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Alternative static-exchange formalism: Low-energy electron scattering with heavy alkaline-earth atoms

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A static-exchange formalism is proposed based on the assumption that the scattering electron undergoes the same interaction as the extra electron in the negative ion of the target atom. In this method the wave function of the negative ion of the target atom is calculated, and the wave function of the frozen neutral core of the negative ion is used in the calculation of the interaction of scattering electron with the target atom. The screening effect of the incident electron on the target atom is approximated by that of the absorbed extra electron on the neutral core of the corresponding negative ion. The spin-polarization effect of the incident electron on the closed-shell target atoms is also considered by spin-polarized self-consistent field calculations for the negative-ion structures. A parameter-free spin-polarized correlation-polarization potential is included to represent the correlation and polarization effects in both the structure and scattering calculations. In order to account for the relativistic effects for heavy targets, a quasirelativistic approach is applied to the calculations of the negative-ion structures and the scattering processes. The results of low-energy electron scattering with Ca, Sr, Ba, and Ra atoms are given for energies between 0.01 and 5 eV.

I. INTRODUCTION

Generally in the static-exchange approximation the static and exchange interactions between the scattering electrons and the targets are calculated using free atomic wave functions; the dynamical correlation and polarization effects are neglected. In order to incorporate the neglected effects in the one-particle model of the scattering processes, various model polarization potentials have been used in the static-exchange plus polarization-potential calculations.[1] At very low energies, where the coupling between the elastic and inelastic channels is not strong, the one-particle model of static-exchange plus polarization potential can give quite reliable results for the elastic cross sections of closed-shell targets when a suitable model polarization potential is used.[2] In the static-exchange plus polarization formalism the long-range polarization effect is taken into account by the long-range polarization potential, while the short-range distortion, or the changes of the target electron-density distribution, caused by the screening effect of the incident electron generally is not considered explicitly in the construction of the model potential. The short-range polarization potential is modified empirically or semiempirically by a cutoff function.[1] In a modification by Padial and Norcross[3] of the original proposal of O'Connell and Lane,[4] a correlation potential, obtained from a local-density-functional theory, was used instead of the cutoff function in the short-range polarization potential. In a series of papers,[2,5] we have demonstrated that by combining the method of Padial and Norcross with the exact treatment of the static and exchange interactions, reliable results can be obtained for closed-shell targets, but in these calculations free atomic Hartree-Fock wave functions were used in evaluating the interactions between scattering electron and targets.

In the calculations of the low-lying shape resonances of electron-atom scattering processes the screening effect of the incident electron on the target atom is relatively more important because of the temporary absorption of the incident electron by the target atom in a quasistationary state. In a recent proposal of Haberland *et al.*,[6] the screening effect of the incident electron was taken into account by treating the scattering electron and the target atom as an entire system and self-consistently solving the $N+1$ one-particle equation as in atomic-structure calculations in the density-functional theory, but in their scheme the contribution of the continuum state to the total charge density was included by means of an arbitrary envelope function, and the exchange interaction of the incident electron with the electrons in the target was approximated by a local model exchange potential. In the continuum multiple-scattering method of Bloor and Sherrod,[7] the screening effect of the projectile was taken into account by the transition-state theory, but also a local model exchange potential was used in their method. Nevertheless, up to now no local model exchange potential has been confirmed to be suitable for representing the exchange effect in electron-atom scattering processes for a varity of target atoms, therefore the error caused by the local exchange approximation can reduce the reliability of the analysis of the validity and suitability of the polarization potential to account for the distortion, correlation, and polarization effects.

In the most recent calculations of Fischer *et al.*,[8] Vosko *et al.*,[9] Guo and Whitehead,[10] and Fuentealba *et al*,[11] one-particle self-consistent-field calculations predicted successfully stable negative ions of heavy alkaline-earth atoms by including the correlation correction potential. Bound orbitals were produced for the extra np electrons by Vosko *et al.* including a correlation potential in the Hartree-Fock method, and by Guo and Whitehead and Fuentealba *et al.* including correlation potential in the local-density-functional formalism. For heavy atoms the relativistic effects were considered in the calculations of Guo and Whitehead by means of the quasirelativistic approach of Cowan and Griffin.[12] We[13] have shown primarily that the quasirelativistic method of Cowan and Girffin is also very effective of taking the relativistic effects into account for the low-energy electron scattering with heavy atoms.

In the present paper the negative ions Ca^-, Sr^-, Ba^-, and Ra^- are calculated by introducing a spin-polarized correlation-polarization potential in the quasirelativistic Ξ method of Selvaraj and Gopinathan.[14] The neutral core part of the wave functions of the negative ions are used in the calculations of low-energy electron scattering with the neutral atoms. In this way the screening and spin-polarization effects of the incident electron on the targets are represented approximately by that of the absorbed electrons on the neutral core. The Ξ method uses a local approximation for exchange. In order to correct the error of the local exchange approximation, exact treatment of the exchange interaction is applied to the scattering processes. Because the core wave functions are spin polarized in the negative ions, spin-polarized correlation-polarization potentials are also included to represent the short-range correlation and long-range polarization effects in the scattering processes. The scattering processes of electrons with Ca, Sr, Ba, and Ra atoms are calculated while paying attention to the low-lying shape resonances. In order to make an indirect examination of the accuracy of the phase shifts, the bound energies of the np orbitals of the absorbed extra electrons in the negative ions are estimated by transforming the corresponding *p*-wave phase shifts at very low energies into the polarization quantum defects (PQD) defined by Watanabe and Greene[15] in the generalized quantum-defect theory (QDT). In this way the error in the bound energies caused by the local exchange approximation in Ξ method can be corrected. Unless otherwise specified, atomic units are used throughout the paper.

II. THEORETICAL FORMALISM

Because of the nonclosed shell structure of the negative ions Ca^-, Sr^-, Ba^-, and Ra^-, the spin-polarized quasirelativistic Ξ method is used in the calculations of the negative-ion structure. The details of the method were given by Selvaraj and Gopinathan.[14] Here only the construction of the spin-polarized correlation-polarization potential, which is included in the original Ξ method to produce bound orbitals for the extra *np* electrons, is given by

$$V_{cp}^{\uparrow}(r)=\begin{cases}V_c^{\uparrow}(r), & r\le r_c^{\uparrow}\\ V_p(r), & r>r_c^{\uparrow}\end{cases} \tag{1a}$$

and

$$V_{cp}^{\downarrow}(r)=\begin{cases}V_c^{\downarrow}(r), & r\le r_c^{\downarrow}\\ V_p(r), & r>r_c^{\downarrow},\end{cases} \tag{1b}$$

where $V_c^{\uparrow}$ and $Vc^{\downarrow}$ are the correlation potentials of spin-up and spin-down electrons, respectively, given by Perdew and Zunger,[16] $V_p(r)=-\alpha/2r^4$ is the long-range polarization potential, α is the polarizability of the neutral atom, and $r_c^{\uparrow}$ and $r_c^{\downarrow}$ are the inner intersection points of the corresponding correlation potential with the long-range polarization potential.

