Application of the quasirelativistic approach to low-energy electron–atom scattering: Xe

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Abstract. A quasirelativistic approach is applied to the calculation of the atomic wavefunc-tion and the low-energy e-Xe scattering process. For the scattering calculation the exchange and static interactions are treated exactly; the correlation, distortion and polarization effects are accounted for approximately by a parameter-free correlation-polarization potential. The relativistic, correlation, distortion and polarization effects are considered effectively and very good agreement between theory and experiment is obtained for the elastic total, differential and momentum transfer cross sections in the energy range 0.1-20.0 eV.

1. Introduction

The low-energy e-Xe scattering process has been investigated extensively by both theory and experiment. However, no satisfactory agreement has been obtained between the theoretical and experimental results, particularly around the top of the d wave shape resonance. Compared with the measured values (Dababneh *et al* 1980, Jost *et al* 1983, Nickel *et al* 1985, Register *et al* 1986, Subramanian and Kumar 1987) all the reported calculations (see for example Sin Fai Lam 1982, McEachran and Stauffer 1984, 1987, Yuan and Zhang 1989a) overestimated the total cross section by about 6–15 Å² near the maximum point. In the calculations of Sin Fai Lam (1982) and McEachran and Stauffer (1987), although the exchange interaction was included exactly and the relativistic effects were considered adequately, their results showed apparent discrepancy with experiment near the peak because of the excessive strength of the polarization potentials. In our previous papers (Yuan 1988, Yuan and Zhang 1989a) we have calculated the elastic cross sections of electron scattering from He, Ne, Ar, Kr and Xe atoms by combining the exact treatment of exchange with the parameter-free correlation-polarization (CP) potential of Padial and Norcross (1984), which is a modification of the proposal of O'Connell and Lane (1983). Reliable results and demonstration of the adequacy of the CP potential were given for He, Ne, Ar and Kr atoms, but for the Xe atom the result showed some discrepancy from the experiments because of the relativistic effects being neglected. We have pointed out (Yuan and

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Zhang 1989a) that neglecting relativistic effects was the predominant reason for the deviation of our result from the measured values. Therefore, the influence of the relativistic effects on the calculation would be interesting to investigate.

Cowan and Griffin (1976) proposed a quasirelativistic approach for the calculations of heavy atomic structures. Their scheme is successful in dealing with the relativistic effects with results very close to the corresponding Dirac–Fock values. Cowan and Griffin originally combined their method with Hartree–Fock theory; in a later paper Selvaraj and Gopinathan (1984) applied Cowan and Griffin's scheme successfully with the Ξ method (Vaidehi and Gopinathan 1984) in the structural calculations of atoms. They gave the values of total energies, orbital eigenvalues and the expectation of r^n ($n = -1, 1, 2$) very close to those of Cowan and Griffin and Dirac–Fock calculations.

The purpose of the present paper is to estimate the applicability of Cowan and Griffin's quasirelativistic approach to the scattering process of low-energy electrons with heavy atoms and to give much better agreement between theory and experiment for the low-energy e-Xe scattering than the previous reported calculations by incorporating relativistic effects via the quasirelativistic approach. The atomic wavefunction is calculated based on the quasirelativistic Ξ method of Selvaraj and Gopinathan (1984), while the calculation of the scattering process is the same as in our previous papers (Yuan 1988, Yuan and Zhang 1989a) except the inclusion of the relativistic correction in the scattering equations. Unless otherwise specified atomic units are used in this paper.

2. Quasirelativistic approach

The quasirelativistic Ξ method of Selvaraj and Gopinathan (1984) is used in the calculation of the Xe structure. The details of the method were given by Selvaraj and Gopinathan (1984). In this section only the relativistic corrected scattering equation is given. By incorporating the relativistic correction, V_{rc}, the radial equation of scattering wavefunction becomes

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - 2V_s(r) - 2V_{cp}(r) - 2V_{rc}(r) + k^2\right)U_l(r) = K_l(r)U_l(r) \quad (1)$$

where $V_s(r)$ is the static potential, $V_{cp}(r)$ is the CP potential of Padial and Norcross (1984) with the recommended correlation potential of Perdew and Zunger (1981), which is slightly weaker than the form used by Padial and Norcross (1984) and in our previous papers (Yuan 1988, Yuan and Zhang 1989a), $K_l(r)U_l(r)$ is the exchange kernel arising from the exchange effect of the incident electron with the electrons in the target. The relativistic correction is given by

