

Elastic scattering of electrons from krypton and xenon

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Abstract. Results are given for the low-energy elastic scattering of electrons from krypton and xenon. The calculations were carried out by treating exchange exactly and including only the dipole part of the polarisation potential. Values are given for the phaseshifts, differential, total elastic and momentum transfer cross sections. Comparison are given with recent experimental and theoretical work for these processes.

1. Introduction

We have previously examined the effects of polarisation and exchange in the elastic scattering of electrons from helium, neon and argon (McEachran and Stauffer 1983a,b). In these papers we have found that to obtain reliable results electron exchange must be treated exactly and only the dipole part of the polarisation potential should be retained. We have used this model to calculate scattering of electrons from krypton and xenon in the low-energy region.

Absolute differential cross section measurements have been made by Holtkamp and Jost (1983) and Register *et al* (1980) for xenon, by Jost and Otto (1983) and Srivastava *et al* (1981) for krypton and by Williams and Crowe (1975) for krypton and xenon. Srivastava *et al* have also presented elastic phaseshifts which were extracted from their scattering data. Very low energy results for both gases have been reported by Weyhreter *et al* (1983). Relative data have been published by Heindorff *et al* (1976), Klewer *et al* (1980) (xenon), Lewis *et al* (1974), Mehr (1967) and Zhou Qing *et al* (1982) (krypton). Total elastic cross sections have been measured by Dababneh *et al* (1980), Gus'kov *et al* (1978), Jost *et al* (1983), Nickel (1983) and Wagenaar and de Heer (1980) for both these gases. Experimentally derived momentum transfer cross sections have been reported by Frost and Phelps (1964) for both krypton and xenon.

Theoretical calculations for these two gases have been carried out in an optical potential model by McCarthy *et al* (1977) who gave results for differential cross sections and by Sin Fai Lam (1982) who used a relativistic approximation to calculate elastic phaseshifts and cross sections. Local exchange approximations have been employed for scattering calculations by Awe *et al* (1983) for xenon and by Berg (1982), O'Connell and Lane (1983), Woolfson *et al* (1982) and Yau *et al* (1980) for both gases.

2. Theoretical method

We have used an adiabatic exchange (AE) method in our calculations which included the polarisation potentials previously used for positron scattering from these gases (McEachran *et al* 1980). These polarisation potentials are calculated in a frozen-core

Table 1. Elastic scattering phaseshifts δ_i for krypton.

| k | δ_0 | δ_1 | δ_2 | δ_3 | δ_4 | δ_5 | δ_6 |
|--------|------------|------------|------------|------------|------------|------------|------------|
| 0 | -3.102 897 | | | | | | |
| 0.0857 | 0.122 183 | 0.016 966 | 0.003 668 | 0.001 208 | 0.000 549 | 0.000 296 | 0.000 178 |
| 0.1000 | 0.119 968 | 0.021 153 | 0.005 029 | 0.001 644 | 0.000 747 | 0.000 403 | 0.000 242 |
| 0.1212 | 0.109 121 | 0.026 871 | 0.007 376 | 0.002 417 | 0.001 097 | 0.000 591 | 0.000 355 |
| 0.1485 | 0.084 771 | 0.032 485 | 0.011 380 | 0.003 632 | 0.001 648 | 0.000 887 | 0.000 533 |
| 0.1715 | 0.057 421 | 0.034 922 | 0.015 623 | 0.004 849 | 0.002 198 | 0.001 183 | 0.000 710 |
| 0.1917 | 0.029 490 | 0.035 321 | 0.020 397 | 0.006 060 | 0.002 747 | 0.001 478 | 0.000 887 |
| 0.2000 | 0.017 143 | 0.034 449 | 0.022 163 | 0.006 607 | 0.002 991 | 0.001 609 | 0.000 966 |
| 0.2100 | 0.001 686 | 0.033 159 | 0.025 065 | 0.007 292 | 0.003 298 | 0.001 774 | 0.001 064 |
| 0.2269 | -0.025 705 | 0.029 792 | 0.029 953 | 0.008 530 | 0.003 851 | 0.002 071 | 0.001 242 |
| 0.2424 | -0.052 031 | 0.025 266 | 0.035 042 | 0.009 750 | 0.004 397 | 0.002 364 | 0.001 418 |
| 0.2573 | -0.078 250 | 0.019 621 | 0.040 490 | 0.011 004 | 0.004 955 | 0.002 664 | 0.001 598 |
| 0.2711 | -0.103 214 | 0.013 281 | 0.044 195 | 0.012 235 | 0.005 503 | 0.002 958 | 0.001 774 |
| 0.2844 | -0.127 805 | 0.006 185 | 0.050 291 | 0.013 491 | 0.006 059 | 0.003 255 | 0.001 952 |
| 0.2970 | -0.151 518 | -0.001 400 | 0.058 311 | 0.014 736 | 0.006 610 | 0.003 550 | 0.002 129 |
| 0.3000 | -0.157 217 | -0.003 326 | 0.059 867 | 0.015 044 | 0.006 744 | 0.003 623 | 0.002 172 |
| 0.3092 | -0.174 813 | -0.009 514 | 0.064 729 | 0.016 010 | 0.007 167 | 0.003 849 | 0.002 307 |
| 0.3209 | -0.197 425 | -0.017 975 | 0.071 579 | 0.017 283 | 0.007 722 | 0.004 146 | 0.002 485 |
| 0.3321 | -0.219 287 | -0.026 672 | 0.078 661 | 0.018 555 | 0.008 274 | 0.004 441 | 0.002 662 |
| 0.4000 | -0.355 026 | -0.090 288 | 0.134 848 | 0.027 416 | 0.012 038 | 0.006 449 | 0.003 863 |
| 0.4696 | -0.497 013 | -0.170 385 | 0.226 281 | 0.038 807 | 0.016 670 | 0.008 899 | 0.005 327 |
| 0.5000 | -0.559 207 | -0.208 663 | 0.281 145 | 0.044 628 | 0.018 944 | 0.010 096 | 0.006 041 |
| 0.6000 | -0.762 211 | -0.343 198 | 0.539 134 | 0.067 923 | 0.027 618 | 0.014 584 | 0.008 708 |
| 0.6062 | -0.774 661 | -0.351 829 | 0.558 687 | 0.069 595 | 0.028 218 | 0.014 891 | 0.008 890 |
| 0.7000 | -0.960 224 | -0.484 233 | 0.870 255 | 0.098 516 | 0.038 227 | 0.019 957 | 0.011 876 |
| 0.7425 | -1.042 330 | -0.544 592 | 1.001 742 | 0.114 065 | 0.043 362 | 0.022 514 | 0.013 379 |
| 0.8000 | -1.151 223 | -0.625 784 | 1.154 361 | 0.137 822 | 0.050 948 | 0.026 236 | 0.015 560 |
| 0.8573 | -1.257 094 | -0.705 590 | 1.275 819 | 0.164 813 | 0.059 295 | 0.030 247 | 0.017 899 |
| 0.9000 | -1.334 221 | -0.764 097 | 1.347 615 | 0.187 106 | 0.066 071 | 0.033 442 | 0.019 745 |
| 1.0000 | -1.508 846 | -0.897 446 | 1.458 267 | 0.245 965 | 0.083 924 | 0.041 705 | 0.024 417 |
| 1.0500 | -1.593 013 | -0.962 205 | 1.487 181 | 0.278 385 | 0.093 864 | 0.046 300 | 0.026 964 |
| 1.1000 | -1.675 117 | -1.025 710 | 1.502 996 | 0.312 581 | 0.104 396 | 0.051 212 | 0.029 689 |
| 1.2000 | -1.833 301 | -1.149 043 | 1.512 848 | 0.386 604 | 0.127 008 | 0.061 821 | 0.035 719 |
| 1.2124 | -1.852 370 | -1.163 980 | 1.513 150 | 0.396 340 | 0.129 958 | 0.063 191 | 0.036 514 |
| 1.3000 | -1.983 794 | -1.267 093 | 1.513 318 | 0.468 175 | 0.151 939 | 0.073 156 | 0.042 275 |
| 1.4000 | -2.127 052 | -1.379 567 | 1.505 744 | 0.553 192 | 0.179 844 | 0.085 531 | 0.048 919 |
| 1.4849 | -2.243 350 | -1.471 128 | 1.486 949 | 0.624 113 | 0.205 309 | 0.097 492 | 0.054 987 |
| 1.5000 | -2.263 546 | -1.487 090 | 1.482 504 | 0.636 586 | 0.209 900 | 0.099 759 | 0.056 176 |
| 1.6000 | -2.393 745 | -1.590 607 | 1.450 148 | 0.719 912 | 0.240 257 | 0.115 172 | 0.065 153 |
| 1.7000 | -2.518 111 | -1.690 240 | 1.421 913 | 0.805 399 | 0.271 577 | 0.129 965 | 0.074 828 |
| 1.7146 | -2.535 807 | -1.704 431 | 1.418 328 | 0.817 744 | 0.276 401 | 0.132 073 | 0.076 120 |
| 1.8000 | -2.637 079 | -1.785 548 | 1.397 123 | 0.886 443 | 0.306 215 | 0.145 053 | 0.082 674 |
| 1.9000 | -2.751 046 | -1.876 762 | 1.365 120 | 0.957 852 | 0.342 397 | 0.163 573 | 0.090 354 |
| 1.9170 | -2.769 949 | -1.891 930 | 1.358 747 | 0.969 442 | 0.348 328 | 0.167 064 | 0.092 056 |
| 2.0000 | -2.860 373 | -1.964 838 | 1.326 480 | 1.026 689 | 0.375 712 | 0.183 977 | 0.102 892 |

