partial-wave phase shifts and total  $\sigma_{el}$  and momentum-transfer cross sections  $\sigma_m$  for electrons elastically scattered from argon. The entry for  $k=0$  under  $s$  wave is the scattering length. All phase shifts are in rad and are normalized to be between  $-\pi/2$  and  $\pi/2$ .

$k$ (a.u.)	$E$ (eV)	$s$ wave	$p$ wave	$d$ wave	$f$ wave	$g$ wave	$\sigma_{el}$ ( $\pi a_0^2$ )	$\sigma_m$ ( $\pi a_0^2$ )
0.0000	0.000	-1.4613	0.0000	0.0000	0.0000	0.0000	8.5414	8.5414
0.0857	0.100	0.0445	0.0118	0.0024	0.0008	0.0003	1.3203	0.6827
0.1000	0.136	0.0392	0.0148	0.0033	0.0011	0.0005	0.9031	0.3505
0.1212	0.200	0.0273	0.0192	0.0048	0.0016	0.0007	0.5439	0.1403
0.1486	0.300	0.0050	0.0244	0.0074	0.0024	0.0011	0.3886	0.1889
0.1715	0.400	-0.0189	0.0273	0.0101	0.0032	0.0014	0.4295	0.3706
0.1917	0.500	-0.0416	0.0289	0.0129	0.0040	0.0018	0.5688	0.6247
0.2000	0.544	-0.0518	0.0291	0.0141	0.0044	0.0020	0.6421	0.7304
0.2100	0.600	-0.0645	0.0291	0.0157	0.0049	0.0022	0.7406	0.8610
0.2711	1.000	-0.1505	0.0214	0.0279	0.0082	0.0037	1.5470	1.6669
0.3000	1.225	-0.1950	0.0129	0.0357	0.0100	0.0045	2.0190	2.0349
0.3834	2.000	-0.3317	-0.0283	0.0669	0.0167	0.0074	3.6355	3.1387
0.4000	2.177	-0.3602	-0.0392	0.0751	0.0183	0.0081	4.0071	3.3941
0.4696	3.000	-0.4822	-0.0928	0.1186	0.0258	0.0112	5.7567	4.6984
0.5000	3.401	-0.5362	-0.1198	0.1432	0.0297	0.0127	6.6275	5.4185
0.5422	4.000	-0.6123	-0.1601	0.1835	0.0356	0.0150	7.9643	6.6022
0.6000	4.898	-0.7163	-0.2194	0.2523	0.0448	0.0185	10.0420	8.5633
0.6062	5.000	-0.7278	-0.2261	0.2607	0.0459	0.0189	10.2920	8.8031
0.6641	6.000	-0.8315	-0.2895	0.3490	0.0569	0.0230	12.7494	11.1641
0.7000	6.667	-0.8954	-0.3301	0.4131	0.0645	0.0257	14.4366	12.7304
0.7173	7.000	-0.9261	-0.3498	0.4463	0.0684	0.0271	15.2828	13.4860
0.7668	8.000	-1.0129	-0.4068	0.5502	0.0803	0.0313	17.7929	15.5612
0.8000	8.708	-1.0705	-0.4453	0.6261	0.0889	0.0344	19.4700	16.7696
0.8133	9.000	-1.0933	-0.4609	0.6576	0.0925	0.0356	20.1237	17.1909
0.8573	10.000	-1.1681	-0.5118	0.7655	0.1049	0.0401	22.1268	18.2526
0.9000	11.021	-1.2394	-0.5612	0.8729	0.1177	0.0447	23.7200	18.7187
1.000	13.606	-1.4009	-0.6747	1.1187	0.1504	0.0567	25.5542	17.6821
1.0500	15.000	-1.4788	-0.7300	1.2311	0.1678	0.0633	25.4695	16.3836
1.1000	16.463	-1.5548	-0.7843	1.3336	0.1858	0.0703	24.8771	14.8763
1.2124	20.000	1.4230	-0.9022	1.5253	0.2277	0.0874	22.5114	11.5992
1.4859	30.040	1.0634	-1.1636	-1.3308	0.3324	0.1340	16.2845	6.9675
1.5000	30.613	1.0463	-1.1761	-1.3210	0.3377	0.1365	16.0184	6.8349
1.9170	50.000	0.5906	-1.5123	-1.1584	0.4950	0.2112	10.5274	4.7385
2.0000	54.423	0.5103	1.5694	-1.1443	0.5263	0.2259	9.8374	4.5119
2.7111	100.0	-0.0739	1.1288	-1.1138	0.7793	0.3539	6.4334	3.0790

stead of  $0.24a_0$ , we would have obtained the positronic effective radius  $r_0^+ = 1.5$ , which, in turn, produces the positron-scattering length  $-0.563a_0$  and total cross sections very close to those of Schrader,<sup>34</sup> which lie in the middle of the experimental data. On the other hand, had we chosen  $0.30a_0$ , we would have obtained electron-neon total cross sections very close to the results of McEachran and Stauffer<sup>56</sup> shown in Fig. 1. This illustrates great sensitivity to the polarization potential in positronic systems. Thus the opposite fitting procedure, i.e., using the positron-scattering length as a reference, will provide satisfactory results for both positronic and electronic systems if more precise positronic scattering lengths become available.