$$V_{rc} = -\frac{\alpha^2}{2}\left(\frac{k^2}{2} - V'(r)\right)^2$$

$$-\delta_{l,0}\frac{\alpha^2}{4}\left[1 + \frac{\alpha^2}{2}\left(\frac{k^2}{2} - V'(r)\right)\right]^{-1}\frac{dV'(r)}{dr}\left[\frac{dU_l(r)}{dr}(U_l(r))^{-1} - \frac{1}{r}\right] \quad (2)$$

where $V'(r) = V_s(r) + V_{cp}(r) + V_{ex}(r)$, $V_{ex}(r)$ is the free-electron gas exchange potential

of Hara (1967), and α, the fine-structure constant, is equal to $1/137.036$. The details of solving equation (1) are the same as in Yuan and Zhang (1989a).

3. Results and discussion

In the calculations of Cowan and Griffin (1976) and Selvaraj and Gopinathan (1984), the major relativistic effects were incorporated effectively by the quasirelativistic approach for the structural calculations. Their results of total energies, orbital eigenvalues and the expectations of r^n ($n = -1, 1, 2$) were in very good agreement with that of the exact relativistic Dirac–Fock calculations for a variety of atoms. Therefore, one can expect that the same good agreement can be obtained by the quasirelativistic method for the wavefunctions and electron densities as for the quantities mentioned above, and then the major indirect relativistic effects in the low-energy electron–atom scattering mentioned by Sin Fai Lam (1982) can be incorporated adequately by the method. The wavefunction of Xe obtained by the quasirelativistic Ξ method (Selvaraj and Gopinathan 1984) is used in the calculations of $V_s(r)$, $V_{cp}(r)$, $V_{rc}(r)$ and the exchange kernel, $K_1(r)U_1(r)$, in equation (1).

The Ξ method provides a very successful way to approximate the exchange interaction by a local model exchange potential in atomic structure calculations, but no local approximation for the exchange interaction in electron–atom scattering process works satisfactorily at such low energies. Therefore, equation (1) is solved without any approximation for the exchange kernel on the right-hand side of the equation. In the calculations of Cowan and Griffin (1976) and Selvaraj and Gopinathan (1984) the model exchange potential of HX (Hartree-exchange potential in Cowan and Griffin (1976), and Cowan (1967)) and Ξ were used respectively in the calculations of the relativistic correction $V_{rc}(r)$, while the free electron gas exchange potential (Hara 1967) is used in the present calculation of the relativistic correction because Hara's potential generally gives better results than HX as well as the Ξ-exchange potential for electron–atom scattering processes.

In figure 1 our results for the total elastic cross section are plotted and compared with several sets of recent experimental and theoretical results. In the Ramsauer–Townsend (RT) minimum region the agreement of the present quasirelativistic corrected result with the plotted experiments is apparently better than our previous non-relativistic calculation (Yuan and Zhang 1989a). As we expected in the previous paper, compared with our non-relativistic result the RT minimum point is moved to a higher energy by 0.1 eV via the inclusion of the relativistic effects in the present case. Below 2 eV, our quasirelativistic result is in very good agreement with the semirelativistic calculation of Sin Fai Lam (1982), and shows some discrepancy from the complete relativistic result of McEachran and Stauffer (1987), but the agreement of the present curve with the plotted experimental points is as good as that of McEachran and Stauffer except the deviation is in the opposite direction from the experimental points below 0.6 eV. In the calculations of Sin Fai Lam (1982) and McEachran and Stauffer (1987), because the polarization potentials were too large to represent the polarization effect adequately for the d partial wave, the calculated total elastic cross sections were much higher than the measured data around the maximum point, although the relativistic effects were considered adequately, while because of the neglect of the relativistic effects we also obtained a much higher peak than the measurements in our non-relativistic calculation
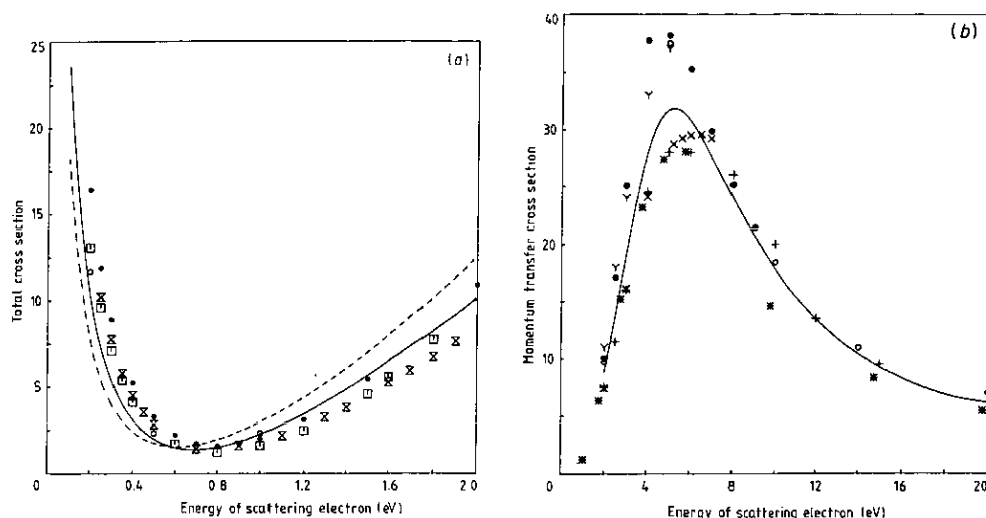
Figure 1. Total cross sections, (*a*) from 0.1 eV to 2.0 eV, (*b*) from 1.0 eV to 20 eV: ——, present elastic total cross section; ----, non-relativistic elastic total cross section of Yuan and Zhang (1989a); ●, relativistic elastic total cross section of McEachran and Stauffer (1987); ○, semirelativistic elastic total cross section of Sin Fai Lam (1982); *, total cross section estimated by adding the total excitation cross section of Hayashi (1983) to the present total elastic cross section; □, total cross section measured and revised by Jost *et al* (1983, quoted by McEachran and Stauffer 1987 and Subramanian and Kumar 1987); ⅀, experiment by Ferch *et al* (1987, quoted by McEachran and Stauffer 1987); +, total cross section by Dababneh *et al* (1980); Y, total cross section by Nickel *et al* (1985); ×, total cross section of Subramanian and Kumar (1987). The typical estimated accuracy of the experiment is better than 3.5% (Dababneh *et al* 1980).

