

## A Study of $L^2$ Approximations in Atomic Scattering\*

A. T. Stelbovics and T. Winata<sup>A</sup>

School of Mathematical and Physical Sciences, Murdoch University,  
Perth, W.A. 6150, Australia.

<sup>A</sup> Permanent address: Faculty of Mathematics and Natural Sciences,  
Bandung Institute of Technology, Bandung 40132, Indonesia.

### Abstract

The approximation of Coulomb continuum functions by an  $L^2$  basis is studied using a Laguerre-function basis which can be extended to completeness. Also studied is the convergence rate of  $L^2$  approximations to Born matrix elements for electron impact ionisation as a function of basis-set size. This important class of matrix elements occurs in pseudo-state close-coupling calculations, accounting for scattering to the three-body continuum. Convergence rates in both cases are derived analytically and confirmed numerically. We find that the rate of pointwise convergence of  $L^2$  expansions to the continuum function is slow, and of conditional type; however, it is proven that the corresponding ionisation matrix elements converge geometrically. Our result agrees with the behaviour observed in pseudo-state calculations.

### 1. Introduction

The most sophisticated models of electron-atom scattering employ the close-coupling equations (see for example Burke and Seaton 1971 for a review). A feature of these equations is that they use target-state expansions which when extended over the continuum are complete. It is known that coupling to the continuum channels is important at intermediate energies and must be included. At present there are two approaches to including the continuum, the optical potential method of McCarthy and coworkers (McCarthy and Stelbovics 1983) and the pseudo-state expansion method popularised by Burke and coworkers (see e.g. Burke and Mitchell 1973 and also Burke and Seaton 1971). The present work will concentrate on the pseudo-state method.

In the pseudo-state method the target Hamiltonian is diagonalised in a basis of square integrable ( $L^2$ ) functions. The positive-energy solutions are called pseudo-states because they are not true eigenfunctions of the target and their energy varies with type of basis function and basis-set size. However, it has been established that these functions after a renormalisation can indeed provide a good approximation to a true continuum function, at least for small  $r$ . A recent review of the techniques for different basis sets, properties of the pseudo-states and their relation to exact continuum functions is given by Macias *et al.* (1988). In the calculation of effective-potential matrix elements, the pseudo-states contribute through overlap integrals involving the folding

\* Paper presented at the Workshop on Interfaces in Molecular, Electron and Surface Physics, held at Fremantle, Australia, 4–7 February 1990.

of the wavefunctions between electron-electron and core-electron Coulomb potentials. In the momentum-space formulation (McCarthy and Stelbovics 1983) the effective potentials are the Born matrix elements with exchange included and the momenta taken on and off the energy shell. It is important to note that, while the convergence rates of the  $L^2$  approximations to the continuum wavefunction are of intrinsic interest, it is of more importance to determine the convergence rates of the corresponding Born matrix elements.

Similar reasoning prompted Bransden and Dewangen (1979) to suggest that pseudo-states for a close-coupling calculation may be selected by requiring that they reproduce accurate second-order amplitudes. The approximation is equivalent to a single iteration of the momentum-space close-coupling equations and setting the external momenta on shell. In recent years their suggestion has been used by van Wyngaarden and Walters (1986) and by Callaway and Madison (1987) to optimise pseudo-state basis sets for very large-scale calculations. The optimisation is important because each extra pseudo-state generates a new row and column in the channel indices of the effective potentials. The closure and numerical discretisation of the integral equations over the off-shell momenta extends the row and column size of the final matrix equations by about 25 for each added state. At the present time inclusion of 10 additional states would be regarded as a major increase in the complexity of a typical calculation. Callaway and Madison point out that that 'even if a particular pseudo-state basis set can accurately reproduce a second-order perturbation theory amplitude, there is no guarantee that this same basis set will accurately represent a complete set in a different calculation such as a close-coupling equation'. Nevertheless, because the pseudo-states do converge to the exact continuum functions, one can infer that when enough states are included so convergent Born amplitudes are obtained, such a set will guarantee that the continuum is adequately allowed for in the close-coupling equations.

In this paper we examine the convergence of the Fourier series generated by extending a pseudo-state basis to completion for the ionisation amplitude from the ground state of a hydrogen atom. In the Born approximation the ejected electron is described by a regular Coulomb continuum function. We employ a Laguerre basis used by Yamani and Reinhardt (1975) to construct pseudo-state approximations to the continuum wave for any order of basis. The great advantage of their basis is that the Fourier expansion coefficients have an analytic form. This enables analytic estimates of convergence rates to be made and at the same time permits large-basis pseudo-states to be computed with a high degree of accuracy.

The slow convergence of this type of expansion is emphasised in the second section. Convergence rates for pointwise convergence are derived analytically and are illustrated. In Section 3 the ionisation Born matrix elements to a pseudo-state calculation are discussed. It is shown that the pseudo-state approximations give a matrix element approximation which is essentially geometrically convergent. The optimum exponent for most rapid convergence is derived. The results are illustrated with some examples. Some differential ionisation cross sections are calculated to show that pseudo-states over a substantial range of orbital angular momentum need to be included in realistic calculations at intermediate energies. We compare the convergence rates of our basis set with similar size sets of van Wyngaarden and Walters (1986) and

conclude that the results we find for this basis set are typical of the others used in numerical work. Finally we give some conclusions and suggestions for future work.