### C. Electron-argon

The partial-wave phase shifts calculated with the electronic effective radii given by Eq. (23) are listed in Table IV for incident energies from 0 to 100 eV. The elastic total cross sections are compared graphically in Fig. 5 with recent theoretical results and with recent direct measurements.<sup>9,12,55,63,68,71,72</sup> Datta *et al.* have employed the local exchange potential and the Lane-Geltman polarization potential (see Ref. 29) with a cutoff parameter which was adjusted to produce the best *p*-wave phase shift at 3 eV.

Our method is conceptually the same as theirs, except we use the *s* wave at zero energy, i.e., the scattering length. Our results are markedly better in the neighborhood of the Ramsauer-Townsend minimum, where they lie between the experimental values of Jost *et al.*<sup>9</sup> and of Ferch *et al.*<sup>12</sup> from completely different experimental techniques. MPM calculations of O'Connell and Lane produce reasonably accurate elastic cross sections at low energies.

We emphasize here that all calculations employed some empirical adjustments to produce good results in sub-eV region. RMM calculations of Fon *et al.*,<sup>73</sup> for example, have turned out to be unreliable below 5 eV since their calculated dipole polarizability  $12.8a_0^3$  differs from the accurate value ( $11.08a_0^3$ ). Bell *et al.*<sup>24</sup> have found that the scattering length and the position of the Ramsauer-Townsend minimum are very sensitive to the lowest-lying *R* matrix pole in the  $^2S$  symmetry. Since this pole is strongly coupled to the  $3p^64s^2^2S(N+1)$  quasibound state, its energy is shifted to produce a reasonable scattering length and the Ramsauer-Townsend minimum. POM calculations of McEachran and Stauffer<sup>56</sup> with the exchange-adiabatic approximation include only the dipole part of the polarization potential for electronic systems, while all except the monopole part for positronic systems.

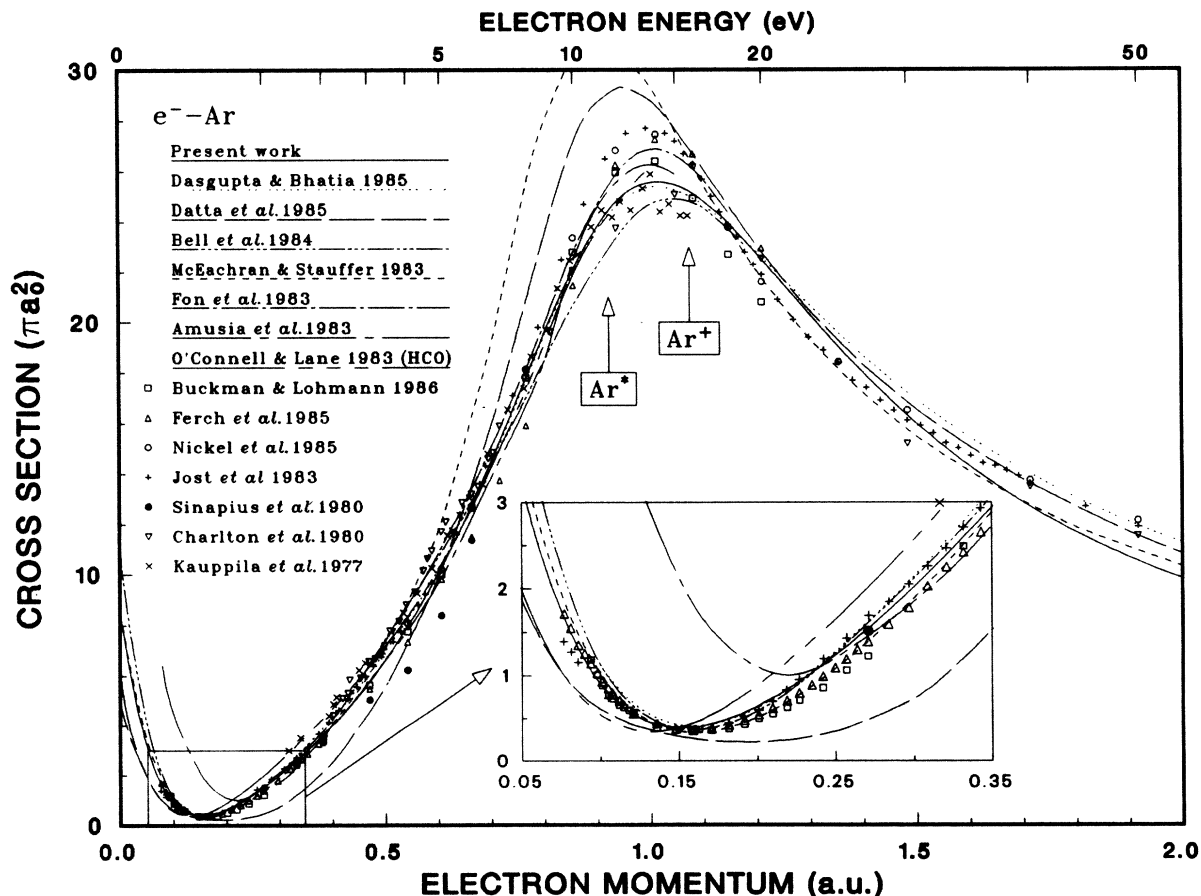


FIG. 5. Total cross sections of electrons elastically scattered from argon. The neighborhood of the Ramsauer-Townsend minimum is expanded in the small window.