(Yuan and Zhang 1989a). In the present case, we gain a much better agreement between theory and experiments below 12 eV than all of the previous calculations (Sin Fai Lam 1982, McEachran and Stauffer 1984, 1987, Yuan and Zhang 1989a) by including the relativistic and polarization effects adequately. Because the inelastic cross sections are also included in the plotted experimental total cross sections, our calculated elastic total cross section is apparently lower than the plotted experimental data at the energies above 12 eV. In order to make a reasonable comparison between theory and experiment at the energies above the inelastic threshold, in figure 1 we also give an estimation for the total cross sections at a few energies above the inelastic threshold by adding the total excitation cross section of Hayashi (1983) to our total elastic cross sections. It is clear that our estimation for the total cross section is in very good agreement with the experiment by Dababneh *et al* (1980). The ionization cross section is not included in our estimation for the total cross section, but by including the ionization cross section the result (not shown in figure 1) is very close to the experimental data of Jost *et al* (1983) and Nickel *et al* (1985) rather than that of Dababneh *et al*. The detailed values of our total elastic and estimated total cross sections are given in table 1.

   The momentum transfer cross section is plotted in figure 2 along with a few sets of experimental data. The agreement of the present results with the experiments is good over the whole plotted energy range. As in figure 1(*b*) our result is much lower and closer to most of the experimental points than the results of Sin Fai Lam (1982) and McEachran and Stauffer (1987) around the peak. As in figure 1(*a*), our momentum

Table 1. Elastic total and momentum transfer cross sections (in 10^{-16} cm^2).

eV	σ_T	σ_m	eV	σ_T	σ_m
0.1	23.60	17.60	6.0	43.05	30.77
0.2	10.43	5.90	6.5	43.57	29.33
0.3	5.42	2.15	7.0	43.58	27.61
0.4	3.10	0.76	7.5	43.23	25.80
0.5	2.00	0.30	8.0	42.66	24.00
0.6	1.49	0.25	8.5	41.96 (41.99)†	22.28
0.7	1.38	0.44	9.0	41.18 (41.31)	20.67
0.8	1.52	0.76	9.5	40.36 (40.49)	19.18
0.9	1.84	1.16	10.0	39.54 (39.72)	17.82
1.0	2.28	1.63	11.0	37.94 (38.36)	15.43
1.5	5.66	4.74	12.0	36.45 (37.29)	13.44
2.0	10.17	8.89	13.0	35.11 (36.39)	11.79
2.5	15.41	13.81	14.0	33.95 (35.65)	10.40
3.0	21.06	19.05	15.0	32.95 (35.09)	9.24
3.5	26.75	23.97	16.0	32.12 (34.67)	8.28
4.0	31.99	27.93	17.0	31.47	7.48
4.5	36.35	30.53	18.0	30.97 (34.32)	6.86
5.0	39.62	31.70	19.0	30.65	6.44
5.5	41.81	31.67	20.0	30.37 (34.10)	6.16