## 2. $L^2$ Wavefunctions

Yamani and Reinhardt (1975) showed that the regular Coulomb partial-wave continuum functions for a hydrogenic target

$$U_l(q, r) = e^{\frac{1}{2}\pi\gamma} \frac{|\Gamma(l+1-i\gamma)|}{\Gamma(2l+2)} (2qr)^{l+1} e^{-iqr} {}_1F_1(l+1+i\gamma, 2l+2, 2iqr) \quad (1)$$

could be expanded in a Laguerre basis as

$$U_l(q, r) = B_l(q) \sum_{n=0}^{\infty} \frac{\Gamma(n+1)}{\Gamma(n+2l+2)} P_n^{l+1}(x) \Phi_n^l(r), \quad (2)$$

where

$$B_l(q) = 2^{l+1} |\Gamma(l+1-i\gamma)| (1-x^2)^{\frac{1}{2}(l+1)} e^{(\theta-\frac{1}{2}\pi)\gamma}, \quad (3)$$

$$\Phi_n(r) = (\lambda r)^{l+1} e^{-\frac{1}{2}\lambda r} L_n^{2l+1}(\lambda r). \quad (4)$$

The  $U_l(q, r)$  are normalised to a  $\delta$  function in  $q/2\pi$ . The variable  $x$  is related to the energy by

$$E_q \equiv \frac{1}{2}q^2 = \frac{\lambda^2}{8} \left( \frac{1+x}{1-x} \right); \quad (5)$$

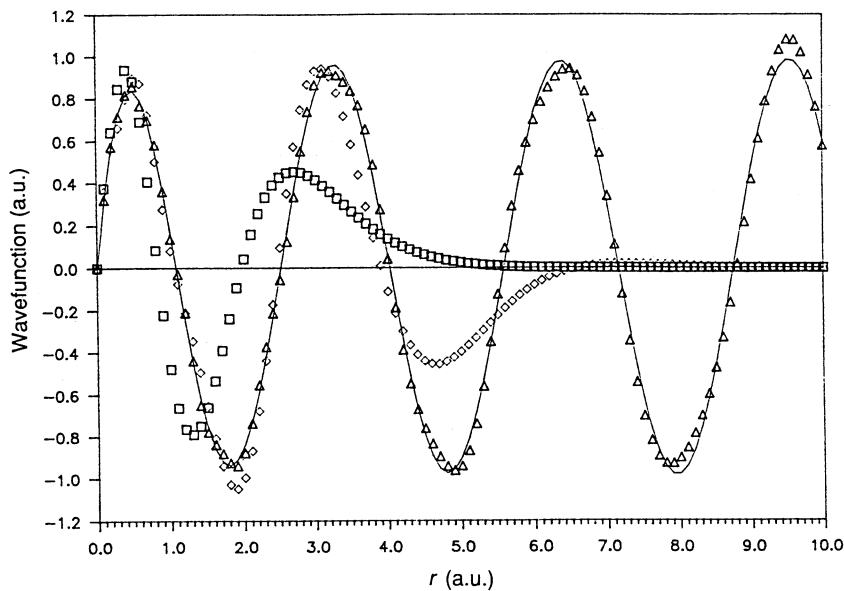
also

$$\gamma = \frac{1}{q}, \quad \text{and} \quad x = \cos\theta, \quad 0 \leq \theta \leq \pi. \quad (6)$$

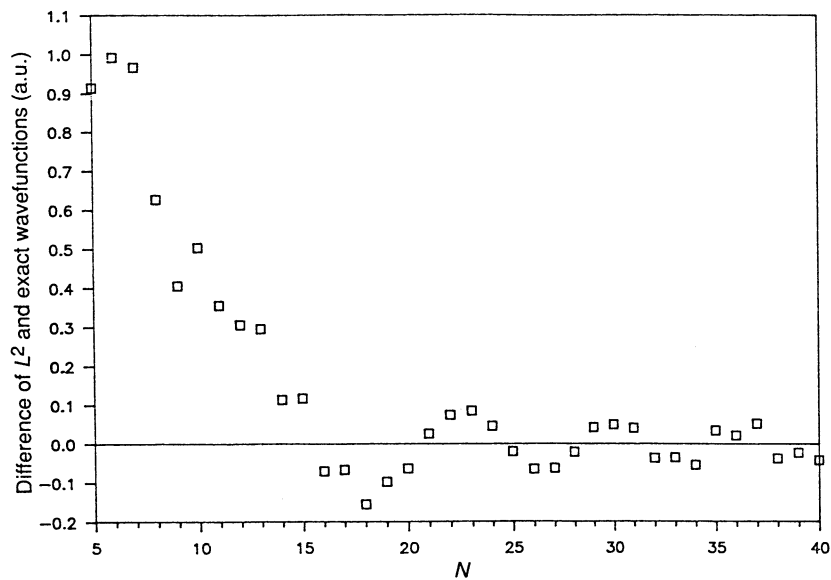
The Fourier coefficients appear complicated but in fact the  $P_n^{l+1}(x)$  are polynomials in the variable  $x$  (Yamani and Reinhardt 1975) defined by a three-term recurrence relation and are easy to calculate. We note that for future reference that they may be expressed in the form