Dasgupta and Bhatia<sup>25</sup> have included the polarized exchange term in their POM calculations with one perturbed orbital  $u_{3p \rightarrow d}$ , which has been found, in turn, to give the dipole polarizability  $14.29a_0^3$ . The perturbed orbital was then multiplied by a factor to generate the correct dipole polarizability.

Our results in the sub-eV region are checked against the momentum-transfer cross sections from the MERT analyses of crossed-beam,<sup>60,74</sup> ECR,<sup>75</sup> from dc swarm,<sup>7,76,77</sup> and from ac swarm.<sup>78</sup> As shown in Fig. 6, our results are within the experimental errors of the most reliable experi-

ments by Milloy *et al.*,<sup>7</sup> even at the minimum. The deviation of the data of Dasgupta and Bhatia at the minimum is due to insufficient data points given in their paper to produce the minimum.

We compare our results with recent POM,<sup>25,56</sup> MPM,<sup>36,56</sup> RMM,<sup>24,73</sup> and OPM (Ref. 26) calculations and the MERT analyses of the dc swarm,<sup>4</sup> ECR,<sup>59</sup> TOF,<sup>12</sup> and the crossed-beam<sup>60,74,79</sup> experiments at 0.136, 5, 10, and 20 eV in Table V. Our results show close agreement with those from more elaborate calculations with various empirical adjustments, and those from MERT and EM-

TABLE V. Comparison of partial-wave phase shifts (rad) for electron-argon collisions with recent theoretical and experimental studies at some selected energies. An asterisk indicates that interpolated values are listed.

$E$ (eV)	Ref.	$s$ wave	$p$ wave	$d$ wave	$f$ wave	$\sigma_{el}$ ( $\pi a_0^2$ )	$\sigma_m$ ( $\pi a_0^2$ )
0.136	PW <sup>a</sup>	0.0392	0.0148	0.0033	0.0011	0.9031	0.3505
	DB <sup>b</sup>	0.0447	0.0156	0.0034	0.0011	1.1188	0.4648
	DMKG <sup>c</sup>	0.0309	0.0129	0.0033	0.0011	0.6060	0.2099
	BSL <sup>*d</sup>	0.0458	0.0152	0.0037	0.0012	1.1488	0.4879
	MS <sup>e</sup>	0.0438	0.0141	0.0033	0.0011	1.0307	0.4523
	OL <sup>f</sup>	0.023	0.016			0.542	0.160
	ACCDR <sup>g</sup>	0.059	0.050	0.007		4.53	1.58
	BL <sup>h</sup>	0.0399	0.0147	0.0033		0.9216	0.3648
	FGMR <sup>i</sup>	0.0411	0.0147	0.0033		0.9617	0.3894
	HO <sup>j</sup>	0.0390	0.0141	0.0033		0.8725	0.3470
GK <sup>k</sup>	0.0349	0.0120	0.0033		0.6861	0.2762	
5.0	PW <sup>a</sup>	-0.7278	-0.2261	0.2607	0.0459	10.2920	8.8031
	DB <sup>b</sup>	-0.7209	-0.2459	0.2580	0.0442	10.4252	8.8563
	BSL <sup>d</sup>	-0.7575	-0.2901	0.2316	0.0453	10.8898	8.7734
	MS <sup>e</sup>	-0.7092	-0.2570	0.3127	0.0434	12.0699	10.7528
	OL <sup>*f</sup>	-0.747	-0.266	0.236		10.424	8.615
	FBBH <sup>l</sup>	-0.7320	-0.2984	0.2440	0.0427	11.0694	9.0629
	STCT <sup>m</sup>	-0.747	-0.256	0.254	0.102	11.402	8.665
	A <sup>n</sup>	-0.733	-0.277	0.260	0.044	11.115	9.342
	W <sup>o</sup>	-0.685	-0.205	0.317	0.031	11.481	10.322
	10.0	PW <sup>a</sup>	-1.1681	-0.5118	0.7655	0.1049	22.1268
DB <sup>b</sup>		-1.1438	-0.5376	0.7539	0.0999	22.0366	17.9612
BSL <sup>d</sup>		-1.1860	-0.6063	0.6610	0.0960	20.6929	16.3135
MS <sup>e</sup>		-1.1279	-0.5410	1.1049	0.0987	30.9621	24.2271
OL <sup>*f</sup>		-1.156	-0.545	0.741		21.700	18.000
FBBH <sup>l</sup>		-1.1554	-0.5865	0.7568	0.0849	22.7987	18.3076
STCT <sup>m</sup>		-1.243	-0.430	0.805	0.171	23.068	18.704
A <sup>n</sup>		-1.143	-0.562	0.840	0.100	24.721	19.738
W <sup>o</sup>		-1.098	-0.528	0.936	0.093	26.558	21.543
20.0		PW <sup>a</sup>	-1.7186	-0.9022	1.5253	0.2277	22.5114
	DB <sup>b</sup>	-1.6743	-0.9300	1.4484	0.2334	22.6220	11.2967
	MS <sup>e</sup>	-1.6529	-0.9176	1.8376	0.2309	21.7367	10.4091
	STCT <sup>m</sup>	-1.818	-0.871	1.679	0.262	22.280	11.861
	A <sup>n</sup>	-1.683	-0.962	1.670	0.232	22.881	10.794
	W <sup>o</sup>	-1.653	-0.935	1.747	0.241	22.500	10.710

<sup>a</sup>PW: present work.