† The data in the parentheses are the total cross sections estimated by adding the excitation cross sections of Hayashi (1983) to the present total elastic cross sections.
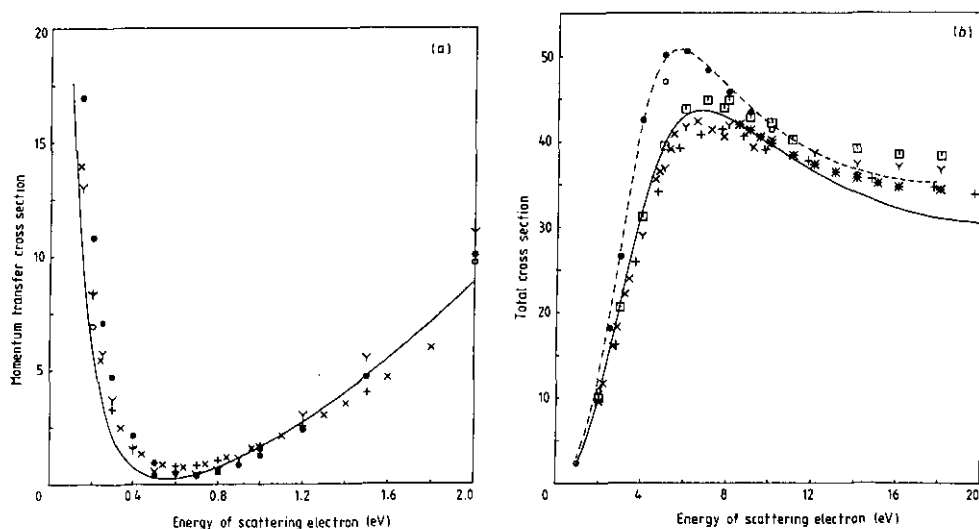
Figure 2. Momentum transfer cross sections, (*a*) from 0.1 eV to 2.0 eV, (*b*) from 1.0 eV to 20 eV: ———, present results; ●, relativistic result of McEachran and Stauffer (1987); ○, semirelativistic result of Sin Fai Lam (1982); +, Hayashi (1983); *, Register *et al* (1986); Y, Koizumi *et al* (1986); ×, Hunter *et al* (1988).

transfer cross section in figure 2(a) is very close to the semirelativistic result of Sin Fai Lam. The details of the present momentum transfer cross section are given in table 1 together with the total elastic cross section.

The phaseshifts of s, p and d waves are plotted in figure 3 along with our previous non-relativistic result. Relativistic contraction of s and p orbitals and expansion of the outer d and f orbitals were observed in the calculations for large atoms by Cowan and Griffin (1976). We had expected (Yuan and Zhang 1989a) that the relativistic contraction of s and p partial waves and expansion of d and f partial waves in the continuum scattering wavefunction would raise the phaseshifts of s and p waves and lower the phaseshifts of d and f waves. In figure 3 our previous expectation has been confirmed by the present calculation. It can be seen that the relativistic corrections for s and d wave phaseshifts are apparent as we expected, but the p wave phaseshift deviates slightly from the non-relativistic curve in the opposite direction to our expectation. The reasons for the lower p wave phaseshift are: (a) the relativistic contraction effect is very small for the outermost p orbital of the Xe atom; (b) the correlation potential of Perdew and Zunger (1981), which was recommended by Padial and Norcross (1984) though they did not use it in their calculation, used in the present case is slightly weaker than the correlation potential in our non-relativistic calculation; (c) the relativistic contraction effect for the p wave has not compensated the weakness of the present correlation potential. The relativistic effects are sufficient for the d wave to lower the phaseshift and the shape resonance peak in the elastic total and momentum transfer cross sections in very good agreement with the experimental data. The present s and p wave phaseshifts agree well with the results of Sin Fai Lam (1982) and McEachran and Stauffer (1986) (not shown in figure 3), but the d wave phaseshift is apparently
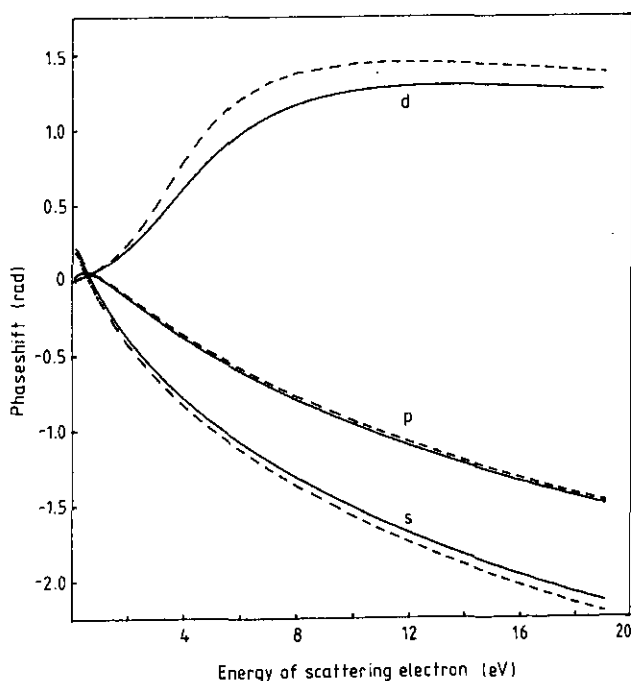