After the self-consistent-field calculations of the negative ions have been completed, the interactions of the scattering electron with the neutral atomic targets are evaluated from the wave functions of the frozen neutral cores of the negative ions, which are different from the corresponding free neutral atomic wave functions because of the screening effects of the absorbed extra electrons. In this way the screening effects of the scattering electrons on the neutral atomic targets are approximated by those of the extra electrons in the negative ions. The scattering equation is given by

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-2V_s(r)\right.$$
$$\left.-2V_{cp}(r)-2V_{\mathrm{RC}}(r)+k^2\right]u_l(r)=K_l(r)u_l(r)\ , \tag{2}$$

where $V_s(r)$ is the static potential, $V_{cp}(R)$ is the correlation-polarization potential of Eq. (1), $V_{\mathrm{RC}}(r)$ is the relativistic correction,[12] $K_1(r)u_1(r)$ is the exchange kernel, $u_1(r)$ is the radial part of the partial wave expansion of the scattering wave function; and k is the momentum of the incident electron. Note that all the quantities in Eq. (2) are calculated with the electron densities and wave functions of the frozen neutral core of the negative ion rather than that of the entire negative ion, and this is the main difference in the calculations of the scattering processes from those of the negative ions. The spin of the incident electron is chosen with the same direction as the extra electron in the negative ion. The relativistic correction $V_{\mathrm{RC}}(r)$ for the scattering electron is given by[12]

$$V_{\mathrm{RC}}(r)=-\frac{\alpha^2}{2}\left[\frac{k^2}{2}-V'(r)\right]^2$$
$$-\delta_{l,0}\frac{\alpha^2}{4}\left[1+\frac{\alpha^2}{2}\left[\frac{k^2}{2}-V'(r)\right]\right]^{-1}$$
$$\times\frac{dV'(r)}{dr}\left[\frac{du_l(r)}{dr}\Big/u_l(r)-\frac{1}{r}\right]\ , \tag{3}$$

where $V'(r)=V_s(r)+V_{cp}(r)+V_{\mathrm{ex}}(r)$, $V_{\mathrm{ex}}(r)$ is the free electron-gas exchange potential of Hara,[17] and α, here the fine-structure constant, is equal to $\frac{1}{137.036}$.

The exchange kernel in Eq. (2) is calculated exactly without any local approximation. The details of solving Eq. (2) are the same as in Yuan and Zhang.[2] It will be seen in the next section that the exact treatment of the exchange will correct the error caused by the local approximation in the bound energies of the absorbed electrons in the negative ions. Because of the screening effects of core electrons on the attraction of the nucleus, the static potential decays more quickly than the exchange interaction outside the neutral core. Therefore the exchange interaction has a relatively long-range effect compared with the static potential, and the exact treatment can apparently produce correction for the bound energies of the extra electrons.

By making an estimation of the bound energies of the extra electrons in the negative ions from the phase shifts of electron scattering at very low energies, the accuracy of the phase shifts at very low energies can be examined indirectly. The p-wave phase shifts can be converted into the PQD parameters, μ^0, as generalized by Watanabe and Greene[15] in the generalized quantum-defect theory, through the equation

$$\mu^0=\pi^{-1}\tan^{-1}[(B\cot\Delta\delta_l+G)^{-1}],\quad \bmod 1 \tag{4}$$

and

$$\Delta\delta_l=\delta_l-\left[\eta+\frac{l}{2}\pi\right], \tag{5}$$

where δ_l is the phase shift relative to spherical Bessel function, and B, G, and η are QDT parameters of polarization potential defined and given in Eqs. (2.12), (2.14), and (2.17) of Ref. 15. Equation (4) is a generalization of the well-known PQD theory for positive energies. μ^0 is smooth over the energy range from positive to negative. One can estimate the behavior of μ^0 and the corresponding negative states at negative energies by extrapolating the PQD number μ^0 from positive to negative energies.

III. RESULTS AND DISCUSSION

A. PQD number and bound state of heavy alkaline-earth negative ions

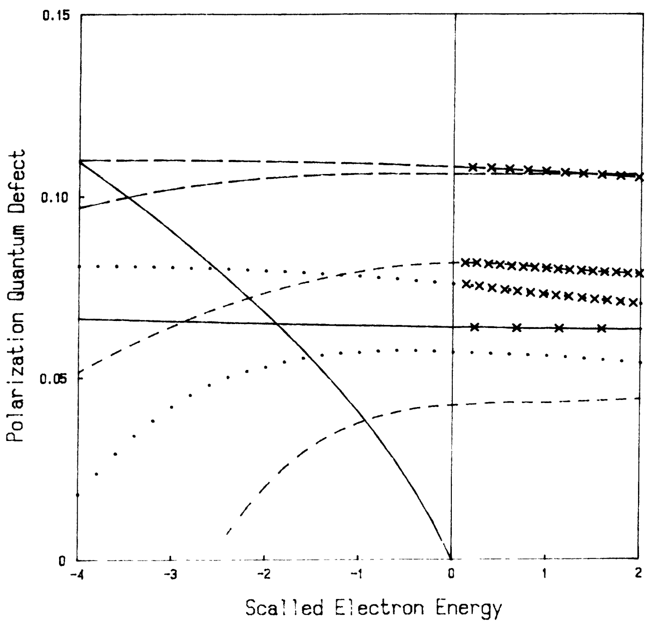

FIG. 1. The converted p-wave PQD μ^0 is shown as a function of the polarization scaled energy $2\varepsilon\alpha$ in (in a.u.), where ε is the electron energy in hartree and α is the polarizability in a.u. – × –, represents the present PQD of e-Ca scattering and the extrapolation at negative energies; – – –, the R-matrix PQD of e-Ca scattering of Kim and Greene in Ref. 18; · × ·, the present PQD of e-Sr scattering and its extrapolation; · · · ·, the R-matrix PQD of e-Sr scattering of Kim and Greene in Ref. 18; — × —, the present PQD of e-Ba scattering and its extrapolation; — — —, the R-matrix PQD of e-Ba scattering of Kim and Greene in Ref. 18; ✕—✕, the present PQD of e-Ra scattering and its extrapolation; ——, the universal relation in polarization potential given by Kim and Greene. The bound energies of the extra electrons of the negative ions are determined by the intersection points of the PQD curves with the solid universal relation.

In our previous papers[5] we have calculated the scattering processes of low-energy electrons with Ca and Sr atoms using the wave functions of free atoms without any consideration of the screening, spin-polarization, and relativistic effects. In Ref. 5 the unpolarized correlation potential was used both with and without an adjustable factor, and the p-wave quantum defects were also calculated from the corresponding phase shifts. In Fig. 1 the present converted p-wave quantum defects are plotted along with the R-matrix results of Kim and Greene.[18] The agreement between our results and their results is poor for Ca, reasonably good for Sr, and very good for Ba. The present p-wave quantum defects of Sr agree well with our previous results (which are not shown in Fig. 1) without the adjustable factor in Ref. 5, although local approximation has been used for exchange in the present calculation for negative ions. As we expected in the last section that the use of an exact treatment of exchange in the scattering calculations can somewhat compensate for the local exchange in structure calculations, we will see in the next paragraph that, compared with the values obtained from the one-electron eigenvalues of the extra electrons using Koopmans' theorem,[19] the bound energies of the absorbed electrons can be improved using the scattering phase shifts. The electron affinities of the corresponding negative ions are estimated approximately by extrapolating the PQD number from positive to negative energies with similar behavior of the curves at negative energies to the corresponding curves of Kim and Greene.[18] The electron affinities are determined by the intersections of the curves of the PQD with the universal solid curve. The estimated electron affinities are given in Table I and are compared with other predictions. The present estimation of the bound-state energies is approximated by the extrapolation of the PQD, but our results yield the same trend in the variation of the electron affinity with atoms as other calculations yield; in particular, a much smaller electron affinity is predicted for Ra compared with the other three atoms. As pointed out by Kim and Greene,[18] the determination of the electron affinity is not sensitive to the accuracy of the evaluated ground-state energies because of the flatness feature of the PQD curves, but it also has to be pointed out that the accuracy is quite sensitive to the values, i.e., the virtual positions, of the PQD curves because of the decrease of the universal curve with energy. Therefore a very accurate PQD is needed to get accurate electron affinities using the generalized quantum-defect theory. Nevertheless, the reflection of the difference in the PQD is not very significant on the positions and magnitudes of the d-wave shape resonances near 1 eV, as we have seen in our previous calculations for Ca and Sr.[5] Thus the apparent deviation of the present PQD of e-Ca scattering from the result of Kim and Greene does not imply that a significant change can be induced for the position and magnitude of the d-wave shape resonance for e-Ca scattering.