<sup>b</sup>DB: POM, Ref. 25.

<sup>c</sup>DMKG: MPM, Ref. 36.

<sup>d</sup>BSL: RMM, Ref. 24.

<sup>e</sup>MS: POM, Ref. 56.

<sup>f</sup>OL: MPM, Ref. 57.

<sup>g</sup>ACCDR: OPM, Ref. 26.

<sup>h</sup>BL: TOF, Ref. 35.

<sup>i</sup>FGMR: TOF, Ref. 12.

<sup>j</sup>HO: dc swarm, Ref. 4.

<sup>k</sup>GK: ECR, Ref. 59.

<sup>l</sup>FBBH: RMM, Ref. 73.

<sup>m</sup>STCT: crossed-beam, Ref. 74.

<sup>n</sup>A: crossed-beam, Ref. 79.

<sup>o</sup>W: crossed-beam, Ref. 60.

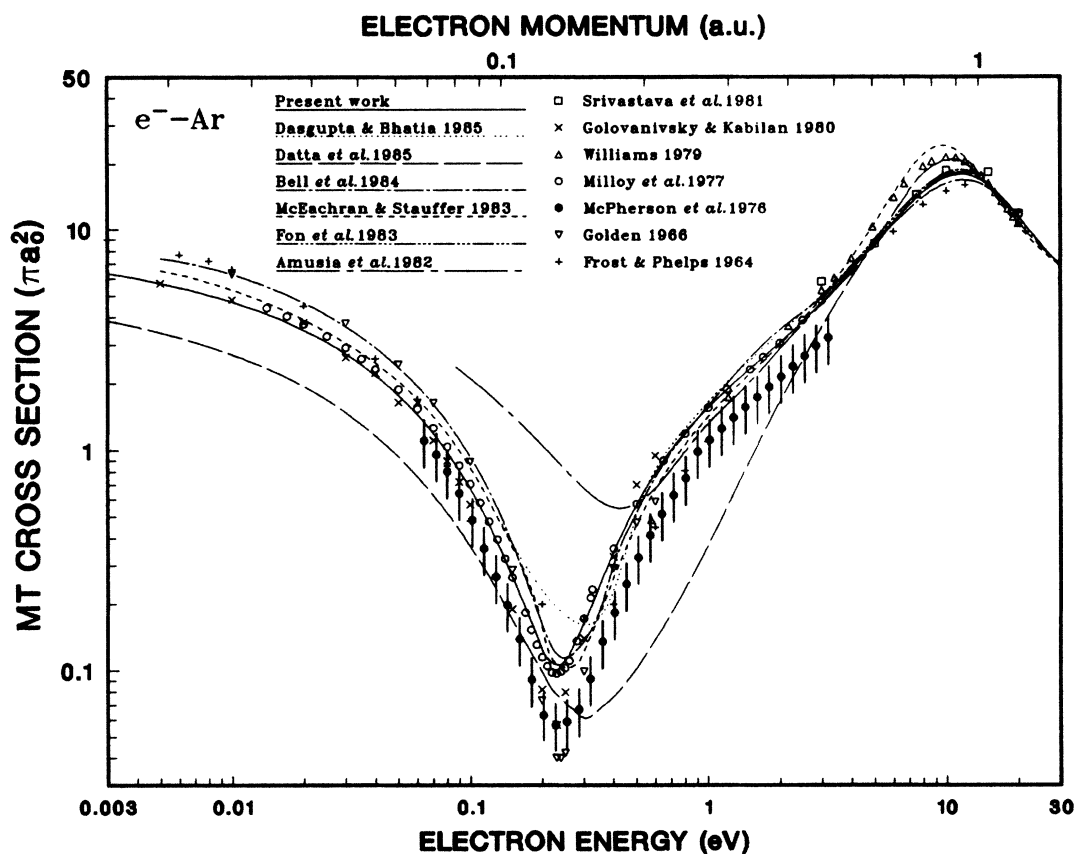


FIG. 6. Momentum-transfer cross sections of electrons elastically scattered from argon.

