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The inner region contains the particles when they are close to the collision center. In this way the most mathematically complex part of the interaction is isolated to a finite region of configuration space, and the collision wave function therein can be expressed in terms of a discrete, complete set of basis functions. In the outer infinite region the collision wave function has its asymptotic form and can be obtained directly from the asymptotic [illegible] equation. To obtain the scattering matrix these wave functions are linked on the boundary surface, through a quantity called the R-matrix.

In the following sections we will set up the various mathematical treatments that have been proposed within this overall concept and compare their mathematical and computational facets.

2 Formulation for Potential Scattering

Many of the mathematical features of R-matrix theory can be illustrated by consideration of a simplified model potential scattering problem. For s-wave scattering by a short-range central potential $V(r)$ the Schrödinger equation is

$$\left(\frac{d^2}{dr^2} + V(r) + k^2\right)\psi(k^2,r) = 0 \tag{2.1}$$

Let us assume that it is an excellent numerical approximation to put $V(r) = 0$ for values of r greater than some radius a. The spherical surface $r = a$ defines the R-matrix boundary. Clearly in the external region the solution is

$$F(k^2,r) = \sin kr + K \cos kr \qquad r \geq a \tag{2.2}$$

where the phase shift δ is related to the unknown R-matrix by $K = \tan \delta$. In the internal region we obtain a set of functions $u_\lambda(r)$ as solutions of

$$\left(\frac{d^2}{dr^2} + V(r) + k_\lambda^2\right)u_\lambda(r) = 0 \tag{2.3}$$

satisfying the R-matrix boundary conditions

$$u_\lambda(0) = 0$$

$$\frac{a}{u_\lambda(a)} \cdot \left.\frac{du_\lambda}{dr}\right|_{r=a} = b \text{ (an arbitrary constant)} \tag{2.4}$$

Equations (2.3) and (2.4) satisfy Sturm-Louisville conditions, and thus the functions $u_\lambda(r)$ constitute a complete discrete set in the region $0 \leq r \leq a$. We may therefore expand the solution of Eq. (2.1) as:

$$F(k^2,r) = \sum_{\lambda=1}^{\infty} A_\lambda(k^2)u_\lambda(r) \qquad 0 \leq r \leq a \tag{2.5}$$

To obtain the coefficients $A_\lambda(k^2)$ we consider Eqs. (2.1) and (2.3), multiply them by u_λ and F, respectively, and integrate their difference to obtain

$$\int_0^a \left(u_\lambda \frac{d^2F}{dr^2} - F\frac{du^2_\lambda}{dr^2}\right) dr = (k_\lambda^2 - k^2)\int_0^a u_\lambda F\, dr \tag{2.6}$$

The left hand side of this equation can be evaluated by Green's Theorem to give:

$$\left.\left(u_\lambda(r)\frac{dF(k^2,r)}{dr} - F(k^2,r)\frac{du_\lambda}{dr}\right)\right|_{r=a} = (k_\lambda^2 - k^2)\int_0^a u_\lambda F\, dr \tag{2.7}$$

From this equation one finds immediately that should we replace F and k^2 by $u_{\lambda'}$ and $k^2_{\lambda'}$, where $\lambda \neq \lambda'$, then the l.h.s. is zero due

to Eq. (2.4) and thus the set of functions u_λ are mutually orthogonal, and can be normalized to satisfy

$$\int_0^a u_\lambda(r)\, u_{\lambda'}(r)\, dr = \delta_{\lambda\lambda'} \tag{2.8}$$

Returning to Eq. (2.7) we have that

$$A_\lambda(k^2) = \int_0^a u_\lambda F\, dr = \frac{1}{a} \cdot \frac{u_\lambda(a)}{k_\lambda^2 - k^2} \left[a \frac{dF}{dr} - bF \right]_{r=a} \tag{2.9}$$

If we now define the R-matrix by

$$R(k^2) = \frac{1}{a} \sum_{\lambda=1}^{\infty} \frac{[u_\lambda(a)]^2}{k_\lambda^2 - k^2} \tag{2.10}$$

then according to Eqs. (2.5) and (2.9)

$$R(k^2) = F(k^2, r) \cdot \left(a \frac{dF(k^2, r)}{dr} - bF(k^2, r) \right)^{-1}_{r=a} \tag{2.11}$$