$$P_n^{l+1}(x) = \frac{\Gamma(n+2l+2)}{n! \Gamma(2l+2)} e^{in\theta} {}_2F_1(-n, l+1-i\gamma; 2l+2; 1-e^{-2i\theta}). \quad (7)$$

The properties of these polynomials have been investigated by Bank and Ismail (1985). The expansion above is formally exact and the spectrum is continuous. In practice we are restricted to a finite basis. If we choose for example the first  $N$  functions from the set (4) and diagonalise the target Hamiltonian in the basis then the positive-energy  $L^2$  states form a set of pseudostates. There are  $N$  solutions spanning both negative and positive energies. The lowest-lying negative energy solutions are excellent approximations to the exact bound state wavefunctions. The approximate  $L^2$  wavefunctions below the continuum represent in some average way the remaining discrete levels.



**Fig. 1.** The  $L^2$  wavefunctions for  $E_q = 50$  eV,  $l = 0$ ,  $\lambda = 6.0$ , and  $N = 5$  (squares),  $N = 10$  (diamonds),  $N = 40$  (triangles), compared with the exact wavefunction (curve).



**Fig. 2.** Convergence of the  $L^2$  wavefunctions shown as a function of number of basis functions  $N$  for  $E_q = 50$  eV,  $l = 0$ ,  $\lambda = 6.0$  and  $r = 5$  a.u.

In the case of the present basis Yamani and Reinhardt have shown that the eigen-energies in the truncated space may be found by imposing the boundary condition

$$P_N^{l+1}(x) = 0. \quad (8)$$

There are  $N$  solutions to this polynomial equation in the variable  $x = x_i^l(N, l)$ ,  $i = 0, 1, \dots, N-1$  and in turn in  $E$  through the mapping (5). The distribution of positive energies is therefore basis dependent and from a physical point of view is a result of the requirement of orthogonality for all the pseudo-states. For the calculations reported here we use the expansion (2) truncated to  $N$  terms. This truncation gives a state which coincides with the pseudo-states at the eigen-energies and thus has the effect of interpolating the  $L^2$  basis solutions to any positive energy. If we denote the  $n$ th term of the Fourier expansion for  $U_l$  by  $S_n^l$  then it is straightforward to prove (see Appendix A) that for large  $n$

$$\begin{aligned} S_n^l(q, r) = & n^{-\frac{3}{4}} 2e^{(2\theta-\pi)\gamma} (\lambda r)^{\frac{1}{4}} \pi^{-\frac{1}{2}} \cos[2(n\lambda r)^{\frac{1}{2}} - (l + \frac{3}{4})\pi] \\ & \times \cos[(n+l+1)\theta + \gamma \ln(2n \sin\theta) - \frac{1}{2}\pi(l+1) \\ & - \arg \Gamma(l+1-iy)] + O(n^{-\frac{5}{4}}). \end{aligned} \quad (9)$$

The feature to note is that the convergence rate will be slow because of the  $n^{-\frac{3}{4}}$  behaviour. In fact the convergence relies on the alternation in sign of the trigonometric factors; i.e. it is only conditionally convergent. The rate of convergence also depends on  $q$ ,  $r$ ,  $l$  and  $\lambda$ .

In Fig. 1 we plot the  $L^2$  approximation to the s-wave continuum function for  $E = 50$  eV, for various basis sizes,  $N = 5, 10$  and  $40$ . The value of  $\lambda = 6a_0^{-1}$  is chosen by a simple optimisation process. We allowed  $\lambda$  to vary over a coarse range from  $1a_0^{-1}$  to  $10a_0^{-1}$  and found the value which gave the least mean square error over the interval from  $0$  to  $10a_0$ . The results are typical of those obtained by Kaufmann *et al.* (1987) and Macias *et al.* (1988). The behaviour of the expansions for arbitrary  $l$  is similar. The most obvious feature of the expansions shown is that there are still minor discrepancies for the largest basis of  $40$  functions. In Fig. 2 we show the nature of the error in the expansion for a fixed value of  $r$ . The rate of convergence and its oscillatory nature matches that of the above asymptotic form. It should be emphasised that the slow rate of convergence is not an artifact of this particular expansion but is germane to all  $L^2$  expansions of functions which are not of bounded variation (continuum functions having an infinite number of undamped oscillations are of unbounded variation).