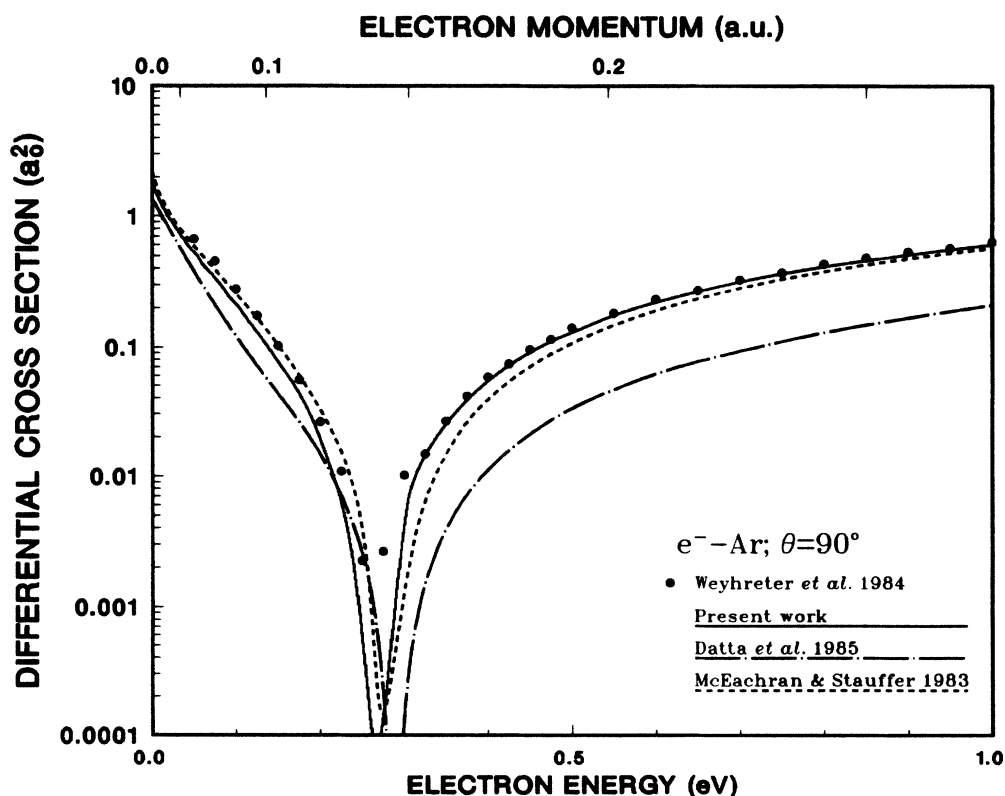


FIG. 7. Differential cross sections of electrons elastically scattered from argon as a function of incident energy at fixed scattering angle  $90^\circ$ . Values of Datta *et al.* are calculated by us with the same polarization and effective exchange potentials used in their paper (Ref. 36).

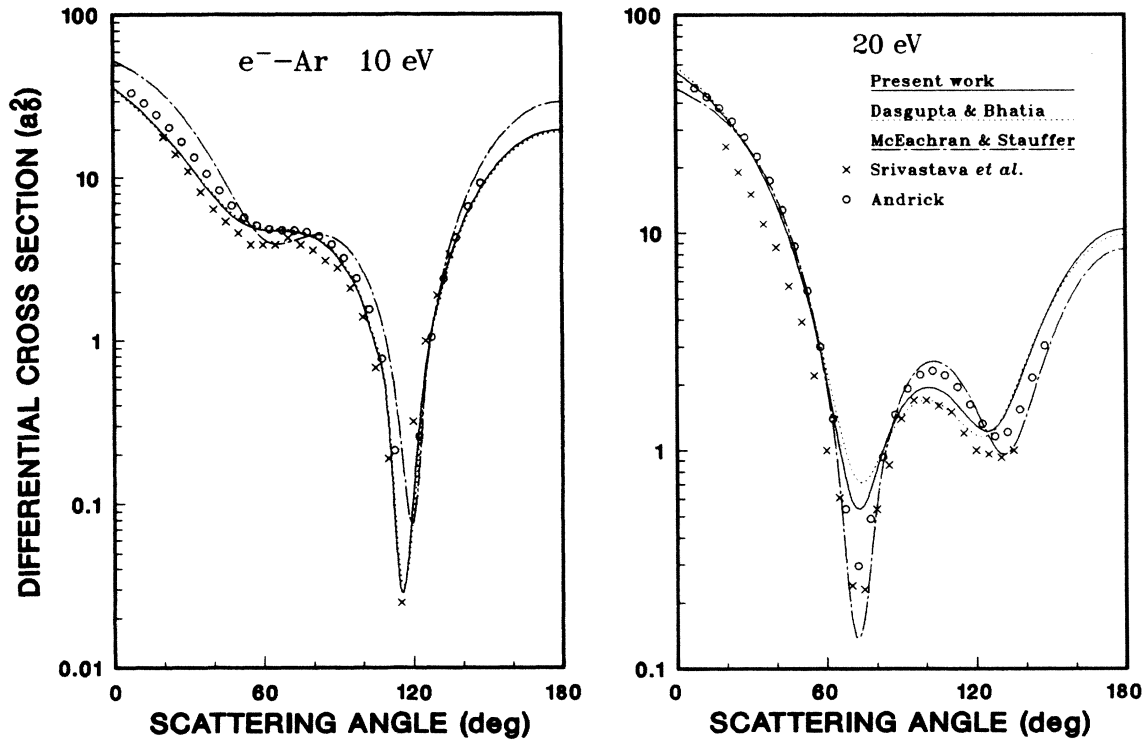


FIG. 8. Differential cross sections of electrons elastically scattered from argon as a function of scattering angle at incident energies 10 and 20 eV.

TABLE VI. Calculated partial-wave phase shifts and total  $\sigma_{el}$  and momentum-transfer cross sections  $\sigma_m$  for positrons elastically scattered from argon. The entry for  $k=0$  under  $s$  wave is the scattering length. All phase shifts are in rad and are normalized to be between  $-\pi/2$  and  $\pi/2$ .