approximation in which only the outermost S and P shells of the atom are polarised. As determined from our earlier work only the dipole part of these potentials was retained and exchange was treated exactly. These calculations should be compared with our earlier calculations (Yau *et al* 1980) where a local exchange approximation was used and the full polarisation potentials retained.

We have calculated the phaseshifts for the partial waves $l = 0$ to $l = 6$. In addition in calculating cross sections we have used the effective-range formula of Ali and Fraser (1977) to produce phaseshift values from $l = 7$ to $l = 100$.

We found that for both krypton and xenon the results were very sensitive to the integration mesh used in our calculations. Since many of the bound-state orbitals for krypton and xenon have nodes very close to the origin it was found necessary in the solution of the integral equations for the scattering functions (cf equation (24) of McEachran and Stauffer 1983a) to have very fine mesh sizes near the origin. For krypton the choice $h = \frac{1}{2048}$ for $0 \leq r \leq 0.25 a_0$, $h = \frac{1}{256}$ for $0.25 a_0 \leq r \leq 1.25 a_0$ and $h = \frac{1}{32}$ for $r > 1.25 a_0$ was found to be sufficient in order to achieve the same accuracy as we did with helium, neon and argon. For xenon it was necessary to use $h = \frac{1}{4096}$ in the innermost region.

3. Results

3.1. Krypton

Our results for the elastic phaseshifts for krypton are given in table 1 and shown in figure 1 where they are compared with the relativistic calculations of Sin Fai Lam

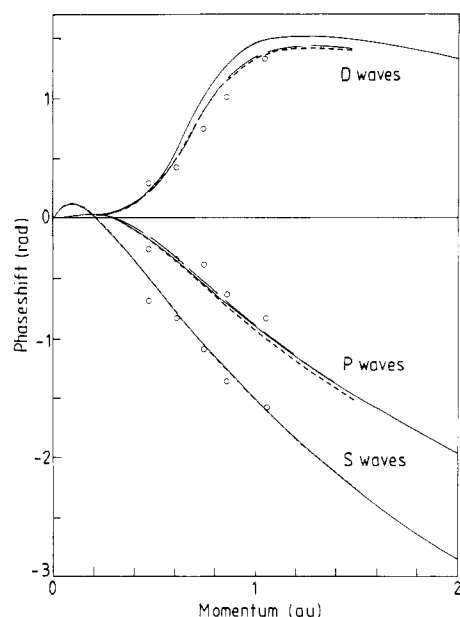


Figure 1. Phaseshifts for elastic scattering of electrons from krypton: —, present results; ----, spin up and —·—, spin down results of Sin Fai Lam (1982); ○, Srivastava *et al* (1981).

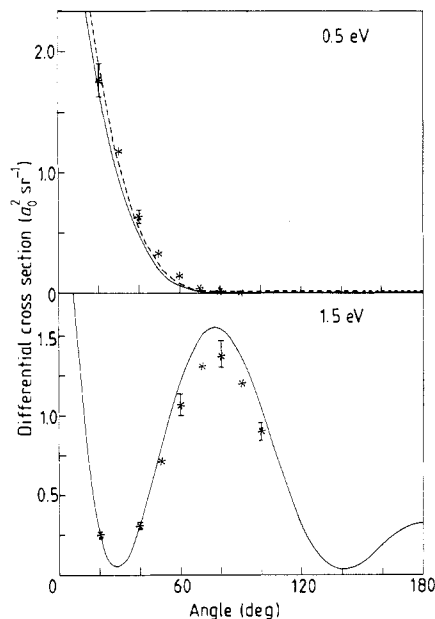


Figure 2. Low-energy differential cross sections for elastic scattering of electrons from krypton: —, present results; ----, Sin Fai Lam (1982); *, Wehyreter *et al* (1983).