Figure 3. Phaseshifts of s, p and d waves: ——, present quasirelativistic result; ----, non-relativistic result of Yuan and Zhang (1989).

lower than theirs, i.e. the polarization potentials in their calculations are too large for the d partial wave. The details of the present phaseshifts are given in table 2.

We have also calculated the differential cross sections at a few energies, the details are given in table 3, the comparisons with measurements are plotted in figure 4. At *the energies below 10 eV our results are in good agreement with the plotted measured* points, especially in (*a*), (*b*), (*c*), (*d*) and (*e*) the agreement between theory and experiment is excellent. The main features of the differential cross sections at higher energies are the minimum and maximum structures with the scattering angle. The accurate determination of the positions and magnitudes of the minimum and maximum structures require high energy resolution ability of the experiments, and generally the coincidences of the measurements are poor. At the energies of 14.75, 19.75 and 20 eV,

Table 2. Elastic scattering phaseshifts δ_l (mod π).

eV	δ_0	δ_1	δ_2	δ_3	δ_4	δ_5	δ_6
0.1	0.2181	0.0277	0.0061	0.0020	0.0009	0.0005	0.0003
0.2	0.1938	0.0431	0.0125	0.0040	0.0018	0.0010	0.0006
0.3	0.1554	0.0511	0.0193	0.0060	0.0027	0.0015	0.0009
0.4	0.1147	0.0539	0.0265	0.0081	0.0036	0.0020	0.0012
0.5	0.0757	0.0527	0.0341	0.0101	0.0046	0.0024	0.0015
0.6	0.0354	0.0486	0.0421	0.0122	0.0055	0.0029	0.0018
0.7	−0.0021	0.0422	0.0507	0.0142	0.0064	0.0034	0.0021
0.8	−0.0383	0.0341	0.0598	0.0163	0.0073	0.0039	0.0024
0.9	−0.0730	0.0247	0.0694	0.0184	0.0082	0.0044	0.0026
1.0	−0.1064	0.0141	0.0796	0.0205	0.0091	0.0049	0.0029
1.5	−0.2573	−0.0483	0.1391	0.0313	0.0138	0.0074	0.0044
2.0	−0.3872	−0.1173	0.2134	0.0425	0.0184	0.0098	0.0059
2.5	−0.5021	−0.1870	0.3017	0.0543	0.0231	0.0123	0.0074
3.0	−0.6056	−0.2552	0.4015	0.0667	0.0279	0.0148	0.0088
3.5	−0.7000	−0.3210	0.5082	0.0797	0.0328	0.0173	0.0103
4.0	−0.7871	−0.3840	0.6165	0.0933	0.0377	0.0198	0.0118
4.5	−0.8679	−0.4443	0.7207	0.1074	0.0426	0.0223	0.0133
5.0	−0.9434	−0.5020	0.8167	0.1221	0.0477	0.0249	0.0148
5.5	−1.0143	−0.5571	0.9019	0.1373	0.0528	0.0274	0.0163
6.0	−1.0813	−0.6098	0.9755	0.1530	0.0580	0.0300	0.0178
6.5	−1.1446	−0.6604	1.0378	0.1691	0.0632	0.0326	0.0193
7.0	−1.2048	−0.7089	1.0898	0.1857	0.0686	0.0352	0.0208
7.5	−1.2621	−0.7554	1.1329	0.2027	0.0739	0.0378	0.0223
8.0	−1.3168	−0.8002	1.1683	0.2202	0.0793	0.0405	0.0238
8.5	−1.3691	−0.8433	1.1971	0.2380	0.0848	0.0431	0.0254
9.0	−1.4193	−0.8849	1.2206	0.2563	0.0902	0.0458	0.0269
9.5	−1.4670	−0.9249	1.2394	0.2750	0.0957	0.0485	0.0284
10.0	−1.5135	−0.9637	1.2545	0.2941	0.1012	0.0512	0.0300
11.0	1.5402	−1.0373	1.2755	0.3338	0.1121	0.0567	0.0331
12.0	1.4584	−1.1064	1.2873	0.3757	0.1230	0.0622	0.0362
13.0	1.3818	−1.1705	1.2924	0.4202	0.1338	0.0677	0.0394
14.0	1.3097	−1.2319	1.2927	0.4678	0.1444	0.0732	0.0426
15.0	1.2416	−1.2900	1.2893	0.5191	0.1549	0.0787	0.0458
16.0	1.1772	−1.3451	1.2831	0.5748	0.1651	0.0841	0.0490
17.0	1.1160	−1.3983	1.2747	0.6354	0.1751	0.0895	0.0522
18.0	1.0576	−1.4482	1.2647	0.7018	0.1850	0.0948	0.0555
19.0	1.0019	−1.4957	1.2597	0.7746	0.1947	0.1001	0.0587
20.0	0.9486	−1.5413	1.2413	0.8543	0.2043	0.1052	0.0619