Koopmans' theorem[19] is a good approximation for the ionization potential of alkali-metal atoms, for which there is an electron outside a closed-shell core. Therefore one can also make an estimation for the electron affinities of the negative ions Ca^-, Sr^-, Ba^-, and Ra^-, in which the extra electrons are absorbed in the np orbitals outside the closed neutral core, from the one-electron eigenvalues of the absorbed electrons. In Table I the present eigenvalues of the extra electrons are also included and com-

TABLE I. Bound ns^2np states of the heavy alkaline-earth negative ions.

	ε (eV)		
Atom	Present		Others
Ca^-	−0.18[a]	−0.349[b]	−0.043±0.007[c] −0.045[d] −0.062[e] −0.13[f] −0.070[g] −0.131[h] −0.057[i] −0.12[j] −0.06[k]
Sr^-	−0.19[a]	−0.349[b]	−0.106[e] −0.16[f] −0.108[g] −0.160[h] −0.093[i] −0.54[j] −0.09[k] −0.17[k]
Ba^-	−0.20[a]	−0.399[b]	−0.148[e] −0.20[f] −0.176[g] −0.199[h] −0.192[i] −0.54[j]
Ra^-	−0.08[a]	−0.252[b]	−0.13[f] −0.075[g] −0.125[h]

[a] Estimated from phase shifts.
[b] Eigenvalues of the valence electrons in the negative ions.
[c] Experimental value of Pegg *et al.* in Ref. 23.
[d] MCHF of Fischer *et al.* in Ref. 8.
[e] MCHF of Fischer in Ref. 21.
[f] Density-functional theory of Vosko, Lagowski, and Mayer in Ref. 9.
[g] R matrix of Kim and Greene in Ref. 18.
[h] Spin-density-functional theory of Guo and Whitehead in Ref. 10.
[i] Many-body theory of Johnson *et al.* in Ref. 20.
[j] Density-functional theory of Fuentealba *et al.* in Ref. 11.
[k] Estimated from phase shifts in Ref. 5.

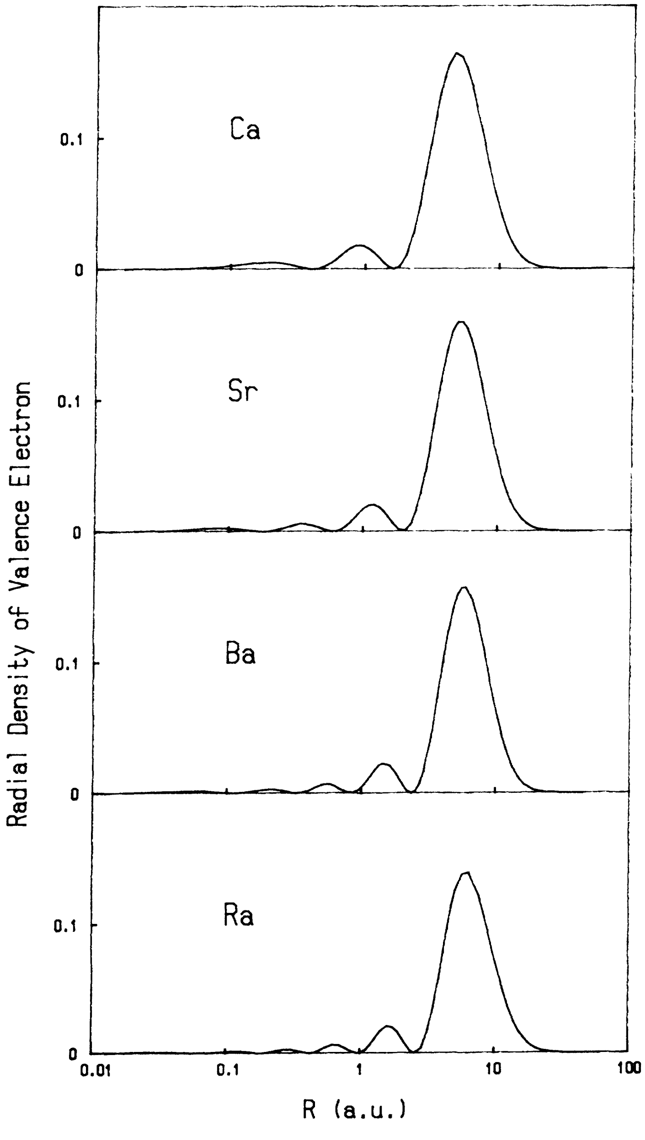

FIG. 2. The radial density distributions of the valence electrons in the alkaline-earth negative ions.

pared with the previous results. It can be seen that the present eigenvalues are much more negative than other data. We attribute these overstrong bound extra electrons to the local exchange approximation in the present structure calculations of the negative ions. In the last paragraph the electron affinities are estimated from the phase shifts, and it is clear that the overestimations are improved considerably by including the exchange exactly in the scattering calculations. Because of the quick decaying of static potential outside the neutral core, the exchange effect has a long interaction range compared with the static potential, and then the local exchange approximation can induce significant error in the extra electrons, for which the static potential is less important than the exchange effect outside the neutral closed shells. No apparent error can be caused by the local exchange potential in the neutral cores where the static potential is predominantly strong. The radial densities of the valence extra electrons are given in Fig. 2. Compared with the many-body theory results of Johnson, Sapirstein, and Blundell,[28] the density distributions are reproduced well in the present case, and the major part of the valence electron density is out the closed neutral core.