(1982) and with the experimentally derived results of Srivastava *et al* (1981). We are in close agreement with the S- and P-wave results of Sin Fai Lam but somewhat higher than his D waves at higher energies. Our previous calculations using a local exchange approximation and the full polarisation potential (Yau *et al* 1980) yield comparable phaseshifts as we noted in the cases of helium, neon and argon (McEachran and Stauffer 1983a, b) but with somewhat greater differences than the previous cases. The experimental phaseshifts of Srivastava *et al* exhibit a certain amount of scatter but are comparable with the theoretical calculations.

Table 2. Differential cross sections $d\sigma/d\Omega(a_0^2 \text{ sr}^{-1})$ for krypton.

| Energy 3.0 (eV) Angle (deg) | 5.0 | 7.5 | 10.0 | 15.0 | 20.0 | 30.0 | 40.0 | 50.0 |
|--------------------------------------|--------|--------|---------|---------|--------|--------|---------|---------|
| 0 | 7.442 | 30.425 | 66.366 | 79.566 | 85.895 | 95.846 | 118.090 | 139.090 |
| 5 | 5.400 | 25.729 | 60.040 | 73.077 | 77.111 | 82.891 | 97.058 | 105.550 |
| 10 | 3.602 | 20.877 | 52.704 | 65.440 | 67.685 | 69.737 | 76.541 | 79.567 |
| 15 | 2.327 | 16.610 | 45.309 | 57.490 | 58.609 | 57.934 | 59.165 | 58.358 |
| 20 | 1.517 | 12.966 | 38.009 | 49.320 | 49.776 | 47.252 | 44.508 | 41.222 |
| 25 | 1.120 | 10.003 | 31.049 | 41.168 | 41.269 | 37.667 | 32.398 | 27.778 |
| 30 | 1.076 | 7.762 | 24.684 | 33.327 | 33.243 | 29.209 | 22.688 | 17.659 |
| 35 | 1.319 | 6.243 | 19.137 | 26.094 | 25.889 | 21.916 | 15.178 | 10.429 |
| 40 | 1.776 | 5.408 | 14.574 | 19.726 | 19.380 | 15.807 | 9.623 | 5.615 |
| 45 | 2.370 | 5.175 | 11.075 | 14.409 | 13.850 | 10.868 | 5.728 | 2.703 |
| 50 | 3.025 | 5.423 | 8.632 | 10.238 | 9.378 | 7.046 | 3.178 | 1.190 |
| 55 | 3.667 | 5.998 | 7.143 | 7.204 | 5.970 | 4.248 | 1.658 | 0.615 |
| 60 | 4.229 | 6.731 | 6.434 | 5.211 | 3.572 | 2.359 | 0.886 | 0.597 |
| 65 | 4.655 | 7.450 | 6.275 | 4.085 | 2.070 | 1.236 | 0.620 | 0.839 |
| 70 | 4.903 | 7.999 | 6.414 | 3.600 | 1.306 | 0.724 | 0.667 | 1.137 |
| 75 | 4.951 | 8.252 | 6.609 | 3.515 | 1.096 | 0.663 | 0.883 | 1.373 |
| 80 | 4.791 | 8.126 | 6.649 | 3.593 | 1.245 | 0.898 | 1.164 | 1.494 |
| 85 | 4.437 | 7.594 | 6.392 | 3.641 | 1.573 | 1.286 | 1.440 | 1.498 |
| 90 | 3.920 | 6.683 | 5.768 | 3.523 | 1.925 | 1.706 | 1.664 | 1.410 |
| 95 | 3.283 | 5.472 | 4.796 | 3.174 | 2.188 | 2.064 | 1.811 | 1.264 |
| 100 | 2.583 | 4.089 | 3.574 | 2.610 | 2.297 | 2.296 | 1.865 | 1.093 |
| 105 | 1.881 | 2.691 | 2.271 | 1.916 | 2.241 | 2.376 | 1.825 | 0.918 |
| 110 | 1.237 | 1.453 | 1.100 | 1.233 | 2.053 | 2.305 | 1.695 | 0.747 |
| 115 | 0.709 | 0.547 | 0.293 | 0.734 | 1.806 | 2.114 | 1.489 | 0.584 |
| 120 | 0.343 | 0.122 | 0.072 | 0.603 | 1.595 | 1.854 | 1.230 | 0.428 |
| 125 | 0.173 | 0.290 | 0.616 | 0.998 | 1.519 | 1.586 | 0.942 | 0.282 |
| 130 | 0.214 | 1.112 | 2.037 | 2.037 | 1.669 | 1.374 | 0.658 | 0.156 |
| 135 | 0.463 | 2.586 | 4.366 | 3.771 | 2.106 | 1.272 | 0.408 | 0.062 |
| 140 | 0.901 | 4.652 | 7.535 | 6.173 | 2.857 | 1.317 | 0.217 | 0.014 |
| 145 | 1.490 | 7.188 | 11.388 | 9.138 | 3.904 | 1.520 | 0.103 | 0.022 |
| 150 | 2.181 | 10.022 | 15.684 | 12.487 | 5.182 | 1.869 | 0.070 | 0.086 |
| 155 | 2.913 | 12.949 | 20.125 | 15.987 | 6.594 | 2.325 | 0.111 | 0.199 |
| 160 | 3.625 | 15.749 | 24.379 | 19.368 | 8.014 | 2.832 | 0.204 | 0.343 |
| 165 | 4.254 | 18.199 | 28.111 | 22.354 | 9.303 | 3.323 | 0.323 | 0.494 |
| 170 | 4.747 | 20.108 | 31.023 | 24.696 | 10.335 | 3.733 | 0.436 | 0.626 |
| 175 | 5.061 | 21.319 | 32.873 | 26.188 | 11.001 | 4.003 | 0.517 | 0.716 |
| 180 | 5.167 | 21.731 | 33.504 | 26.698 | 11.230 | 4.098 | 0.547 | 0.749 |
| $\sigma_{\text{el}}(a_0^2)$ | 33.050 | 78.518 | 118.925 | 119.393 | 98.429 | 83.023 | 65.534 | 55.122 |
| $\sigma_{\text{mt}}(a_0^2)$ | 28.951 | 71.342 | 92.413 | 75.489 | 44.859 | 30.210 | 17.210 | 11.534 |