Table 3. Differential cross sections (in 10^{-16} cm^2 sr^{-1}).

deg	eV 0.5	1.0	1.75	2.75	5.0	9.75	10.0	14.75	19.75	20.0
0	2.702	1.978	2.310	5.133	19.202	33.351	33.744	41.791	51.396	51.796
5	2.585	1.839	2.113	4.781	18.406	32.077	32.442	39.823	48.700	49.071
10	2.270	1.477	1.612	3.875	16.298	28.708	28.997	34.645	41.606	41.902
15	1.850	1.023	1.013	2.767	13.541	24.295	24.490	27.955	32.449	32.645
20	1.424	0.609	0.514	1.801	10.799	19.854	19.964	21.411	23.533	23.633
25	1.057	0.307	0.213	1.157	8.463	15.930	15.977	15.919	16.165	16.184
30	0.773	0.125	0.102	0.840	6.618	12.602	12.607	11.616	10.600	10.561
35	0.564	0.035	0.124	0.765	5.197	9.760	9.741	8.277	6.568	6.494
40	0.409	0.003	0.225	0.850	4.127	7.330	7.296	5.686	3.747	3.661
45	0.291	0.009	0.373	1.047	3.380	5.322	5.280	3.732	1.911	1.831
50	0.198	0.042	0.556	1.328	2.947	3.769	3.722	2.360	0.883	0.821
55	0.127	0.095	0.758	1.665	2.795	2.657	2.608	1.488	0.461	0.423
60	0.075	0.158	0.955	2.006	2.836	1.914	1.863	0.985	0.413	0.399
65	0.041	0.219	1.116	2.288	2.952	1.431	1.379	0.708	0.513	0.518
70	0.021	0.267	1.215	2.457	3.032	1.115	1.063	0.548	0.605	0.621
75	0.010	0.297	1.245	2.491	3.011	0.912	0.861	0.456	0.628	0.648
80	0.004	0.309	1.214	2.400	2.871	0.796	0.749	0.421	0.588	0.604
85	0.001	0.308	1.136	2.209	2.620	0.740	0.700	0.429	0.509	0.517
90	0.000	0.296	1.023	1.942	2.267	0.709	0.678	0.458	0.415	0.413
95	0.000	0.274	0.883	1.615	1.826	0.667	0.647	0.486	0.327	0.316
100	0.001	0.242	0.719	1.247	1.321	0.602	0.594	0.506	0.269	0.253
105	0.001	0.200	0.542	0.865	0.807	0.524	0.528	0.529	0.260	0.242
110	0.001	0.153	0.368	0.514	0.362	0.462	0.477	0.564	0.300	0.283
115	0.000	0.107	0.217	0.241	0.073	0.442	0.463	0.605	0.363	0.347
120	0.000	0.068	0.106	0.082	0.010	0.480	0.500	0.631	0.407	0.392
125	0.000	0.038	0.042	0.055	0.209	0.581	0.592	0.623	0.398	0.384
130	0.000	0.017	0.026	0.162	0.684	0.757	0.749	0.583	0.335	0.322
135	0.001	0.005	0.054	0.398	1.431	1.023	0.988	0.531	0.244	0.232
140	0.001	0.002	0.124	0.753	2.434	1.392	1.323	0.489	0.159	0.149
145	0.003	0.007	0.233	1.213	3.657	1.860	1.750	0.469	0.101	0.097
150	0.005	0.020	0.371	1.747	5.027	2.395	2.241	0.463	0.080	0.086
155	0.008	0.038	0.524	2.305	6.432	2.945	2.746	0.461	0.096	0.117
160	0.010	0.057	0.669	2.828	7.741	3.452	3.209	0.455	0.146	0.183
165	0.011	0.072	0.789	3.261	8.835	3.868	3.589	0.446	0.222	0.277
170	0.011	0.082	0.872	3.572	9.639	4.169	3.863	0.440	0.311	0.381
175	0.011	0.087	0.919	3.754	10.122	4.349	4.026	0.440	0.385	0.466
180	0.011	0.089	0.934	3.814	10.282	4.408	4.081	0.442	0.415	0.499