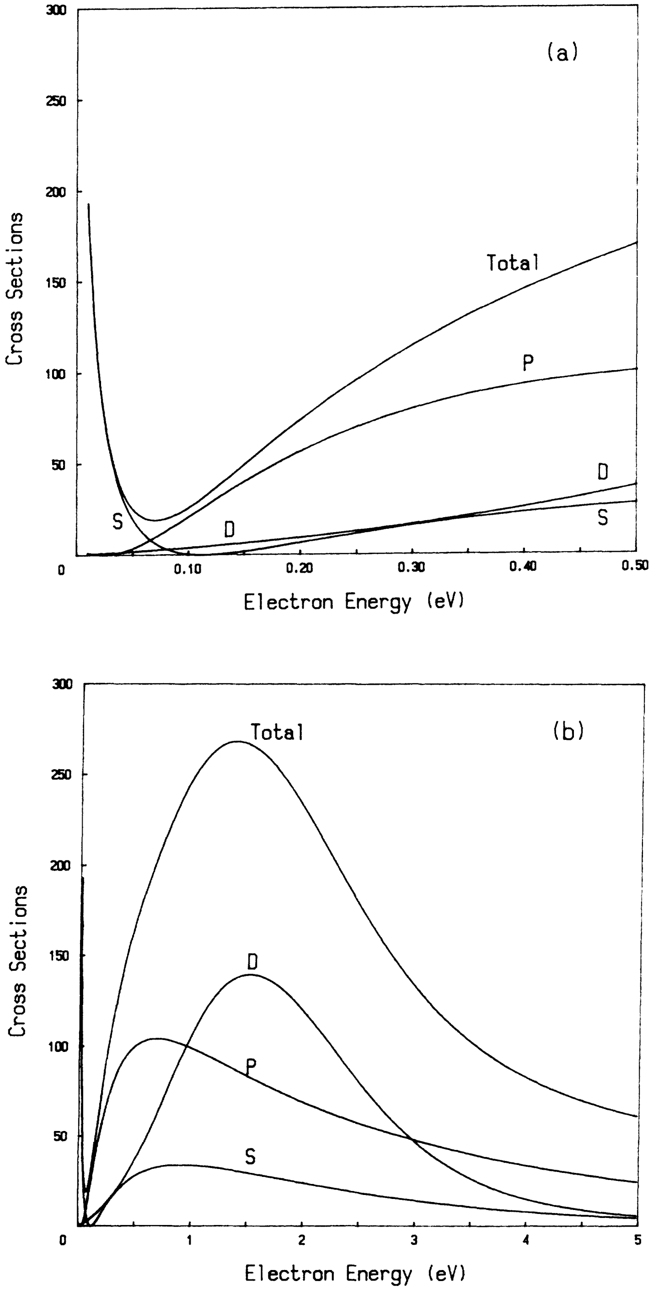

FIG. 3. Energy dependence of the elastic total and partial cross sections (in 10^{-16} cm^2) of e-Ca scattering.

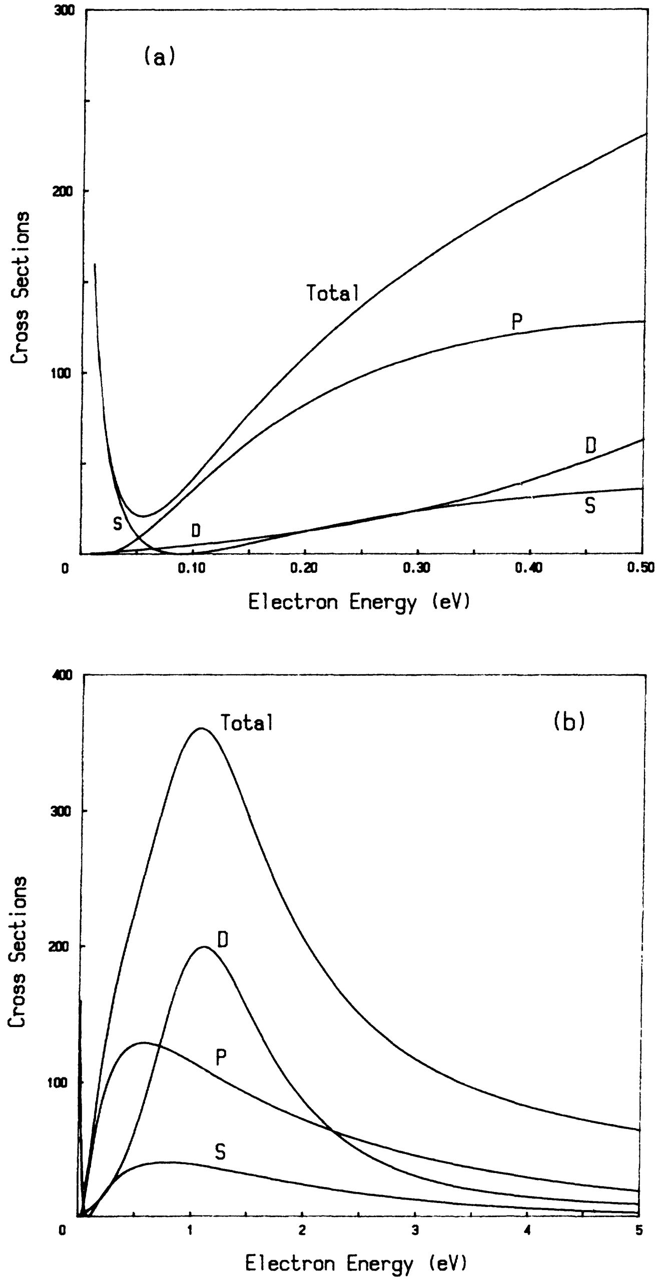

FIG. 4. As in Fig. 3 but for e-Sr scattering.

B. Elastic cross sections

The total cross sections and the partial cross sections of *s*, *p*, and *d* waves of the present calculations are plotted in Figs. 3–6. The main features of the cross sections are the *d*-wave-shape resonances and the Ramsauer-Townsend (RT) minima, which are much like the behavior of the elastic cross sections in the low-energy electron–rare-gas atoms scattering processes. For all the scattering processes in Figs. 3–6, the positions of the RT minimum points are in the range of 0.05–0.07 eV, but the *d*-wave-shape resonance energies are quite different from each other. The trend of the positions of the resonance peaks is that the larger the target is, the smaller the *d*-wave shape resonance energy, except for *e*-Ra process, for which the *d*-wave resonance occurs at higher energy than that of *e*-Ba scattering. This indicates that the attractiveness experienced by the incident electrons in *e*-Ra is weaker than that in *e*-Ba, but this is consistent with the theoretical predictions[8–11,18,20,21] about the stable negative ions of heavy alkalinc-earth elements, which gave a smaller electron affinity for Ra$^-$ than for Ba$^-$. In the last subsection the electron affinities of Ca$^-$, Sr$^-$, Ba,$^-$ and Ra$^-$ with extra electrons in the outmost *np* orbitals