In table 2 we present our differential, total elastic and momentum transfer cross sections at selected energies. We compare our calculations with various experimental and theoretical results for the differential cross section in figures 2 and 3. Overall we

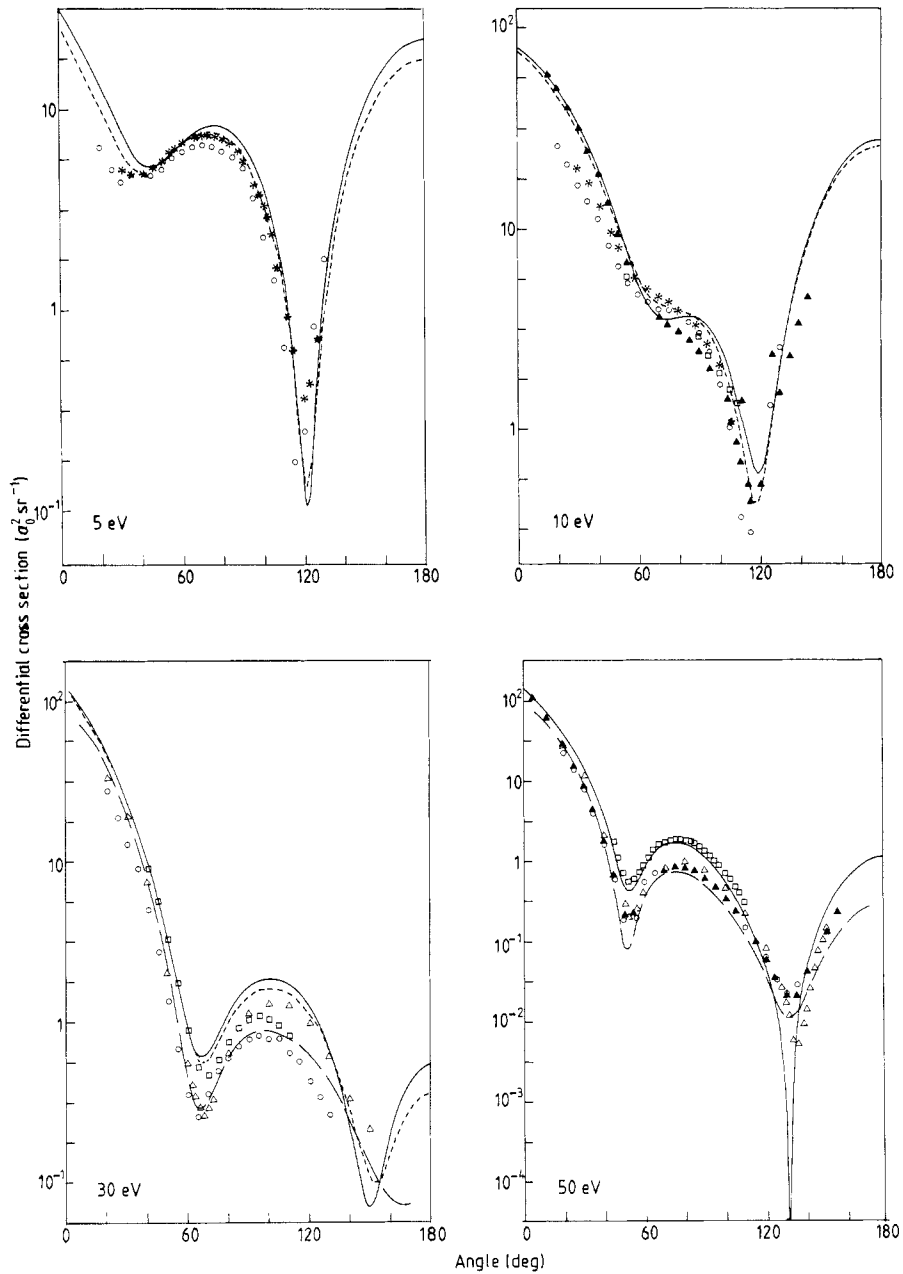


Figure 3. Differential cross sections for elastic scattering of electrons from krypton: —, present results; ---, McCarthy *et al* (1977); ----, Sin Fai Lam (1982); *, Heindorff *et al* (1976); ▲, Jost and Otto (1983); ○, Srivastava *et al* (1981); △, Williams and Crowe (1975); □, Zhou Qing *et al* (1982).

agree very well with the low-energy results of Weyhreter *et al* (1983) in shape and above 0.4 eV also in magnitude although we are some 10% higher in the region of the maximum around 90°. In general the agreement with the experimental results of Jost and Otto, Srivastava *et al* and Williams and Crowe is quite good. The greatest discrepancy occurs in the mid-angular range (80–120°) for energies of 20 (not shown) and 30 eV. These comments hold as well when comparing with the theoretical results of McCarthy *et al* (1977). In contrast we agree quite closely with the results of Sin Fai Lam (1982). We also show the relative results of Heindorff *et al* (1976) and Zhou Qing *et al* (1982) normalised to our results at 60°. These results agree well with ours in shape at 5 and at 50 eV. At 10 eV both sets of relative data fail to show the shallow first minimum. This is also true of the absolute data of Jost and Otto although it appears in the results of Srivastava *et al*.

In figure 4 we compare our total elastic cross sections with the experiments of Dababneh *et al* (1980), Gus'kov *et al* (1978), Jost *et al* (1983), Srivastava *et al* (1981) (whose results are calculated from their derived phaseshifts) and Wagenaar and de Heer (1980) as well as the theoretical calculations of Sin Fai Lam (1982). The agreement at low energies is very good but around the peak of the cross section both sets of theoretical results are higher than the experimental values. At higher energies the agreement between the various results is again good barring those of Srivastava *et al*. The momentum transfer cross section is shown in figure 5. Here we compare with the results of Frost and Phelps (1964) as well as those of Sin Fai Lam and Srivastava *et al*. The agreement between the experimental data of Frost and Phelps and the two theoretical calculations is good at low energies. However at higher energies there is considerable disagreement both in shape and magnitude.