at small scattering angles our results agree well with the experimental points, but for angles larger than 50° the minimum and maximum structures observed in the experiments generally coincide badly with each other; therefore it is difficult to make a quantitative comparison between theory and experiment, but the positions of the minimum and maximum points of our results agree reasonably well with the observations. At 20 eV the present differential cross sections agree well with the semirelativistic result of Sin Fai Lam (1982) (not shown in the figure). In order to make quantitative comparison between theory and experiment much more accurate experimental values are needed for the absolute differential cross section.

In conclusion, the correlation, distortion, polarization and relativistic effects are accounted for adequately in the present calculation. The adequacy and suitability of
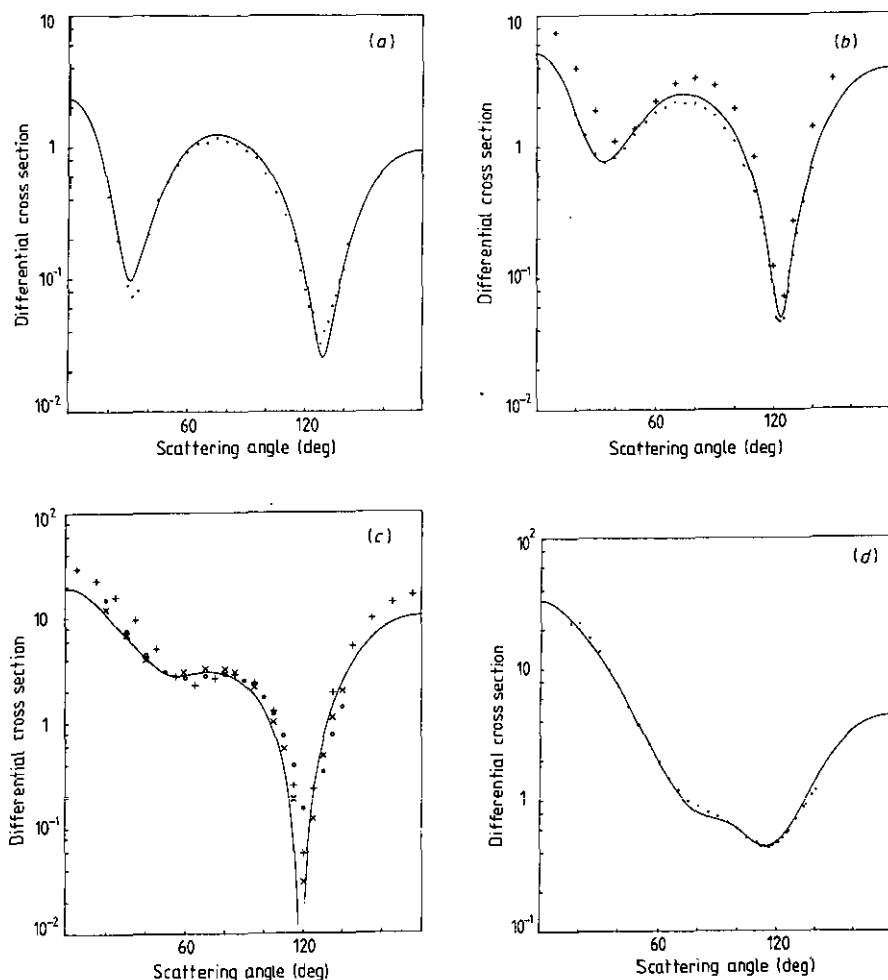
Figure 4. Differential cross sections: ——, present results; +, McEachran and Stauffer (1984); ○, Jost *et al* (1983, quoted by McEachran and Stauffer 1984); ×, Register *et al* (1980) quoted by McEachran and Stauffer 1984); ●, Register *et al* (1986); Y, Williams and Crowe (1975). (*a*) $E = 1.75$ eV, (*b*) $E = 2.75$ eV, (*c*) $E = 5$ eV, (*d*) $E = 9.75$ eV, (*e*) $E = 10$ eV, (*f*) $E = 14.75$ eV, (*g*) $E = 19.75$ eV, (*h*) $E = 20$ eV.