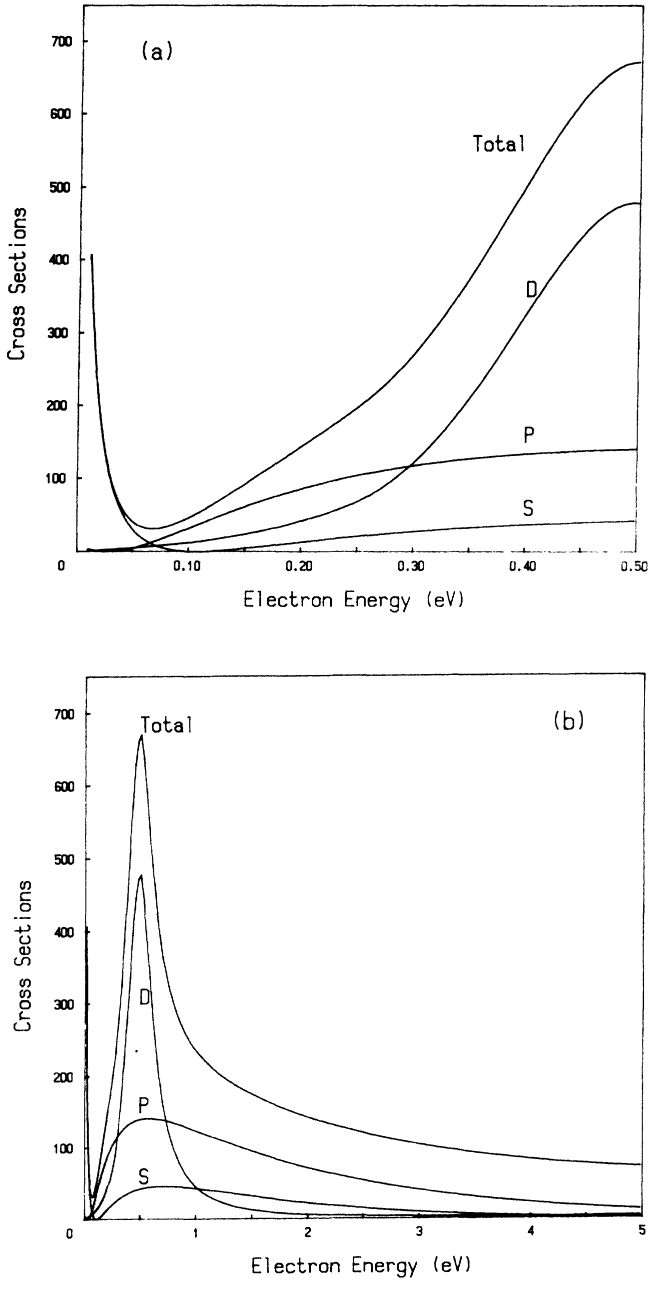

FIG. 5. As in Fig. 3 but for *e*-Ba scattering.

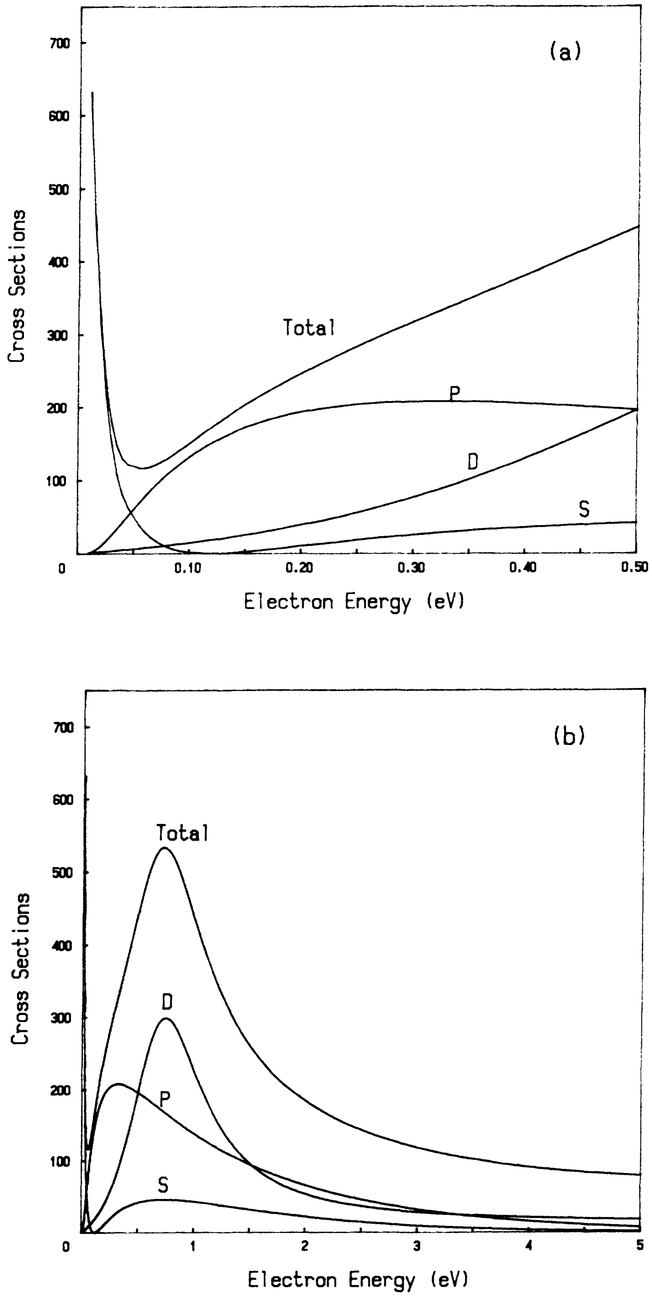

FIG. 6. As in Fig. 3 but for *e*-Ra scattering.

have been estimated from the corresponding *p*-wave phase shifts based on the generalized PQD theory.[15] A smaller electron affinity has been predicted for Ra^- than for Ba^-. Compared with the results in Ref. 5, there are no drastic differences for the results of *e*-Ca and *e*-Sr scattering processes, implying that the combining effects of screening, spin polarization, and relativity are not significant for these two atoms, but this does not mean that each one of these effects is not important separately. The relativistic effects are generally small for Ca and Sr, but are relatively important for Ba and Ra atoms. Nevertheless, comparisons of the total cross sections and phase shifts of *e*-Ba and *e*-Ra processes are not available with other reported theoretical and experimental results.

TABLE II. The total elastic cross sections of electron scattering with Ca, Sr, Ba, and Ra atoms (in 10^{-16} cm^2).

Energy (eV)	Ca	Sr	Ba	Ra
0.01	192.97	159.85	406.27	632.19
0.02	98.79	75.66	186.95	
0.03	57.12	41.50	100.50	180.95
0.04	36.02	26.67	59.86	
0.05	25.24	21.37	40.41	119.52
0.06	20.33	21.33	32.34	
0.07	19.02	24.40	30.94	121.64
0.08	20.00	29.32	33.65	
0.09	22.50	35.37	38.99	139.89
0.10	25.99	42.08	46.05	
0.11	30.13	49.14	54.22	161.78
0.12	34.70	56.36	63.14	
0.13	39.52	63.59	72.55	183.47
0.14	44.49	70.76	82.28	
0.15	49.53	77.80	92.23	203.77
0.16	54.56	84.67	102.33	
0.17	59.56	91.35	112.56	222.45
0.18	64.49	97.82	122.90	
0.19	69.32	104.09	133.38	239.62
0.20	70.04	110.14	144.00	247.71
0.30	114.82	160.48	272.17	317.30
0.40	145.34	198.60	505.47	381.15
0.50	169.34	231.83	670.65	447.04
0.60	189.48	264.13	496.78	504.59
0.70	207.20	296.10	363.00	532.76
0.80	223.03	325.28	296.23	521.62
0.90	236.95	347.53	258.92	482.80
1.00	248.68	359.28	234.80	434.35
1.10	257.87	359.54	217.37	
1.20	264.27	350.05	203.71	346.98
1.30	267.79	333.93	192.43	
1.40	268.52	314.27	182.77	284.33
1.50	266.68	293.40	174.27	
1.60	262.55	272.81	166.67	240.41
1.70	256.49	253.32	159.77	
1.80	248.84	235.31	153.45	208.43
1.90	239.94	218.91	147.62	
2.00	230.12	204.09	142.20	184.18
2.20	208.92	178.75	132.45	165.16
2.40	187.30	158.29	123.88	149.85
2.60	166.76	141.70	116.31	137.32
2.80	148.25	128.13	109.61	126.92
3.00	132.15	116.91	103.67	118.21
3.20	118.49	107.52	98.40	110.86
3.40	107.04	99.58	93.73	104.63
3.60	97.48	92.80	89.59	99.33
3.80	89.48	86.94	85.94	94.81
4.00	82.76	81.84	82.72	90.85
4.20	77.06	77.36	79.88	87.67
4.40	72.18	73.42	77.38	84.87
4.60	67.96	69.91	75.20	82.50
4.80	64.28	66.78	73.29	80.49
5.00	61.05	63.98	71.62	78.80