### 3. Approximation to Born Matrix Elements

The Born ionisation amplitude from the ground state of hydrogen is given by

$$f(\mathbf{q}, \mathbf{K}) = -\frac{2}{K^2} \int \Psi^{(-)}(\mathbf{q}, \mathbf{r})^* e^{i\mathbf{K}\cdot\mathbf{r}} \phi_0(\mathbf{r}) d\mathbf{r}, \quad (10)$$

where

$$\phi_0(\mathbf{r}) = \pi^{-\frac{1}{2}} e^{-r} \quad \text{and} \quad \mathbf{K} = \mathbf{k} - \mathbf{k}'. \quad (11)$$

The integral for (10) is well known and is derived, for example, by Landau and Lifshitz (1977). Our normalisation for the Coulomb function here is to a  $\delta$  function in  $\mathbf{q}/(2\pi)^3$ . A partial-wave analysis gives

$$f(\mathbf{q}, \mathbf{K}) = -\frac{8\pi^{\frac{1}{2}}}{K^2} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} F_l(q, K) P_l\left(\frac{\mathbf{K} \cdot \mathbf{q}}{Kq}\right), \quad (12)$$

with

$$F_l(q, K) = \frac{1}{2q} \int_0^{\infty} r e^{-r} j_l(Kr) U_l(q, r) dr. \quad (13)$$

[The  $P_l$  in (12) is the Legendre polynomial and is not to be confused with the Coulomb polynomials;  $\delta_l$  is the Coulomb partial-wave phase shift.] The Born amplitudes which enter the final close-coupling equations are further partial-wave projected over the scattering angle contained in  $K$ . From the point of view of studying the convergence rates we shall assume that it is sufficient to consider the rate of convergence of the pseudo-state expansions to  $F_l(q, K)$ . This amplitude can be evaluated in closed form (see Jetzke and Broad 1985) in terms of Appell functions. Our interest centres on the series obtained by replacing  $U_l(q, r)$  by its Fourier expansion

$$F_l(q, K) = \frac{B_l(q)}{2q} \sum_{n=0}^{\infty} \frac{\Gamma(n+1)}{\Gamma(n+2l+2)} P_n^{l+1}(x) I_n^l(K), \quad (14)$$

where

$$I_n^l(K) = \int_0^{\infty} r e^{-r} j_l(Kr) \Phi_n^l(r) dr. \quad (15)$$

This integral is evaluated in Appendix B. The result is

$$I_n^l(K) = A^{-(n+l+1)} 2^l \Gamma(l+1)(n+2l+1)(2l+1) \frac{1}{\lambda K} (\sin \omega)^{l+1} \\ \times \left( \frac{2n+2l+2}{n+2l+1} (\cos \omega - A^{-1}) C_n^{l+1}(\cos \omega) + (1-A) C_{n-1}^{l+1}(\cos \omega) \right), \quad (16)$$

where

$$\tan \omega = \frac{K}{1 + K^2 - (\frac{1}{2}\lambda)^2}, \quad 0 \leq \omega \leq \pi, \quad (17)$$

$$A = \left( \frac{(1 + \frac{1}{2}\lambda)^2 + K^2}{(1 - \frac{1}{2}\lambda)^2 + K^2} \right)^{\frac{1}{2}}. \quad (18)$$

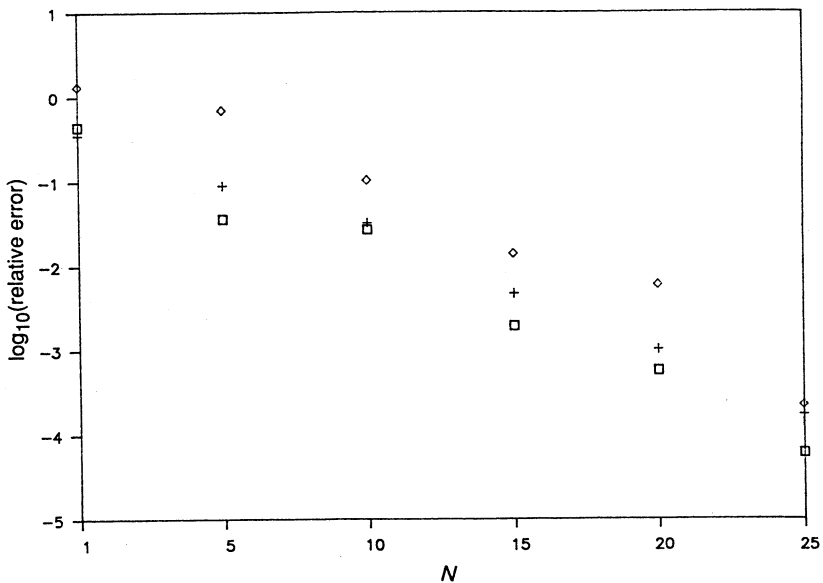
The  $C_n^{l+1}$  are ultraspherical polynomials. The rate of convergence of the series is dominated by the term  $A^{-n}$ . The maximum convergence rate will occur when  $A$  takes its maximum value:

$$\max A = \left( \frac{(1+K^2)^{\frac{1}{2}} + 1}{(1+K^2)^{\frac{1}{2}} - 1} \right)^{\frac{1}{2}}, \quad \text{when } \lambda = 2(1+K^2)^{\frac{1}{2}}. \quad (19)$$

