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Close-coupling calculations of electron scattering by atomic fluorine

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The close-coupling (CC) calculations reported by Ormonde for $e^- + F$ scattering have been repeated using independent CC computer programs. No evidence of very narrow, low-energy shape resonances is observed in the $^1P^o$ and $^1D^o$ d waves.

Ormonde[1] has reported very low energy, and very narrow shape resonances in $e^- + F$ scattering. These were observed for total $\pi LS = {}^1P^o$ and $^1D^o$, at energies between 2×10^{-4} and 2×10^{-3} Ry, even in the static-exchange approximation.[2] We have repeated these calculations using the RMATRX[3] and NIEM[4] close-coupling codes. We have used the F^- orbitals of Bagus[5] for the $1s^2 2s^2 2p^5\,{}^2P^o$ and $1s^2 2s\ 2p^6\,{}^2S$ states of F, since these were used by Ormonde.[2] Our elastic cross sections for the energy range $k^2 = 2.0\times10^{-4}$ to 2.0×10^{-3} Ry in both static-exchange and two-state approximations are presented in Table I.

We had great difficulty in using RMATRX with the asymptotic package ASYM of Norcross[6] at these low energies. Both linear dependence, and the large radial distance at which the Burke-Schey[7] expansion was applicable, gave problems. However, the comparison with the NIEM results, which do not involve a Burke-Schey expansion, indicate that the additional features in ASYM which are specifically designed to handle such low energies problems, provide correct results. Ormonde has used a straight Burke-Schey expansion.[2]

We therefore have no explanation for the features observed by Ormonde, and we support the conclusions of the previous paper.[8] We have observed that the $^1D^o$ d-wave phase shift is adequately given by the Born approximation result, since penetration inside 11 a.u. is negligible, and outside 11 a.u. the potential has its asymptotic form. Further, we are confident that shape resonances could not be induced by inclusion of the states $1s^2 2s 2p^4\ 3l$ into our CC expansion. The thresholds for these states, using the $3s$, $3p$, $3d$ orbitals of Hibbert *et al.*,[9] lie at least 0.8 Ry above the ground state and therefore could not provide R-matrix poles (needed for shape resonances) in the near threshold region.

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TABLE I. Elastic cross sections (in units of πa_0^2) for $e^- + F$ scattering.

	$^1P^o$			$^1D^o$	
	RMATRX		NIEM	RMATRX	NIEM
k^2 (Ry)	Static exchange	2-state	2-state	Static exchange	Static exchange
0.0002	···	0.578	0.576	···	8.88×10^{-3}
0.0004	···	0.583	0.578	···	8.89×10^{-3}
0.0006	···	0.586	0.580	9.04×10^{-3}	8.89×10^{-3}
0.0008	···	0.589	0.582	9.03×10^{-3}	8.89×10^{-3}
0.0010	0.668	0.592	0.583	9.02×10^{-3}	8.89×10^{-3}
0.0012	0.672	0.594	0.585	9.01×10^{-3}	8.89×10^{-3}
0.0014	0.676	0.596	0.586	9.01×10^{-3}	8.89×10^{-3}
0.0016	0.679	0.599	0.587	9.01×10^{-3}	8.89×10^{-3}
0.0018	0.681	0.600	0.588	9.01×10^{-3}	8.89×10^{-3}
0.0020	0.682	0.602	0.590	9.00×10^{-3}	8.89×10^{-3}

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