representing the interactions not included in static-exchange approximation by the parameter-free CP potential have been investigated and confirmed extensively in the present and our previous papers (Yuan 1988, Yuan and Zhang 1989a) for low-energy electron–rare-gas atom scattering processes. The applicability of the CP potential has been investigated for alkaline-earth atoms with encouraging results (Yuan and Zhang 1989b, 1990). The success of the CP potential for a variety of atoms might have some physical basis, then the correlation potential used here not only acts simply as a cut-off function in the short range of the polarization potential, but also has some physical meaning as in the local density functional theory. Compared with our non-relativistic result it has been shown that the major relativistic effects for low-energy e–Xe scattering processes have been considered sufficiently by the quasirelativistic approach as in the structural calculations.
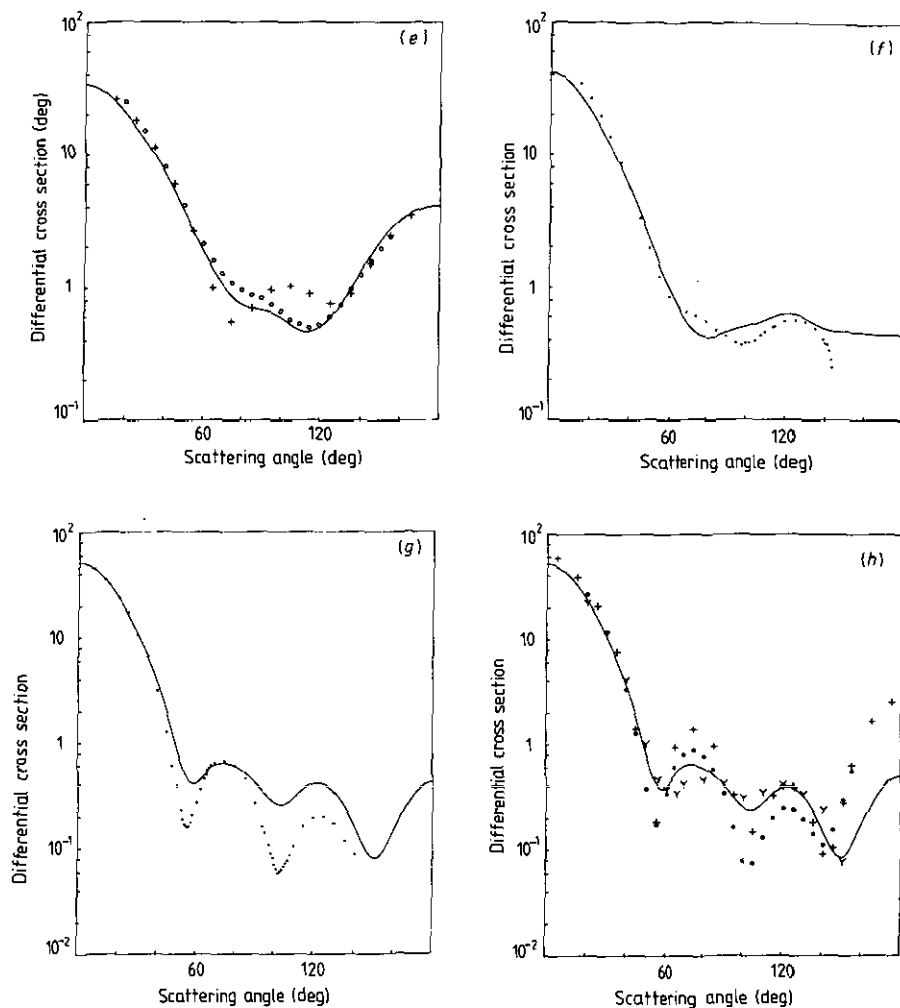
Figure 4. (continued)

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