The only one experimental result for the total cross sections of electron scattering with Ca, Sr, and Ba atoms at very low energies was given by Romanyuk, Shpenik, and Zapesochnyl,[22] but their explanation of the experiment is in disagreement with the most recent experimental and theoretical results for the stable negative ions of Ca^-, Sr^-, Ba^-, and Ra^- with the extra electrons in *np* orbitals. They attributed the maximum peaks of the total cross sections at 0.7 eV for *e*-Ca, 0.1 eV for *e*-Sr, and 0.2 eV for *e*-Ba collisions to the *p*-wave shape resonances caused by the formation and decay of the short-lived states of the negative ions, but in the most recent investigations it has been shown that these atoms have long-lived stable, rather than short-lived decaying, negative ions with extra electron in the outermost *np* orbitals. The stable Ca^- was confirmed in an elegant experiment by Pegg *et al.*[23] In fact, if there are shape resonance states at such low energies as indicated by Romanyuk *et al.* in their experiment, the shape resonance peaks should be much higher than their measured values, and if the second maxima of the total cross sections of *e*-Ca and *e*-

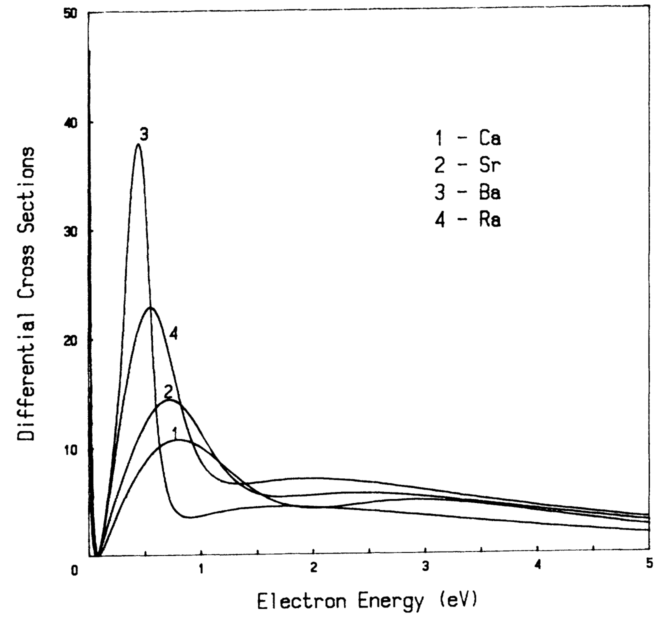

FIG. 7. Energy dependence of the differential cross sections (in 10^{-16} cm^2 sr^{-1}) at an angle of 90°.

TABLE III. The phase shifts of elastic *e*-Ca scattering (in rad, modπ).

Energy (eV)	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
0.01	0.2015	0.0081	0.0037	0.0012	0.0006	0.0003	0.0002
0.03	0.1880	−0.0063	0.0114	0.0037	0.0017	0.0009	0.0005
0.05	0.1436	−0.0349	0.0194	0.0062	0.0028	0.0015	0.0009
0.07	0.0962	−0.0684	0.0276	0.0087	0.0039	0.0021	0.0013
0.09	0.0502	−0.1035	0.0361	0.0113	0.0051	0.0027	0.0016
0.10	0.0279	−0.1211	0.0405	0.0125	0.0056	0.0030	0.0018
0.11	0.0062	−0.1386	0.0450	0.0138	0.0062	0.0033	0.0020
0.13	−0.0355	−0.1730	0.0541	0.0163	0.0073	0.0039	0.0024
0.15	−0.0751	−0.2064	0.0636	0.0189	0.0085	0.0046	0.0027
0.17	−0.1128	−0.2386	0.0733	0.0215	0.0096	0.0052	0.0031
0.20	−0.1659	−0.2848	0.0886	0.0254	0.0113	0.0061	0.0036
0.40	−0.4542	−0.5351	0.2096	0.0520	0.0228	0.0122	0.0073
0.60	−0.6720	−0.7183	0.3623	0.0801	0.0345	0.0183	0.0110
0.80	−0.8502	−0.8623	0.5401	0.1092	0.0464	0.0245	0.0146
1.00	−1.0023	−0.9807	0.7322	0.1391	0.0586	0.0308	0.0183
1.20	−1.1354	−1.0812	0.9276	0.1692	0.0709	0.0371	0.0220
1.40	−1.2541	−1.1687	1.1182	0.1991	0.0833	0.0434	0.0258
1.60	−1.3614	−1.2460	1.3003	0.2282	0.0959	0.0499	0.0295
1.80	−1.4592	−1.3155	1.4725	0.2562	0.1086	0.0563	0.0333
2.00	−1.5492	−1.3787	−1.5070	0.2828	0.1213	0.0628	0.0371
2.20	1.5091	−1.4366	−1.3555	0.3078	0.1338	0.0694	0.0409
2.40	1.4316	−1.4902	−1.2155	0.3310	0.1463	0.0760	0.0447
2.60	1.3591	−1.5402	−1.0879	0.3525	0.1585	0.0826	0.0486
2.80	1.2911	1.5545	−0.9731	0.3723	0.1704	0.0893	0.0525
3.00	1.2271	1.5104	−0.8713	0.3904	0.1820	0.0959	0.0564
3.40	1.1094	1.4289	−0.7035	0.4221	0.2041	0.1091	0.0642
3.80	1.0034	1.3549	−0.5761	0.4488	0.2243	0.1222	0.0722
4.00	0.9541	1.3203	−0.5245	0.4605	0.2337	0.1286	0.0761
4.40	0.8620	1.2550	−0.4399	0.4816	0.2511	0.1411	0.0841
4.80	0.7775	1.1946	−0.3742	0.5002	0.2666	0.1531	0.0921
5.00	0.7378	1.1659	−0.3468	0.5087	0.2737	0.1589	0.0961

Sr in their measurement were caused by ^2D shape resonances as they suspected, the maximum peaks of shape resonances at such high energies should be broad structures rather than small and sharp peaks. From the present calculations it is suspected that the high and large peaks in the experiment of Romanyuk *et al.*, were caused by the *d*-wave shape resonances and the second smaller peaks in *e*-Ca and *e*-Sr scattering in the neighborhood of the high and larger peaks were associated with the $3\,^3D$ and $4\,^4D$ excitations, respectively, and that it is possible that the whole curves of their cross sections were moved to the low-energy direction by about 0.8 eV because of a systematic error in the determination of the electron energy in their measurement. The small structures of the first excitations of the targets were perhaps masked by the shape resonance peaks in the experiment of Romanyuk *et al.* We have noticed the fact that the magnitudes of the peaks agree reasonably well between our results and those of Romanyuk *et al.* for *e*-Ca and *e*-Sr processes, and that the near constant values of the total cross sections at high energies also agree well between our theoretical and their experimental values, but for the *e*-Ba process Romanyuk *et al.*, did not give the value at the top of the peak; their value at 0.2 eV agrees well with our value at 1.0 eV. Based on these facts and the actual positions of the ^3D excitations of Ca and Sr atoms one can also suspect that the curves were systematically moved to lower energy in the experiment of Romanyuk *et al.* The detailed values of the present elastic total cross sections are given in Table II. The detailed values of the phase shifts are given in Tables III–VI.