If we combine the asymptotic forms for  $P_n^l$  and  $I_n^l$  (see Appendix B) we find that the  $n$ th term of the series (14) behaves as

$$\begin{aligned} a_n^l(q, K) = & A^{-(n+l+1)} \frac{1}{\lambda q K} (2l+1) e^{(2\theta-\pi)\gamma} \\ & \times \cos[(n+l+1)\theta + \gamma \ln(2n \sin \theta) - \frac{1}{2}\pi(l+1) - \arg \Gamma(l+1-iy)] \\ & \times \{2(\cos \omega - A^{-1}) \cos[(n+l+1)\omega - \frac{1}{2}\pi(l+1)] \\ & + (1-A) \cos[(n+l)\omega - \frac{1}{2}\pi(l+1)] + O(n^{-1})\}. \end{aligned} \quad (20)$$

In order to illustrate the above theory we have calculated the series (14) in the case  $l=0$  and for several sizes of basis set. The approximations are generated by terminating the expansion (14) after  $N$  terms. The results are shown in Fig. 3 in the form of a logarithm of the relative errors. The error should be of the order of the first neglected term, since apart from the



**Fig. 3.** Relative errors of the  $L^2$  radial integrals compared with the exact radial integrals for  $l=0$ ,  $\lambda=6.0$  and ejected electron energies  $E_q=50$  eV (squares), 100 eV (crosses), 200 eV (diamonds). The scattered electron energy is  $E_{k'}=350$  eV, the incident energy  $E_k=413.6$  eV, and angle of scattering  $\theta_{kk'}=30^\circ$ .

oscillatory terms, the series is geometric. The kinematic regions chosen are ones where the ionisation cross sections take their larger values and are thus of importance in close-coupling applications. The scale chosen shows clearly that the error is dominated by  $-N\log A$  behaviour, although the trigonometric terms have a noticeable effect in the oscillations they produce. For the kinematics shown in Fig. 3 the values of  $A$  are 1.424, 1.426 and 1.400 for  $E_q = 50, 100$  and  $200$  eV respectively. In each case there is a linear trend which agrees with the slopes predicted from the above  $A$ . The optimum value of  $\lambda$  for  $E_q = 50$  eV from (19) is  $\lambda = 5.9 a_0^{-1}$ , leading to optimised  $A$  values which are virtually unchanged from those above. For the other values of  $E_q$  it is very similar. We think it is coincidental that our unrelated primitive optimisation of the continuum wave itself ( $\lambda = 6 a_0^{-1}$ ) gave a result so close to this one. The other main factor contributing to the rate of convergence is from the exponential term in (20) which is governed by the value of  $E_q$ .

#### 4. Discussion and Conclusions

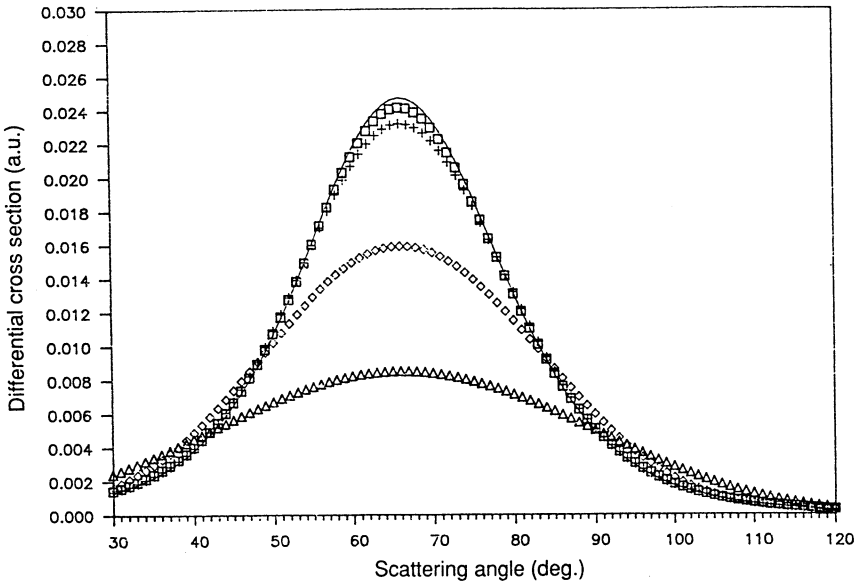
In order to further assess the  $L^2$  approximation technique in the context of the Born matrix elements input to a full close-coupling calculation, we investigated the convergence of the partial-wave expansion to the full amplitude. The differential cross sections are determined using

$$\frac{d^5\sigma}{d\Omega_{\mathbf{k}} d\Omega_{\mathbf{q}} dE_q} = \frac{1}{(2\pi)^3} \frac{k'q}{k} |f(\mathbf{q}, \mathbf{K})|^2. \quad (21)$$