Equations (2.10) and (2.11) give us two independent expressions for the R-matrix. Equation (2.10) says that it can be expressed in terms of quantities determined solely from properties of the basis set in the internal region. Further it says that the interaction in this region can be described solely in terms of eigenenergies and surface amplitudes, without requiring explicit knowledge of the wave function, and that the energy of interaction can be factored out in a simple and explicit way. Equation (2.11) gives us another expression for the R-matrix in terms of the exact solution on the boundary. We can therefore use (2.10) to obtain a value for R on the l.h.s. of (2.11) and then use Eq. (2.2) to obtain

$$K = \tan \delta = \frac{-\sin ka + R(ka \cos ka - b \sin ka)}{\cos ka + k(ka \sin ka + b \cos ka)} \tag{2.12}$$

which can be rewritten as

$$\tan(\delta + ka) = \frac{kaR}{1 + kb} \tag{2.13}$$

Thus once we have R, the K matrix, phase shift and related cross section can be easily determined.

Pictorially we see that in the R-matrix treatment we have replaced the continuum spectrum of the whole of configuration space, Fig. 2a, by the discrete spectrum, Fig. 2b, in the internal region.

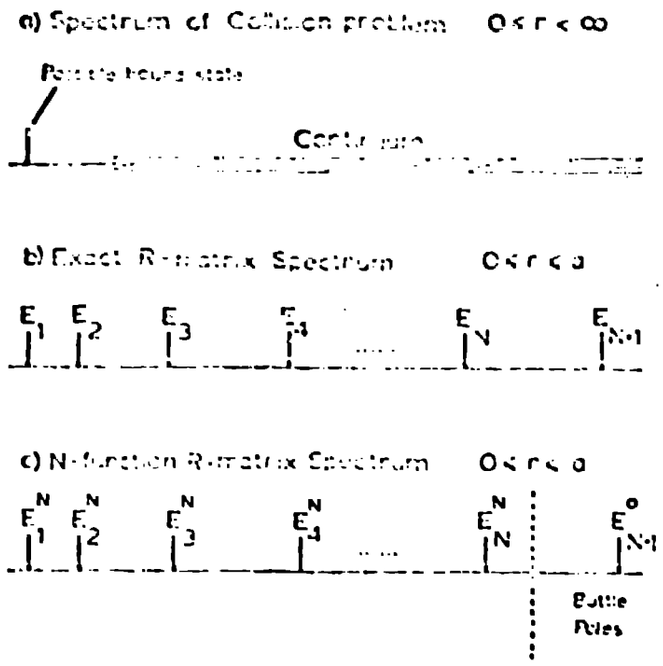

Fig. 2. R-matrix energy spectra.

3 Computation of the R-matrix

The main problem now is how to compute the R-matrix given by Eq. (2.10). Clearly we cannot deal with an infinite, albeit discrete, set of functions, and so as in most other atomic and molecular computations we have to obtain a finite representation of that set. In addition, it is not usually possible to solve the original Schroedinger equation exactly and so we must use

basis sets which satisfy some lower order, but physicaly significant, equation. The discussion in this section relates to these two problems and provides us an introduction to the practicalities of solving the multichannel problem.

Two approaches have been adopted, the first has obvious appeal to numerical integrators of coupled equations, while the second is a more natural approach for analytic basis set manipulators.

3a Expansion in an Orthogonal R-matrix Basis

Let us consider the eigensolutions of some simpler zero-order equation:

$$\left(\frac{d^2}{dr^2} + V_0(r) + k_{0\lambda}^2\right) V_\lambda^0(r) = 0 \tag{3.1}$$

subject to the same boundary conditions (2.4). We now approximate the first N eigensolutions $u_\lambda(r)$ of Eq. (2.3) by:

$$u_\lambda^{(N)}(r) = \sum_{\lambda'=1}^{N} c_{\lambda\lambda'}^{(N)} V_{\lambda'}^0(r) \qquad \lambda = 1, N \tag{3.2}$$

where the expansion coefficients $c_{\lambda\lambda'}^{(N)}$ are obtained by diagonalizing the symmetric matrix

$$H_{\lambda\lambda'}^{(N)} = -\int_0^a V_\lambda^0 \left(\frac{d^2}{dr^2} + V(r)\right) V_{\lambda'}^0 \, dr \qquad \lambda, \lambda' = 1, N \tag{3.3}$$

In matrix notation we can write

$$\underset{\sim}{c}^{(N)^T} \underset{\sim}{H}^{(N)} \underset{\sim}{c}^{(N)} = \underset{\sim}{k}^{(N)^2} \tag{3.4}$$

where $\underset{\sim}{k}^{(N)^2}$ is diagonal.