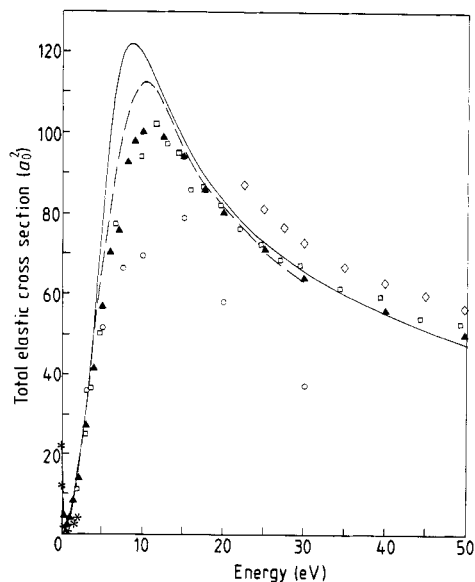


Figure 4. Total elastic cross sections for the elastic scattering of electrons from krypton: —, present results; ---, Sin Fai Lam (1982); □, Dababneh *et al* (1980); *, Gus'kov *et al* (1978); ▲, Jost *et al* (1983); ○, Srivastava *et al* (1981); ◇, Wagenaar and de Heer (1980).

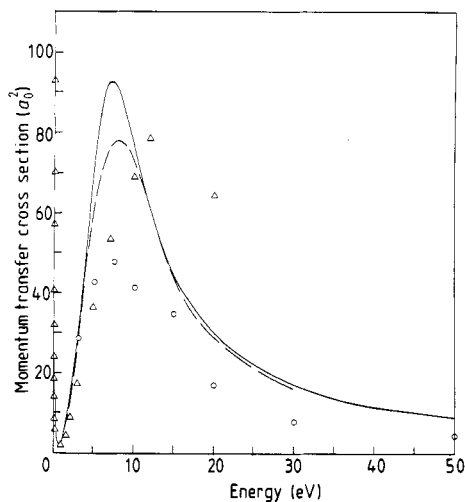


Figure 5. Momentum transfer cross sections for elastic scattering of electrons from krypton: —, present results; ---, Sin Fai Lam (1982); △, Frost and Phelps (1964); ○, Srivastava *et al* (1981).

Table 3. Elastic scattering phaseshifts d_l for xenon.

| k | δ_0 | δ_1 | δ_2 | δ_3 | δ_4 | δ_5 | δ_6 |
|--------|------------|------------|------------|------------|------------|------------|------------|
| 0.0000 | -5.231 769 | | | | | | |
| 0.0857 | 0.185 297 | 0.027 220 | 0.006 080 | 0.001 986 | 0.000 903 | 0.000 486 | 0.000 292 |
| 0.1000 | 0.178 539 | 0.033 658 | 0.008 364 | 0.002 706 | 0.001 228 | 0.000 662 | 0.000 397 |
| 0.1212 | 0.157 965 | 0.042 129 | 0.012 534 | 0.003 979 | 0.001 804 | 0.000 972 | 0.000 583 |
| 0.1485 | 0.118 500 | 0.049 689 | 0.019 484 | 0.005 986 | 0.002 710 | 0.001 458 | 0.000 875 |
| 0.1715 | 0.077 374 | 0.052 006 | 0.026 993 | 0.008 001 | 0.003 616 | 0.001 945 | 0.001 167 |
| 0.1917 | 0.037 035 | 0.051 081 | 0.035 103 | 0.010 021 | 0.004 521 | 0.002 430 | 0.001 458 |
| 0.2000 | 0.019 592 | 0.049 426 | 0.038 914 | 0.010 919 | 0.004 922 | 0.002 646 | 0.001 587 |
| 0.2100 | -0.001 990 | 0.046 592 | 0.043 920 | 0.012 056 | 0.005 428 | 0.002 917 | 0.001 749 |
| 0.2269 | -0.039 654 | 0.039 691 | 0.053 530 | 0.014 113 | 0.006 340 | 0.003 406 | 0.002 042 |
| 0.2424 | -0.075 279 | 0.031 576 | 0.063 792 | 0.016 154 | 0.007 240 | 0.003 888 | 0.002 331 |
| 0.2573 | -0.110 306 | 0.021 918 | 0.077 041 | 0.018 258 | 0.008 163 | 0.004 382 | 0.002 627 |
| 0.2711 | -0.143 300 | 0.011 437 | 0.089 484 | 0.020 335 | 0.009 067 | 0.004 866 | 0.002 916 |
| 0.2844 | -0.175 510 | 0.000 013 | 0.100 653 | 0.022 456 | 0.009 985 | 0.005 356 | 0.003 210 |
| 0.2970 | -0.206 328 | -0.011 939 | 0.114 472 | 0.024 579 | 0.010 897 | 0.005 843 | 0.003 501 |
| 0.3000 | -0.213 703 | -0.014 939 | 0.118 073 | 0.025 028 | 0.011 120 | 0.005 962 | 0.003 572 |
| 0.3092 | -0.236 399 | -0.024 494 | 0.129 757 | 0.026 946 | 0.011 818 | 0.006 334 | 0.003 795 |
| 0.3209 | -0.265 411 | -0.037 385 | 0.146 112 | 0.029 095 | 0.012 738 | 0.006 824 | 0.004 088 |
| 0.3321 | -0.293 311 | -0.050 455 | 0.163 486 | 0.031 183 | 0.013 653 | 0.007 310 | 0.004 378 |
| 0.3834 | -0.422 066 | -0.118 158 | 0.269 198 | 0.042 419 | 0.018 265 | 0.009 755 | 0.005 839 |
| 0.4000 | -0.463 871 | -0.142 371 | 0.314 403 | 0.046 590 | 0.019 911 | 0.010 623 | 0.006 357 |
| 0.4496 | -0.588 563 | -0.219 718 | 0.487 670 | 0.060 754 | 0.025 290 | 0.013 441 | 0.008 036 |
| 0.5000 | -0.714 249 | -0.303 868 | 0.718 953 | 0.078 152 | 0.031 498 | 0.016 655 | 0.009 946 |
| 0.6000 | -0.958 263 | -0.479 352 | 1.191 012 | 0.124 073 | 0.046 247 | 0.024 110 | 0.014 350 |
| 0.6063 | -0.973 342 | -0.490 583 | 1.214 867 | 0.127 574 | 0.047 293 | 0.024 629 | 0.014 656 |
| 0.7000 | -1.192 895 | -0.657 650 | 1.459 022 | 0.190 282 | 0.064 674 | 0.033 075 | 0.019 586 |
| 0.7301 | -1.261 452 | -0.710 914 | 1.501 278 | 0.215 271 | 0.071 027 | 0.036 086 | 0.021 329 |
| 0.8000 | -1.416 805 | -0.833 031 | 1.556 015 | 0.284 333 | 0.087 342 | 0.043 673 | 0.025 680 |
| 0.8573 | -1.540 091 | -0.931 079 | 1.570 299 | 0.354 650 | 0.102 424 | 0.050 537 | 0.029 574 |
| 0.9000 | -1.629 588 | -1.002 772 | 1.569 236 | 0.416 917 | 0.114 702 | 0.056 044 | 0.032 672 |
| 1.0000 | -1.831 385 | -1.165 775 | 1.542 100 | 0.605 298 | 0.147 024 | 0.070 302 | 0.040 601 |
| 1.1000 | -2.022 650 | -1.321 763 | 1.494 942 | 0.874 943 | 0.184 328 | 0.086 536 | 0.049 508 |
| 1.2000 | -2.203 995 | -1.470 859 | 1.437 136 | 1.254 148 | 0.226 381 | 0.104 751 | 0.059 426 |
| 1.2124 | -2.225 824 | -1.488 882 | 1.429 488 | 1.308 592 | 0.231 912 | 0.107 146 | 0.060 725 |
| 1.3000 | -2.376 103 | -1.613 385 | 1.373 612 | 1.714 818 | 0.272 857 | 0.124 923 | 0.070 341 |
| 1.3555 | -2.467 893 | -1.689 787 | 1.337 097 | 1.965 187 | 0.300 349 | 0.136 949 | 0.076 840 |
| 1.4000 | -2.539 667 | -1.749 712 | 1.307 403 | 2.146 413 | 0.323 170 | 0.146 995 | 0.082 282 |
| 1.4849 | -2.672 328 | -1.860 881 | 1.250 024 | 2.428 866 | 0.368 487 | 0.167 096 | 0.093 191 |
| 1.5000 | -2.695 357 | -1.880 234 | 1.239 763 | 2.470 738 | 0.376 775 | 0.170 799 | 0.095 198 |
| 1.6000 | -2.843 802 | -2.005 344 | 1.171 871 | 2.698 862 | 0.433 058 | 0.196 303 | 0.109 033 |
| 1.7000 | -2.985 586 | -2.125 399 | 1.104 363 | 2.862 842 | 0.491 191 | 0.223 293 | 0.123 866 |
| 1.8000 | -3.121 241 | -2.240 748 | 1.037 387 | 2.983 597 | 0.550 771 | 0.251 598 | 0.139 446 |
| 1.9000 | -3.251 254 | -2.351 715 | 0.971 500 | 3.077 449 | 0.610 867 | 0.281 240 | 0.155 944 |
| 1.9174 | -3.273 333 | -2.370 598 | 0.960 158 | 3.091 514 | 0.621 324 | 0.286 491 | 0.158 923 |
| 2.0000 | -3.376 064 | -2.458 594 | 0.906 664 | 3.150 386 | 0.671 029 | 0.311 707 | 0.173 278 |