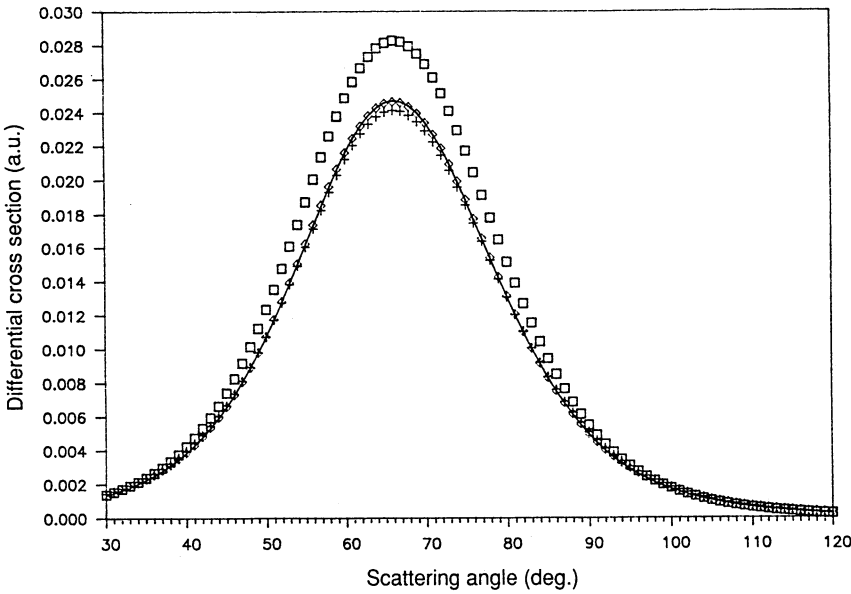
Some results are shown in Fig. 4, where it can be seen that including less than 10 partial waves leads to errors of the order of 100% in the cross section. If one therefore assumes that total cross sections from a full calculation will have an error related to that of the input Born terms one must conclude that pseudo-state bases need to be extended beyond the s, p and d waves typical of current calculations. In order to assess how far in basis size one must go we have also calculated the differential cross sections for  $l$  large enough to ensure convergence in the partial-wave sum. The results in Fig. 5 are typical. With a basis  $N=5$  in each partial wave we reproduce the correct values to the order of 10% which improves to 1–2% by the time  $N=10$ . For the Laguerre basis studied, it would appear that if one is using the close-coupling formalism to compute inelastic and ionisation scattering at intermediate energies one should be careful to include pseudo-state functions up to  $l \approx 5-10$ , otherwise there is no additional gain in accuracy in extending the basis size  $N$  beyond 2–3.

A question which naturally arises is how our basis compares with some of the other modern calculations, for example that of van Wyngaarden and Walters (1986). In order to test that there is nothing peculiar to our choice of basis we carried out a comparison with the pseudo-state data of van Wyngaarden and Walters. We used their second Born testing criterion for initial and final  $1s$  states and compared the second Born amplitudes for intermediate  $l=0$  pseudo-states. The results are shown in Table 1, where we also include the earlier data of Fon *et al.* (1981). We add Laguerre pseudo-states terminating at the same basis size as van Wyngaarden and Walters. Our second Born result for the same number of states is very similar. We conclude that an optimised Laguerre basis has convergence properties that are not dissimilar





**Fig. 4.** Convergence of the  $L^2$  differential cross sections shown for 3 (triangles), 5 (diamonds), 10 (crosses) and 15 (squares) partial waves, for  $N = 10$ ,  $\lambda = 6.0$  and  $E_q = 50$  eV. The remaining kinematics are the same as for Fig. 3.



**Fig. 5.** Convergence of the  $L^2$  differential cross sections shown for varying basis size  $N$ . The number of partial waves used is 15 and  $\lambda = 6.0$ . The remaining kinematics are the same as for Fig. 3.

to other optimised sets. it is also apparent that the second Born amplitudes have not yet converged to two significant figures.

**Table 1. Partial-wave second Born terms of  $L^2$  expansions shown for intermediate  $l=0$  pseudo-states at 100 eV for  $1s \rightarrow 1s$  scattering, compared with data from Fon *et al.* (F) and van Wyngaarden and Walters (vW)**

Powers of 10 are denoted by a superscript and a.u. are used. R labels the real part and I the imaginary part of the amplitudes. The exact wavefunctions for  $1s$  and  $2s$  states are employed. The notation  $3s-8s$  for example implies 6,  $l=0$  pseudostates are included. A value  $\lambda=6.0$  was used to generate the Laguerre basis states under the heading  $L^2$  expansions

	F	vW	$L^2$ expansions (Laguerre bases)				
	3s-4s	3s-8s	3s-4s	3s-5s	3s-6s	3s-7s	3s-8s
R	$1.6^{-2}$	$3.0^{-2}$	$3.2^{-3}$	$1.1^{-2}$	$1.7^{-2}$	$2.3^{-2}$	$2.9^{-2}$
I	$7.8^{-2}$	$8.6^{-2}$	$5.1^{-2}$	$7.0^{-2}$	$7.9^{-2}$	$8.4^{-2}$	$8.6^{-2}$