$k$ (a.u.)	$E$ (eV)	$s$ wave	$p$ wave	$d$ wave	$f$ wave	$g$ wave	$\sigma_{el}$ ( $\pi a_0^2$ )	$\sigma_m$ ( $\pi a_0^2$ )
0.0000	0.000	-4.5076	0.0000	0.0000	0.0000	0.0000	81.2751	81.2751
0.1000	0.136	0.2633	0.0210	0.0032	0.0011	0.0005	27.6471	23.2807
0.2000	0.544	0.2632	0.0736	0.0133	0.0044	0.0020	8.4975	4.3029
0.2711	1.000	0.2036	0.1180	0.0245	0.0081	0.0037	4.6874	1.3954
0.3000	1.225	0.1730	0.1354	0.0299	0.0100	0.0045	3.9923	1.1084
0.3834	2.000	0.0749	0.1789	0.0482	0.0164	0.0074	3.1248	1.3108
0.4000	2.177	0.0543	0.1857	0.0521	0.0178	0.0080	3.0494	1.4158
0.4696	3.000	-0.0340	0.2067	0.0698	0.0246	0.0111	2.8647	1.8343
0.5000	3.401	-0.0730	0.2121	0.0778	0.0278	0.0126	2.8203	1.9791
0.5422	4.000	-0.1272	0.2155	0.0890	0.0326	0.0148	2.7684	2.1208
0.6000	4.898	-0.2012	0.2132	0.1041	0.0397	0.0182	2.7136	2.2290
0.6062	5.000	-0.2091	0.2126	0.1057	0.0405	0.0186	2.7087	2.2361
0.6641	6.000	-0.2822	0.2022	0.1199	0.0481	0.0223	2.6637	0.2609
0.7000	6.667	-0.3270	0.1927	0.1280	0.0531	0.0247	2.6401	2.2528
0.7173	7.000	-0.3483	0.1874	0.1317	0.0555	0.0259	2.6305	2.2439
0.7668	8.000	-0.4089	0.1695	0.1413	0.0625	0.0295	2.6057	2.2093
0.8000	8.708	-0.4489	0.1558	0.1469	0.0673	0.0321	2.5912	2.1799
0.8133	9.000	-0.4649	0.1499	0.1489	0.0692	0.0331	2.5868	2.1680
0.8573	10.000	-0.5169	0.1291	0.1546	0.0755	0.0367	2.5714	2.1250
0.9000	11.021	-0.5666	0.1072	0.1588	0.0816	0.0402	2.5592	2.0826
1.0000	13.605	-0.6799	0.0505	0.1631	0.0951	0.0488	2.5364	1.9847
1.0500	15.000	-0.7346	0.0201	0.1622	0.1004	0.0533	2.5257	1.9370
1.1000	16.463	-0.7883	-0.0114	0.1595	0.1071	0.0577	2.5159	1.8910
1.2124	20.000	-0.9050	-0.0850	0.1467	0.1179	0.0677	2.4953	1.7930
1.4000	26.667	-1.0875	-0.2118	0.1080	0.1277	0.0831	2.4636	1.6435
1.4859	30.040	-1.1660	-0.2702	0.0844	0.1283	0.0892	2.4502	1.5802
1.5000	30.613	-1.1787	-0.2797	0.0802	0.1282	0.0901	2.4481	1.5701
1.9170	50.000	-1.5157	-0.5525	-0.0685	0.0948	0.1050	2.4037	1.3080
2.0000	54.423	1.5667	-0.6035	-0.1018	0.0821	0.1045	2.3997	1.2640
2.7111	100.0	1.1592	-0.9789	-0.3886	-0.0770	0.0525	2.4434	1.0018