3.2. Xenon

Our phaseshifts for electron-xenon scattering are shown in table 3 and plotted in figure 6 along with the relativistic calculations of Sin Fai Lam. The agreement between these two sets of results is quite good except for the D wave where, as in the case of krypton, our results are somewhat higher. There is also some deviation for higher

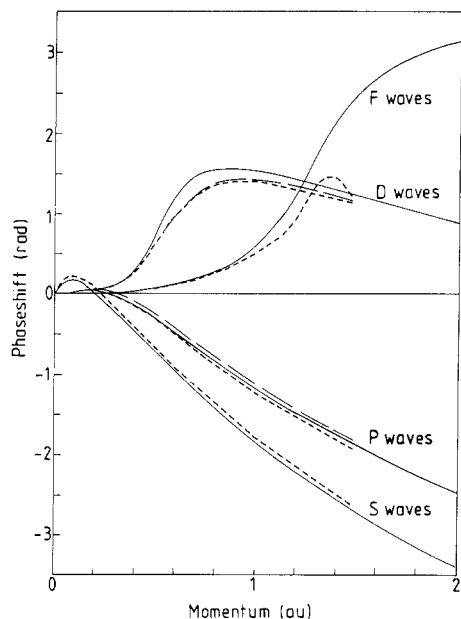


Figure 6. Phaseshifts for elastic scattering of electrons from xenon; —, present results; ----, spin up and — —, spin down results of Sin Fai Lam (1982).

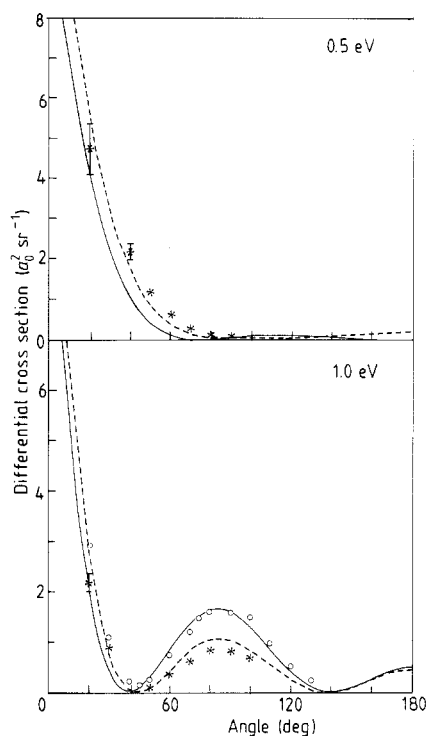


Figure 7. Low-energy differential cross sections for elastic scattering of electrons from xenon: —, present results; ----, Sin Fai Lam (1982); ○, Register *et al* (1980); *, Wehyreter *et al* (1983).

energies in the F wave. For this atom the relativistic effects are becoming appreciable in the P wave.

Table 4 gives our results for the differential, total elastic and momentum transfer cross sections at selected energies. In figures 7 and 8 we show a selection of the differential cross section results along with experimental and other theoretical values. As in krypton we agree quite well in shape with the low-energy results of Weyhreter *et al* (1983) but not as well in magnitude. Good agreement in magnitude occurs only for small angles (20–40°) at energies between 1 and 1.5 eV. At higher energies (20 eV and above) the structure of the differential cross section is quite complex having three distinct minima. All of the experimental and theoretical results have these three minima although there is some disagreement in their positions as well as in the magnitudes of the cross sections in the angular range at which these minima occur. Around 10 eV our theoretical calculations and those of Sin Fai Lam both predict two distinct minima but the experiments of Holtkamp and Jost (1983) and of Register *et al* (1980) do not show the first minimum as fully developed. We also note the increased discrepancy between our results and those of Sin Fai Lam especially at 30 eV.