This analysis demonstrates that pseudo-states give ionisation matrix elements which are geometrically convergent and so can provide accurate inputs to close-coupling equations for a large enough basis. We have not attempted to calculate ionisation matrix elements for arbitrary initial states. However, by using parametric differentiation, a general calculation will yield combinations of the fundamental integrals already derived and therefore our results can be extended to the wider class of ionisation amplitudes. There are some qualifications that need to be made. First, while the convergence is geometric, the value of  $A$  is often in the neighbourhood of 1, even for the optimum value of  $\lambda$ . The rate of convergence is thus slow; larger basis sets, say of the order of 10 states for each partial wave are required to obtain convergent amplitudes. Second, in a momentum-space close-coupling calculation, off-shell matrix elements are required as well as the on-shell ones. This means that the momentum transfer  $K$  varies over a wide range and thus affects the choice of  $\lambda$ . In practice we assume that a value of  $\lambda$  which is optimum for the kinematic regions that have the larger ionisation amplitudes would need to be used. Also the value will depend on the exact specification of states included in  $P$ -space, so choosing the optimum  $\lambda$  in a calculation needs careful consideration.

A related question we have not attempted to consider here but which should receive attention at some future stage is how the exchange matrix elements are approximated by pseudo-states. The implicit assumption in previous work has been that once pseudo-states approximate the direct Born amplitudes to sufficient accuracy then the exchange amplitudes will be similarly approximated. It would be nice to have some evidence for this.

## Acknowledgment

One of us (A.T.S.) gratefully acknowledges the financial support of the Australian Research Council for this work.

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## Appendix A

We derive the asymptotic form for the  $n$ th term of the Fourier expansion of the radial Coulomb function  $U_l(q, r)$ . The  $n$ th term contains two  $n$ -dependent quantities  $P_n^{l+1}(x)$  and  $\phi_n^{l+1}(r)$ . We begin by considering the behaviour of  $P_n^{l+1}(x)$ . The large- $n$  behaviour of this polynomial is analysed by using the hypergeometric function representation of equation (7). The asymptotic behaviour is most conveniently determined with the aid of the estimate (Luke 1969, Vol. I, p. 241)

$${}_2F_1(a, b-n; c; z) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c-a)} \{ \Gamma(a)(nz)^{-a} [1 + O(n^{-1})] + \Gamma(c-a)(nze^{-i\pi})^{a-c} (1-z)^{c-a-b+n} [1 + O(n^{-1})] \}. \quad (\text{A1})$$

After simplification one finds that

$$\frac{\Gamma(n+1)}{\Gamma(n+2l+2)} P_n^{l+1}(x) = 2e^{y[\theta - \frac{1}{2}\pi]} \frac{(2n \sin \theta)^{-(l+1)}}{|\Gamma(l+1-iy)|} \{ \cos[(n+l+1)\theta + y \ln(2n \sin \theta) - \frac{1}{2}\pi(l+1) - \arg \Gamma(l+1-iy)] + O(n^{-1}) \}. \quad (\text{A2})$$

To determine the form of  $\phi_n^{l+1}(r)$  for large  $n$  we note (Magnus *et al.* 1966, p. 245) that

$$L_n^\alpha(y) = \pi^{-\frac{1}{2}} e^{\frac{1}{2}y} y^{-\frac{1}{2}} \alpha^{-\frac{1}{4}} n^{\frac{1}{2}} \alpha^{-\frac{1}{4}} \cos[2(ny)^{\frac{1}{2}} - \frac{1}{2}\alpha\pi - \frac{1}{4}\pi] + O(n^{\frac{1}{2}}\alpha^{-\frac{3}{4}}). \quad (\text{A3})$$

Hence, we get

$$\phi_n^l(r) = (\lambda r)^{\frac{1}{4}} \pi^{\frac{1}{2}} n^{l+\frac{1}{4}} \cos[2(n\lambda r)^{\frac{1}{2}} - (l + \frac{3}{4})\pi] + O(n^{l-\frac{1}{4}}). \quad (\text{A4})$$

Combining (A2) and (A4) we have for the  $n$ th term of the expansion (2) the representation

$$S_n^l(q, r) = n^{-\frac{3}{4}} 2 e^{(2\theta - \pi)y} (\lambda r)^{\frac{1}{4}} \pi^{-\frac{1}{2}} \cos[2(n\lambda r)^{\frac{1}{2}} - (l + \frac{3}{4})\pi] \times \cos[(n+l+1)\theta + y \ln(2n \sin \theta) - \frac{1}{2}\pi(l+1) - \arg \Gamma(l+1-iy)] + O(n^{-\frac{5}{4}}). \quad (\text{A5})$$

## Appendix B

Here we evaluate the integral

$$I_n^l(K) = \int_0^\infty r e^{-r} j_l(Kr) \phi_n^l(r) dr$$

and determine its asymptotic form. We begin by noting the representations

$$j_l(Kr) = 2 \frac{(l+1)!}{(2l+2)!} (2Kr)^l e^{-iKr} {}_1F_1(l+1; 2l+2; 2iKr), \quad (B1)$$

$$L_n^{2l+1}(\lambda r) = \frac{(n+2l+1)!}{n!(2l)!} {}_1F_1(-n; 2l+2; \lambda r). \quad (B2)$$