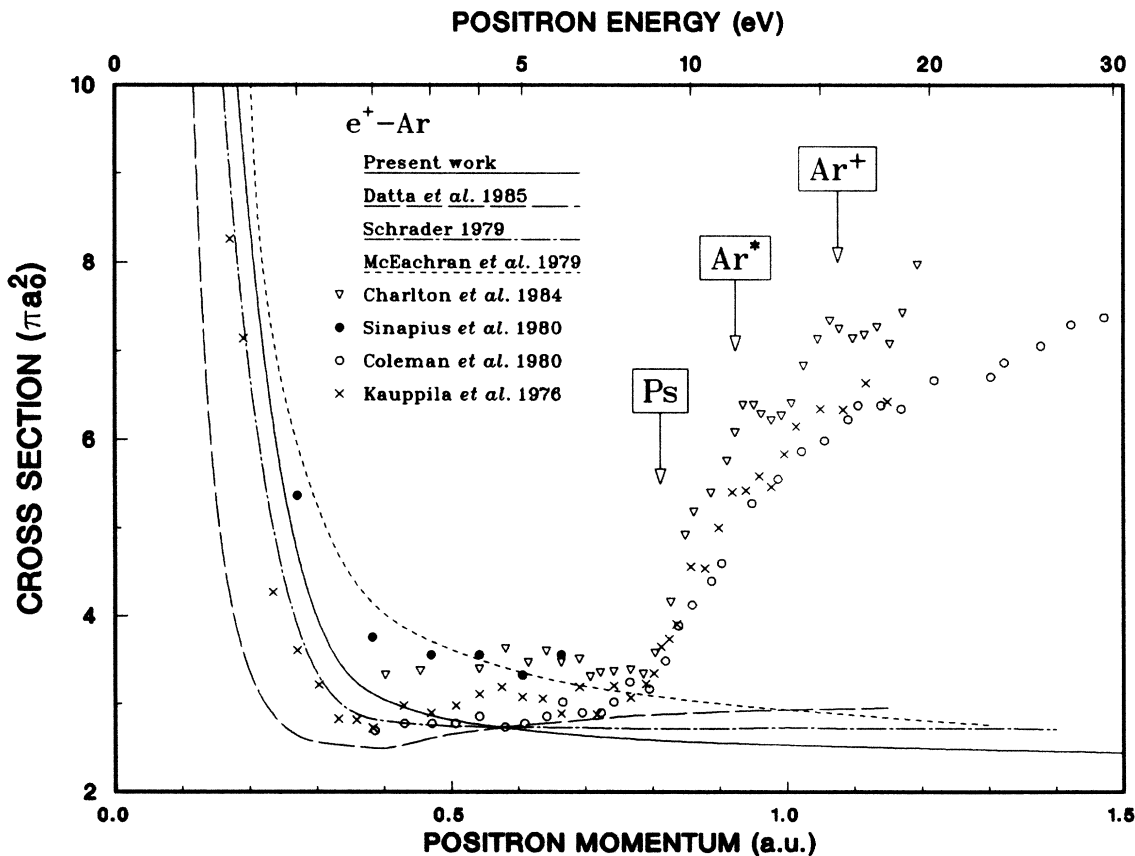


FIG. 9. Total cross sections of positrons elastically scattered from argon.

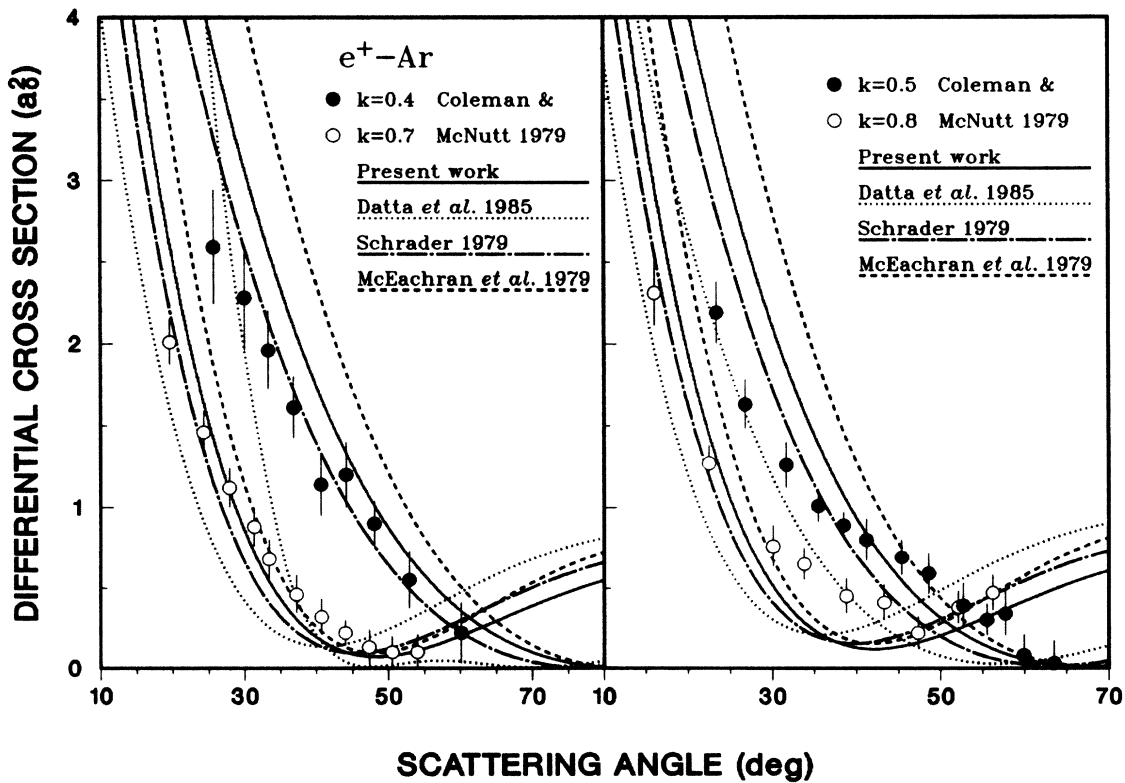


FIG. 10. Differential cross sections of positrons elastically scattered from argon for incident momentum from 0.4 to 0.8 a.u.

ERT analyses of experimental data. The large discrepancy in the results of McEachran and Stauffer above 5 eV (see Fig. 5) is due to their excessive  $d$ -wave phase shifts.

Recently, Weyhreter *et al.*<sup>13</sup> made direct measurements of the differential cross sections at the energies from 50 meV to 2 eV and found a deep minimum and a large increase of the cross sections toward zero energy. Their measurements at the scattering angle  $90^\circ$  are shown in Fig. 7 along with our and other theoretical calculations. Our results are in very good agreement with the experimental values, and very close to those of McEachran and Stauffer.<sup>56</sup> The values of Datta *et al.* are calculated by us with the same polarization potential and the local exchange potential used in their paper.<sup>36</sup> Figure 8 shows our differential cross sections for 10 and 20 eV, along with those from other work.<sup>25,56,74,79</sup> Our results for 10 eV are almost identical to those of Dasgupta and Bhatia,<sup>25</sup> and are between experimental values of Srivastava *et al.*<sup>74</sup> and Andrick<sup>79</sup> (values of Andrick were calculated from the partial-wave phase shifts listed in Table V).