Figure 9 compares various results for the total elastic cross section. The theoretical results of ourselves and Sin Fai Lam show a large peak at about 5 eV. This peak is typical of the heavier noble gases and the theoretical values are considerably higher in this region than the experimental results with the exception of those by Jost *et al*

Table 4. Differential cross sections $d\sigma/d\Omega(a_0^2 \text{ sr}^{-1})$ for xenon.

| Energy 2.750 Angle (deg) | 5.000 | 7.250 | 10.000 | 20.000 | 25.000 | 30.000 | 50.000 |
|-----------------------------|---------|----------|----------|----------|----------|----------|----------|
| 0 | 42.0580 | 114.6800 | 122.3500 | 139.0900 | 248.5700 | 177.3900 | 169.9500 |
| 5 | 34.3700 | 105.1500 | 112.7200 | 123.8700 | 213.4400 | 148.3100 | 107.2800 |
| 10 | 26.5620 | 93.6550 | 101.6400 | 107.7400 | 175.2400 | 120.3100 | 59.9280 |
| 15 | 19.8520 | 81.5300 | 90.0930 | 92.4580 | 138.6400 | 95.2540 | 31.1990 |
| 20 | 14.2740 | 69.0370 | 78.0520 | 77.8210 | 104.2400 | 72.0710 | 14.8670 |
| 25 | 9.8920 | 56.6490 | 65.7870 | 63.9640 | 73.4240 | 51.0230 | 6.4353 |
| 30 | 6.7369 | 44.9070 | 53.7080 | 51.1240 | 47.5300 | 32.9160 | 2.5874 |
| 35 | 4.7776 | 34.3340 | 42.2940 | 39.5690 | 27.4640 | 18.5870 | 1.0582 |
| 40 | 3.9284 | 25.3640 | 31.9880 | 29.5190 | 13.4740 | 8.5239 | 0.5055 |
| 45 | 4.0397 | 18.2800 | 23.1530 | 21.1200 | 5.0968 | 2.6648 | 0.2688 |
| 50 | 4.9087 | 13.1890 | 16.0200 | 14.4200 | 1.2922 | 0.3851 | 0.1229 |
| 55 | 6.2868 | 10.0020 | 10.6630 | 9.3599 | 0.6721 | 0.6434 | 0.0425 |
| 60 | 7.9077 | 8.4654 | 7.0119 | 5.8081 | 1.7915 | 2.2213 | 0.0457 |
| 65 | 9.5008 | 8.1869 | 4.8570 | 3.5588 | 3.3950 | 3.9962 | 0.1098 |
| 70 | 10.8210 | 8.6960 | 3.8908 | 2.3666 | 4.6020 | 5.1591 | 0.1748 |
| 75 | 11.6700 | 9.5073 | 3.7509 | 1.9683 | 4.9781 | 5.3305 | 0.1828 |
| 80 | 11.9140 | 10.1740 | 4.0601 | 2.0977 | 4.5018 | 4.5656 | 0.1280 |
| 85 | 11.4970 | 10.3550 | 4.4806 | 2.5129 | 3.4463 | 3.2276 | 0.0677 |
| 90 | 10.4470 | 9.8475 | 4.7460 | 3.0064 | 2.2183 | 1.8154 | 0.1049 |
| 95 | 8.8680 | 8.6110 | 4.6924 | 3.4208 | 1.1990 | 0.7690 | 0.3352 |
| 100 | 6.9382 | 6.7744 | 4.2717 | 3.6560 | 0.6240 | 0.3276 | 0.7950 |
| 105 | 4.8807 | 4.6100 | 3.5502 | 3.6752 | 0.5359 | 0.4733 | 1.4258 |
| 110 | 2.9481 | 2.5011 | 2.6925 | 3.4998 | 0.7991 | 0.9690 | 2.0830 |
| 115 | 1.3921 | 0.8872 | 1.9331 | 3.2040 | 1.1761 | 1.4700 | 2.5763 |
| 120 | 0.4369 | 0.2056 | 1.5393 | 2.9011 | 1.4279 | 1.6674 | 2.7330 |
| 125 | 0.2564 | 0.8311 | 1.7662 | 2.7205 | 1.4031 | 1.4220 | 2.4743 |
| 130 | 0.9527 | 3.0226 | 2.8198 | 2.7917 | 1.0979 | 0.8277 | 1.8476 |
| 135 | 2.5446 | 6.8813 | 4.8188 | 3.2168 | 0.6571 | 0.2076 | 1.0406 |
| 140 | 4.9625 | 12.3280 | 7.7709 | 4.0526 | 0.3278 | 0.0207 | 0.3361 |
| 145 | 8.0545 | 19.1030 | 11.5650 | 5.2992 | 0.3778 | 0.7201 | 0.0331 |
| 150 | 11.5960 | 26.7780 | 15.9730 | 6.8904 | 1.0014 | 2.5981 | 0.3599 |
| 155 | 15.3120 | 34.8050 | 20.6750 | 8.7028 | 2.2489 | 5.6700 | 1.3911 |
| 160 | 18.9040 | 42.5590 | 25.2870 | 10.5670 | 3.9932 | 9.6275 | 3.0110 |
| 165 | 22.0720 | 49.4070 | 29.4070 | 12.2920 | 5.9489 | 13.8760 | 4.9224 |
| 170 | 24.5530 | 54.7720 | 32.6630 | 13.6870 | 7.7424 | 17.6810 | 6.7268 |
| 175 | 26.1310 | 58.1910 | 34.7490 | 14.5950 | 9.0005 | 20.3130 | 8.0111 |
| 180 | 26.6680 | 59.3610 | 35.4660 | 14.9110 | 9.4509 | 21.2420 | 8.4686 |
| $\sigma_{\text{el}}(a_0^2)$ | 98.464 | 201.298 | 178.043 | 152.524 | 134.567 | 103.933 | 69.291 |
| $\sigma_{\text{mt}}(a_0^2)$ | 92.938 | 155.895 | 104.002 | 67.447 | 32.399 | 38.865 | 36.772 |

(1983) which exhibit a pronounced peak in this region with a magnitude much closer to the theoretical values. This discrepancy in the experimental results is unlikely to arise from the neglect of forward scattered electrons since the amount of forward scattering in the peak region is less than at 15 eV where all experimental and theoretical results are in tolerably good agreement. In figure 10 we show the momentum transfer cross sections. The experimental results of Frost and Phelps (1964) exhibit a much broader and lower peak than our theoretical results and those of Sin Fai Lam although the agreement between these data is very good at lower energies.