The differential cross sections (DCS) are calculated at an angle of 90° and plotted in Fig. 7 for all the four atoms. In the experiment of Kazakov and Khristoforov,[24] the relative elastic DCS of *e*-Ca scattering at an angle of 90° was measured with the electron energy. The main features of the variation of the DCS with the scattering energy are the very deep minimum structure near zero energy, a high peak around 1 eV, and a relatively shallow minimum structure in 2–3 eV. In the experiment of *e*-Sr scattering by Kazakov *et al.*,[25] the resonances caused by the formation of short-lived negative

TABLE IV. The phase shifts of elastic *e*-Sr scattering (in rad, modπ).

Energy (eV)	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
0.01	0.1832	0.0065	0.0041	0.0014	0.0006	0.0003	0.0002
0.03	0.1564	−0.0163	0.0127	0.0041	0.0019	0.0010	0.0006
0.05	0.1042	−0.0539	0.0216	0.0069	0.0031	0.0017	0.0010
0.07	0.0514	−0.0957	0.0309	0.0097	0.0044	0.0023	0.0014
0.09	0.0005	−0.1380	0.0407	0.0124	0.0056	0.0030	0.0018
0.10	−0.0237	−0.1588	0.0457	0.0138	0.0062	0.0033	0.0020
0.11	−0.0472	−0.1794	0.0509	0.0152	0.0069	0.0037	0.0022
0.13	−0.0923	−0.2194	0.0616	0.0181	0.0081	0.0044	0.0026
0.15	−0.1350	−0.2578	0.0729	0.0209	0.0094	0.0050	0.0030
0.17	−0.1754	−0.2946	0.0846	0.0238	0.0106	0.0057	0.0034
0.20	−0.2324	−0.3468	0.1033	0.0281	0.0125	0.0067	0.0040
0.40	−0.5380	−0.6242	0.2642	0.0579	0.0253	0.0135	0.0081
0.60	−0.7677	−0.8246	0.4970	0.0895	0.0382	0.0203	0.0121
0.80	−0.9550	−0.9814	0.7971	0.1227	0.0515	0.0271	0.0162
1.00	−1.1145	−1.1105	1.1240	0.1569	0.0650	0.0341	0.0202
1.20	−1.2541	−1.2201	1.4231	0.1915	0.0788	0.0410	0.0243
1.40	−1.3783	−1.3156	−1.4745	0.2259	0.0928	0.0481	0.0285
1.60	−1.4905	−1.4001	−1.2831	0.2594	0.1070	0.0552	0.0326
1.80	1.5487	−1.4761	−1.1322	0.2915	0.1213	0.0624	0.0368
2.00	1.4563	−1.5452	−1.0112	0.3218	0.1355	0.0697	0.0409
2.20	1.3676	1.5330	−0.9125	0.3502	0.1497	0.0770	0.0451
2.40	1.2866	1.4743	−0.8311	0.3765	0.1636	0.0843	0.0494
2.60	1.2109	1.4195	−0.7633	0.4006	0.1773	0.0917	0.0536
2.80	1.1398	1.3682	−0.7066	0.4228	0.1906	0.0991	0.0579
3.00	1.0729	1.3198	−0.6590	0.4430	0.2035	0.1065	0.0622
3.40	0.9497	1.2304	−0.5856	0.4785	0.2279	0.1212	0.0709
3.80	0.8386	1.1492	−0.5335	0.5085	0.2501	0.1356	0.0796
4.00	0.7870	1.1111	−0.5134	0.5219	0.2603	0.1426	0.0840
4.40	0.6904	1.0394	−0.4820	0.5462	0.2791	0.1563	0.0927
4.80	0.6016	0.9727	−0.4596	0.5681	0.2957	0.1693	0.1014
5.00	0.5598	0.9411	−0.4509	0.5784	0.3032	0.1755	0.1057

Sr^- ion are detected in the energy dependence of the flux of elastically scattered electrons, but the differential cross sections were not evaluated. The main features of the experiment of *e*-Ca scattering by Kazakov and Khristoforov[24] are reproduced well in our calculations as plotted in Fig. 7, but the minimum point near 0.08 eV is caused by an RT minimum structure in our calculation rather than by a *p*-wave shape resonance as suggested by Kazakov and Khristoforov[24] in their experiment. The maximum peak near 0.8 eV of *e*-Ca scattering in Fig. 7 is caused by a *d*-wave shape resonance in agreement with the experiment. The second shallow minimum structure is predicted at 2 eV in our calculation for *e*-Ca. In the experiment for *e*-Sr scattering,[25] the deep minimum point near zero energy, the high and larger maximum peak near 1 eV, and the second shallow minimum structure were detected, although only the scattered electron flux was measured without evaluating the differential cross sections, but they also attributed the deep minimum point near zero energy to a very low-lying *p*-wave shape resonance. As shown in Fig. 7, similar features are predicted for *e*-Sr scattering, and as for Ca, the minimum point below 0.1 eV is caused by an RT structure rather than a low-lying *p*-wave shape resonance. The suspicion of Kazakov *et al.*[24,25] about the *p*-wave shape resonances associated with the deep minimum points near zero energy was based on the experiment of Romanyuk *et al.*,[22] but in the last paragraph we have pointed out that their experiment should be reexamined. All the curves in Fig. 7 have the similar dependence with electron energy except for the difference in the positions of the minimum and maximum structures. No measurement is available for *e*-Ba and *e*-Ra differential cross sections for comparison with our results. In Fig. 7, the *d*-wave shape resonance of *e*-Ra scattering occurs at higher energy with smaller peak than *e*-Ba scattering, as in the total elastic cross sections, although it is heavier and has larger polarizability than Ba.

TABLE V. The phase shifts of elastic *e*-Ba scattering (in rad, modπ).