#### D. Positron-argon

Our results for positron-argon elastic scattering are listed in Table VI along with the elastic total and momentum-transfer cross sections up to positron incident energy 100 eV. The calculated scattering length is  $-4.5a_0$ , which can be compared with  $-(4.4 \pm 0.5)a_0$  obtained by Lee and Jones<sup>80</sup> from electric field and temperature dependences of their positron-lifetime data,  $-(2.8 \pm 0.7)a_0$  by Tsai *et al.*<sup>49</sup> from their total cross-section data analysis, and  $-(3.5 \pm 0.5)a_0$  by Hara and Fraser<sup>81</sup> from the temperature dependence of the annihilation rate. The theoretical values are  $-3.5a_0$  by Datta *et al.*<sup>36</sup> and  $-4.11a_0$  by Schrader<sup>34</sup> from MPM calculations, and  $-5.30a_0$  by McEachran *et al.*<sup>82</sup> from a POM calculation. The elastic total cross sections are compared in Fig. 9 with recent MPM (Refs. 34 and 36) and POM (Ref. 82) calculations and with experimental measurements.<sup>64,68,83,84</sup> It should be noted that Datta *et al.* have used the same polarization potential for both positron and electron-argon systems without any justification. Our results lie between those of Schrader<sup>34</sup> and of McEachran *et al.*<sup>82</sup> below 5 eV. It is interesting to note that all MPM calculations seem to have a common point at  $k \sim 0.58$  regardless of the choice of the cutoff function. It is difficult at present to conclude which calculation is more reliable since there are large discrepancies among the experimental data. (See Sec. III B.)

Coleman and McNutt<sup>19</sup> have obtained differential cross sections for positrons scattering from argon for the positron incident momentum from 0.4 to 0.8 in the scattering angles from  $20^\circ$  to  $60^\circ$  from the analysis of the TOF histograms. In Fig. 10 we have compared our results with the experimental values as well as other theoretical calculations. Our results are about 20% higher than those obtained by Schrader<sup>34</sup> (below  $\sim 40^\circ$ ) and some 30% lower than those by McEachran *et al.*<sup>82</sup> The results of Datta *et al.* at  $k=0.4$ , which we calculated from the partial-wave phase shifts given in their paper,<sup>36</sup> are very different from those given in Fig. 6 in their paper. For  $k=0.4$  and

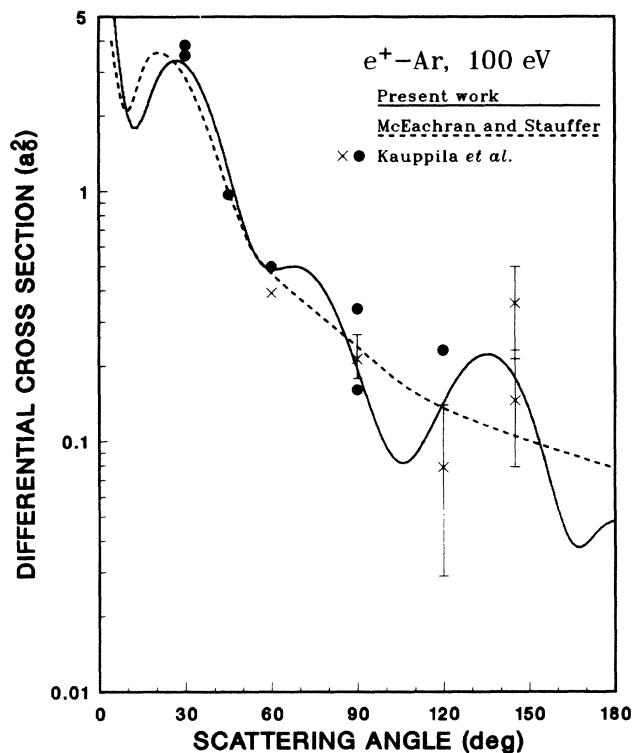


FIG. 11. Differential cross sections of positrons elastically scattered from argon for incident energy 100 eV. Values of McEachran and Stauffer are taken from Fig. 2 of Ref. 21.

0.7 Schrader's and our results seem to show reasonable agreement with the experimental values, while no calculations are able to reproduce accurately the experimental values for  $k=0.5$  and  $0.8$ . Thus it is difficult at the present moment to conclude which calculation is more reliable. Very recently, the first crossed-beam experiments were reported by the Kauppila *et al.*,<sup>21</sup> for electron-argon at 100 and 200 eV. Although at such a high energy the polarization effect has little effect, we have extended our calculation to 100 eV and the calculated phase shifts are listed in Table VI. Our differential cross sections are shown in Fig. 11, along with the experimental values of Kauppila *et al.* and the POM calculation of McEachran and Stauffer. Unexpectedly, our results are different from the POM calculation, and show several minima.

#### IV. CONCLUSIONS

We have performed calculations of low-energy electron and positron elastic scattering from neon and argon atoms using a model polarization potential for the target. The potential includes an effective radius. The *ad hoc* content of our approach is reduced to a single radius for each target atom by extending empirical relationships obtained previously for one- and two-electron targets to neon and argon. For the electronic systems a local exchange potential has been employed with parameters which are adjusted to generate the correct static-exchange phase shifts and the Hartree-Fock scattering length without explicitly con-



sidering the orthogonality conditions for the scattering wave.

In spite of great simplicity of our method, our results for the electronic systems are very accurate at low energy, where most other MPM calculations and more elaborate calculations yield less accurate results. For positronic systems, which are more sensitive to errors in potentials, our method give reasonably good results. Although it may be too early to conclude the validity of our empirical relations among the effective radii, they have worked well for neon and argon.

## ACKNOWLEDGMENTS

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