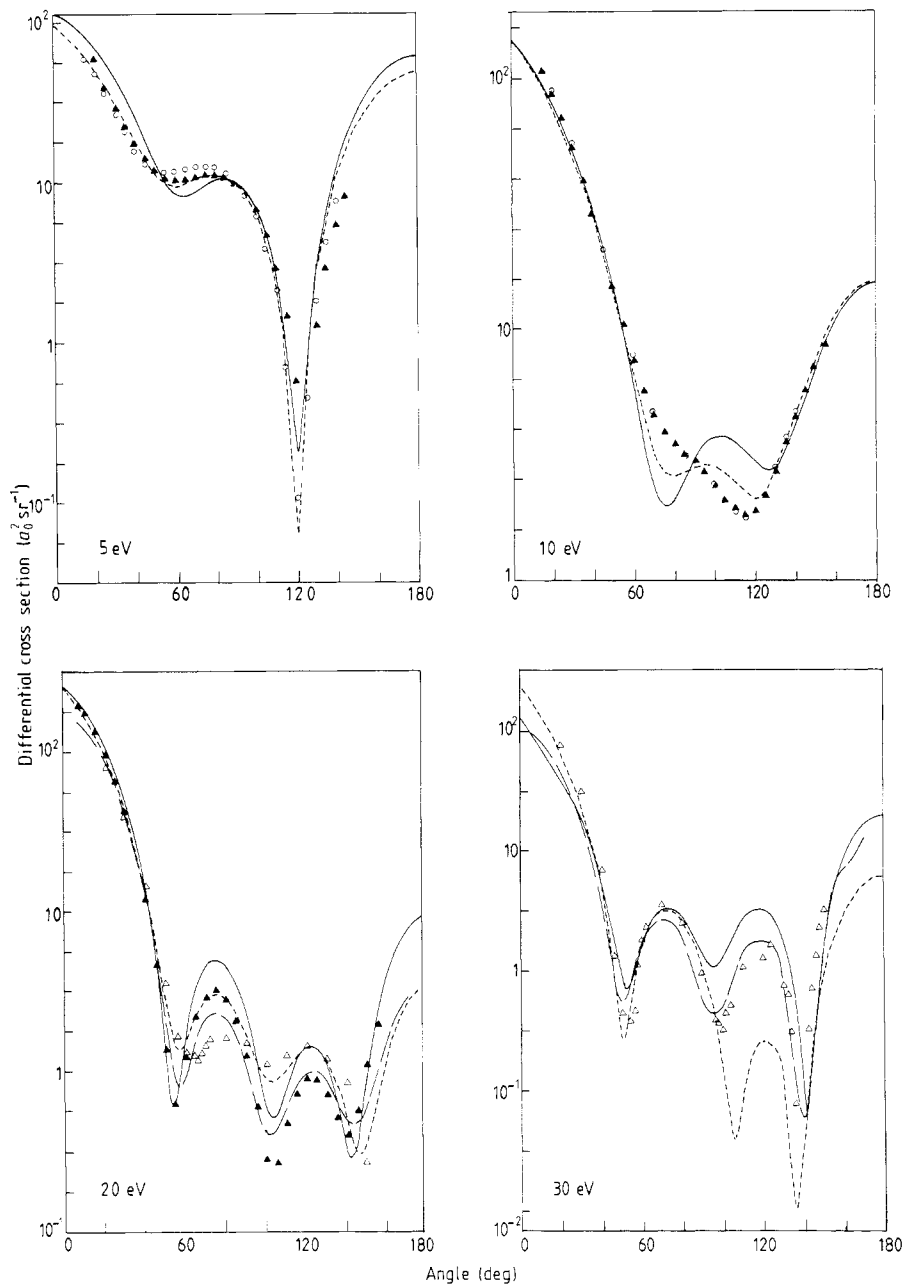


Figure 8. Differential cross sections for elastic scattering of electrons from xenon: —, present results; — — —, McCarthy *et al* (1977); - - - -, Sin Fai Lam (1982); ▲, Jost (1982); ○, Register *et al* (1980); △, Williams and Crowe (1975).

4. Conclusions

We have presented a detailed study of elastic scattering of electrons by krypton and xenon in the energy region from 0 to 50 eV in the adiabatic exchange approximation.

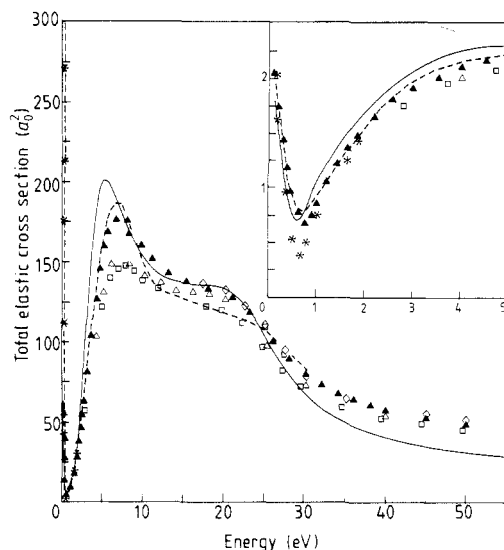


Figure 9. Total elastic cross sections for electron scattering from xenon: —, present results; ----, Sin Fai Lam (1982); \square , Dababneh *et al* (1980); *, Gus'kov *et al* (1978); \blacktriangle , Jost *et al* (1983); \triangle , Nickel *et al* (1983); \diamond , Wagenaar and de Heer (1980).

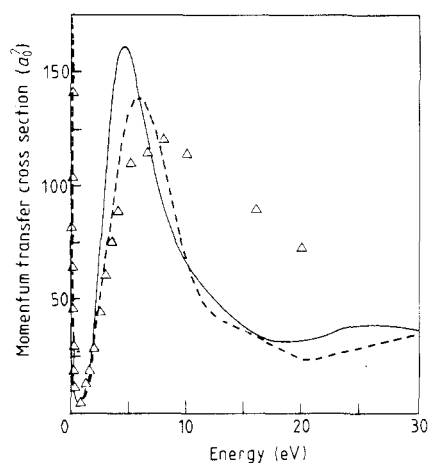


Figure 10. Momentum transfer cross sections for elastic scattering of electrons from xenon: —, present results; ----, Sin Fai Lam (1982); \triangle , Frost and Phelps (1964).

On the whole the results seem quite reliable as was the case for the other noble gases previously reported (McEachran and Stauffer 1983a, b). However for xenon the accuracy is not as good partly because of the complexity of the atom and partly because relativistic effects are becoming important. We intend to investigate this latter effect further within our AE approximation. Another possibility for improving the accuracy of our calculations would be to use polarisation potentials derived from calculations in which all of the electron shells in the atom are polarised instead of just the valence shells as in the present results. Comparisons between these two types of potentials

were reported in the case of argon by Yau *et al* (1980) and suggest that smaller peak total cross sections would result. However the calculation of these potentials is very time consuming in the case of the large atoms considered in this paper. In general, however, this approximation has lived up to our expectation for calculations on krypton and xenon.

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