The integral can then be evaluated in terms of the following basic integral:

$$\begin{aligned} \int_0^\infty e^{-zt} t^{c-1} {}_1F_1(a; c; t) {}_1F_1(a'; c; \Lambda t) dt \\ = \Gamma(c)(z-1)^{-a}(z-\Lambda)^{-a'} z^{a+a'-c} {}_2F_1(a, a'; c; s), \end{aligned} \quad (B3)$$

where

$$s = \frac{\Lambda}{(z-1)(z-\Lambda)}. \quad (B4)$$

All our integrals have the following parameters:

$$z = \frac{1}{2} + \frac{1}{\lambda} - i\frac{K}{\lambda}, \quad \Lambda = -2i\frac{K}{\lambda}, \quad c = 2a' = 2l+2, \quad a = -m, \quad m = 0, 1, \dots \quad (B5)$$

We denote the integrals with these values as  $G(m, l, K, \lambda)$ . With the above it follows that  $1-s = u^2$  where  $u$  is a complex number of unit modulus. We can thus write

$$s = -\frac{2iK\lambda}{(1-\frac{1}{2}\lambda-iK)(1+\frac{1}{2}\lambda+iK)} = 1-e^{2i\omega}, \quad \text{where } 0 \leq \omega \leq \pi. \quad (B6)$$

Further with the above values for  $s$ ,  $z$  and  $\Lambda$  it may be shown that

$$\begin{aligned} \frac{z}{z-1} &= e^{i\omega} A, \quad \text{where } A = \left( \frac{(1+\frac{1}{2}\lambda)^2 + K^2}{(1-\frac{1}{2}\lambda)^2 + K^2} \right)^{\frac{1}{2}} > 1, \\ \tan \omega &= \frac{K}{1+K^2-(\frac{1}{2}\lambda)^2}, \quad 0 \leq \omega \leq \pi. \end{aligned} \quad (B7)$$

Then we have

$$G(m, l, K, \lambda) = A^{-m} \Gamma(2l+2) \left[ \left( \frac{1}{2} + \frac{1}{\lambda} \right)^2 + \left( \frac{K}{\lambda} \right)^2 \right]^{-(l+1)} e^{-im\omega} {}_2F_1(-m, l+1; 2l+2; s). \quad (B8)$$

Suppressing all the constant indices in  $G$  one deduces

$$\begin{aligned} I_n^l(K) &= \frac{\Gamma(l+2)\Gamma(n+2l+2)2^{l+1}}{\Gamma(n+1)\Gamma(2l+1)\Gamma(2l+3)} \frac{K^l}{\lambda^{l+2}} [- (n+2l+2)G(n+1) \\ &\quad + (2n+2l+2)G(n-nG(n-1))]. \end{aligned} \quad (B9)$$

A simplification of this complex form is achieved by noting that the hypergeometric function in the  $G$  functions is related to the ultraspherical polynomials  $C_n^{l+1}$ :

$$C_n^{l+1}(\cos\omega) = \frac{\Gamma(n+2l+2)}{n!\Gamma(2l+2)} e^{-in\omega} {}_2F_1(-n, l+1; 2l+2; 1-e^{2i\omega}). \quad (\text{B10})$$

After some rearrangement one finally finds

$$I_n^l(K) = A^{-n}\Gamma(l+1)(n+2l+1)(2l+1) \frac{(2K)^l}{\lambda^{l+2}} \left[ \left( \frac{1}{2} + \frac{1}{\lambda} \right)^2 + \left( \frac{K}{\lambda} \right)^2 \right]^{-(l+1)}, \\ \times \left( \frac{2n+2l+2}{n+2l+1} (\cos\omega - A^{-1}) C_n^{l+1}(\cos\omega) + (1-A) C_{n-1}^{l+1}(\cos\omega) \right). \quad (\text{B11})$$

To obtain the asymptotic form for large  $n$  we note (Magnus *et al.* 1966, p. 224)

$$C_n^{l+1}(\cos\omega) = 2 \frac{\Gamma(n+l+1)}{\Gamma(n+1)\Gamma(l+1)} \frac{\cos[(n+l+1)\omega - \frac{1}{2}\pi(l+1)]}{(2\sin\omega)^{l+1}} + O(n^{l-1}). \quad (\text{B12})$$

Thus we arrive at the estimate

$$I_n^l(K) = A^{-(n+l+1)} n^{l+1} (2l+1) \frac{1}{\lambda K} \{ 2(\cos\omega - A^{-1}) \cos[(n+l+1)\omega - \frac{1}{2}\pi(l+1)] \\ + (1-A) \cos[(n+l)\omega - \frac{1}{2}\pi(l+1)] \} + O(n^{-1}). \quad (\text{B13})$$