Energy (eV)	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
0.01	0.2943	0.0143	0.0060	0.0019	0.0009	0.0005	0.0003
0.03	0.2495	−0.0026	0.0185	0.0059	0.0027	0.0014	0.0009
0.05	0.1783	−0.0394	0.0321	0.0099	0.0045	0.0024	0.0014
0.07	0.1097	−0.0825	0.0469	0.0139	0.0063	0.0034	0.0020
0.09	0.0462	−0.1271	0.0630	0.0180	0.0081	0.0043	0.0026
0.10	0.0163	−0.1493	0.0717	0.0200	0.0090	0.0048	0.0029
0.11	−0.0126	−0.1713	0.0808	0.0221	0.0099	0.0053	0.0032
0.13	−0.0673	−0.2143	0.1004	0.0263	0.0117	0.0063	0.0038
0.15	−0.1184	−0.2558	0.1221	0.0303	0.0135	0.0072	0.0043
0.17	−0.1666	−0.2956	0.1463	0.0345	0.0153	0.0082	0.0049
0.20	−0.2339	−0.3523	0.1881	0.0409	0.0181	0.0097	0.0058
0.40	−0.5868	−0.6557	0.8326	0.0851	0.0366	0.0194	0.0116
0.60	−0.8467	−0.8757	−1.0439	0.1321	0.0556	0.0293	0.0174
0.80	−1.0565	−1.0482	−0.6091	0.1812	0.0750	0.0393	0.0233
1.00	−1.2339	−1.1905	−0.4480	0.2306	0.0949	0.0493	0.0292
1.20	−1.3883	−1.3118	−0.3607	0.2789	0.1150	0.0595	0.0352
1.40	−1.5251	−1.4178	−0.3047	0.3250	0.1353	0.0698	0.0411
1.60	1.4934	−1.5120	−0.2663	0.3679	0.1554	0.0802	0.0471
1.80	1.3816	1.5444	−0.2397	0.4073	0.1753	0.0907	0.0532
2.00	1.2792	1.4666	−0.2216	0.4431	0.1946	0.1012	0.0593
2.20	1.1846	1.3949	−0.2100	0.4754	0.2133	0.1116	0.0654
2.40	1.0969	1.3283	−0.2031	0.5046	0.2311	0.1220	0.0715
2.60	0.0151	1.2659	−0.2001	0.5311	0.2480	0.1324	0.0777
2.80	0.9385	1.2073	−0.1998	0.5553	0.2639	0.1425	0.0838
3.00	0.8666	1.1519	−0.2018	0.5777	0.2788	0.1525	0.0900
3.40	0.7345	1.0495	−0.2103	0.6186	0.3055	0.1717	0.1023
3.80	0.6158	0.9564	−0.2227	0.6563	0.3283	0.1896	0.1144
4.00	0.5607	0.9128	−0.2297	0.6746	0.3385	0.1980	0.1204
4.40	0.4576	0.8308	−0.2450	0.7108	0.3567	0.2137	0.1321
4.80	0.3629	0.7549	−0.2613	0.7474	0.3726	0.2278	0.1433
5.00	0.3183	0.7189	−0.2697	0.7659	0.3799	0.2343	0.1487

IV. CONCLUSION

In conclusion, the screening, spin-polarization, and relativistic effects are accounted for in the present static-exchange plus correlation-polarization potential formalism based on the assumption that the incident electron experiences the same interaction as the extra absorbed electron in the negative ion of the target. The present correlation-polarization potential is not exactly the same as the original one of Padial and Norcross, in which the spin-polarization was neglected, but the present potential is also different from that used in the local-density-functional theory, where the long-range polarization potential is ignored, though it is very important for the loosely bound extra electrons in the negative ions. The results for *e*-Ca and *e*-Sr scattering processes show that the combined effects of the screening, spin-polarization, and relativity are not very significant for these two atoms. The present cross sections of the four heavy alkaline-earth atoms have similar dependences with electron energy, but they are drastically different from the earlier experiment of Romanyuk *et al.* Because the conclusions of the short-lived ^2P shape resonance states in the experiment of Romanyuk *et al.* disagree with the most recent experimental prediction for stable Ca^- and theoretical predictions for all the stable heavy alkaline-earth negative ions, quantitative comparisons between theory and experiment need more reliable experimental data of total cross sections, but the reliability of the present calculations is examined indirectly from the estimated electron affinities from phase shifts, and our results agree reasonably well with other investigations. The present predictions of the DCS dependences with electron energy has been confirmed in the experiment of Kazakov and Khristoforov for *e*-Ca scattering, although they attributed the deep minimum structure near zero energy to a low-lying *p*-wave shape resonance, while we give the minimum point by an RT structure. Further, more complete calculations are needed for electron–alkaline-earth-atom scattering. The present scheme cannot be applied to account for the screening effect for the atoms, for example, rare-gas atoms, for which stable negative ions do not exist; a new formalism has to be developed for these atoms.

TABLE VI. The phase shifts of elastic *e*-Ra scattering (in rad, modπ).

Energy (eV)	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
0.01	0.3716	−0.0046	0.0068	0.0022	0.0010	0.0005	0.0003
0.03	0.3142	−0.0714	0.0212	0.0068	0.0030	0.0016	0.0010
0.05	0.2341	−0.1457	0.0363	0.0114	0.0051	0.0027	0.0016
0.07	0.1585	−0.2153	0.0524	0.0160	0.0072	0.0038	0.0023
0.09	0.0894	−0.2787	0.0694	0.0206	0.0093	0.0050	0.0030
0.11	0.0261	−0.3365	0.0873	0.0253	0.0113	0.0061	0.0036
0.13	−0.0323	−0.3894	0.1063	0.0301	0.0134	0.0072	0.0043
0.15	−0.0867	−0.4383	0.1263	0.0349	0.0155	0.0083	0.0050
0.17	−0.1376	−0.4836	0.1474	0.0397	0.0176	0.0094	0.0056
0.20	−0.2086	−0.5460	0.1812	0.0469	0.0207	0.0111	0.0066
0.40	−0.5764	−0.8571	0.4846	0.0968	0.0420	0.0223	0.0133
0.60	−0.8438	−1.0727	0.9371	0.1474	0.0637	0.0336	0.0200
0.80	−1.0579	−1.2410	1.4340	0.1970	0.0856	0.0451	0.0268
1.00	−1.2378	−1.3805	−1.3327	0.2439	0.1073	0.0566	0.0335
1.20	−1.3936	−1.5004	−1.0952	0.2872	0.1286	0.0681	0.0404
1.40	−1.5311	1.5356	−0.9453	0.3266	0.1491	0.0796	0.0472
1.60	1.4873	1.4409	−0.8467	0.3622	0.1687	0.0910	0.0540
1.80	1.3756	1.3550	−0.7795	0.3944	0.1871	0.1022	0.0609
2.00	1.2734	1.2762	−0.7323	0.4239	0.2044	0.1131	0.0677
2.20	1.1793	1.2033	−0.6987	0.4510	0.2203	0.1236	0.0744
2.40	1.0919	1.1355	−0.6746	0.4762	0.2351	0.1338	0.0811
2.60	1.0105	1.0722	−0.6573	0.5001	0.2487	0.1436	0.0877
2.80	0.9341	1.0126	−0.6451	0.5229	0.2613	0.1528	0.0942
3.00	0.8623	0.9564	−0.6369	0.5449	0.2729	0.1616	0.1005
3.40	0.7302	0.8527	−0.6288	0.5873	0.2939	0.1778	0.1127
3.80	0.6108	0.7586	−0.6286	0.6286	0.3123	[illegible]	0.1240
4.00	0.5552	0.7147	−0.6306	0.6490	0.3208	0.1986	0.1294
4.40	0.4509	0.6320	−0.6378	0.6903	0.3366	0.2106	0.1394
4.80	0.3547	0.5553	−0.6481	0.7326	0.3513	0.2214	0.1486
5.00	0.3096	0.5189	−0.6542	0.7543	0.3582	0.2264	0.1529

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