We now proceed by augmenting the N functions $u_\lambda^{(N)}(r)$ with the zero-order functions $V_\lambda^0(r)(\lambda = N + 1, \infty)$. For convenience we denote this whole set by $u_\lambda^{(N)}(r)$ and expand for the exact solution as:

$$F^{(N)}(k^2,r) = \sum_{\lambda=1}^{\infty} a_\lambda^{(N)}(k\ )\ u_\lambda^{(N)}(r) \tag{3.5}$$

The analysis proceeds as for Eqs. (2.6) through (2.11) where now we assume that the operator $\frac{d^2}{dr^2} + V(r)$ is diagonal in our basis $u_\lambda^{(N)}(r)$. This assumption introduces some error which however becomes small as N becomes large provided V_0 is chosen appropriately.

In practice the contribution from the k-matrix poles $\lambda = N + 1, \infty$ is added in by the procedure due to Battle [c]. Since the zero-order Eq. (3.1) can be solved exactly at the energy k^2, with solution V^0, we can write the exact expression for the R-matrix from Eq. (2.11) as

$$R^0 = \left[\frac{a}{V^0(a)} \left. \frac{dV^0}{dr} \right|_{r=a} - b \right]^{-1} \tag{3.6}$$

and the contribution from the poles $\lambda = N + 1, \infty$ is

$$R_C^{0(N)} = R^0 - \frac{1}{a} \sum_{\lambda=1}^{N} \frac{V_\lambda^{0^2}(a)}{k_{0\lambda}^2 - k^2} \tag{3.7}$$

This gives the total R-matrix within the representation of states $u_\lambda^{(N)}(r)$ as:

$$R^{(N)} = \frac{1}{a} \sum_{\lambda=1}^{N} \frac{\left[u_\lambda^{(N)}(a)\right]^2}{k^{(N)^2} - k^2} + R_C^{0(N)} \tag{3.8}$$

The effect of this finite set diagonalization is shown in Fig. 2c. The Hylleraas-Undheim Theorem tells us that the pole positions in Figs. 2b and 2c must satisfy

$$k_\lambda^{(N)^2} \geq k_\lambda^2 \tag{3.9}$$

Clearly the lowest $k_\lambda^{(N)^2}$ will converge on k_λ^2 fastest with increasing N, and so incident energies in their neighborhood will be best represented for small N values. From Eqs. (3.8) and (3.9) we see that $R \geq R^{(N)}$ and so from Eq. (2.13) the approximate phase shift δ^N approaches the exact phase shift δ from below. Such effective minimum principles in the orthogonal basis R-matrix methods are discussed in greater detail by Burke and Robb [3].

3b Expansion in an Arbitrary Basis Set

It is clear that the computation of the R-matrix in the region $0 \leq r \leq a$ as described above has many features of obtaining bound state configuration interaction wave functions. Namely, one has to compute a Hamiltonian matrix H in terms of some effectively finite range basis. When one comes to considering such a complex problem as electron-molecule scattering it would be foolish not to take advantage of the available bound state software available to evaluate Hamiltonian matrices in terms of arbitrary Slater-type-orbital (STO) of Gaussian-type-orbital (GTO) bases. We therefore consider the expansion of $F(k^2,r)$ in (1) in terms of such a basis set.

Bloch [2] has shown that the operator

$$\frac{d^2}{dr^2} + V(r) + L_b \tag{3.10}$$

where

$$L_b = \delta(r - a)\left[\frac{d}{dr} - b\right] \tag{3.11}$$

is Hermitian in the region $0 \leq r \leq a$ with respect to an arbitrary set of functions. We therefore introduce a complete set of functions u_λ satisfying

$$\left(\frac{d^2}{dr^2} + V(r) + L_b + k_\lambda^2\right)u_\lambda(r) = 0 \tag{3.12}$$

These functions $u_\lambda(r)$ may be expanded in terms of arbitrary functions, since the Bloch operator L_b guarantees that the $u_\lambda(r)$ satisfy the boundary condition (2.4) even though the expansion functions do not. We may then proceed as in the previous section to evaluate the R-matrix and phase shift.

In contrast to the method described in §3a the present approach may not require the inclusion of a contribution from distant levels to obtain reasonable convergence. The arbitrary basis can be chosen essentially to cover the whole interior configuration space and so the idea of "nearby" or "distant" levels is essentially lost.

4 Multichannel Electron-Atom and Electron Molecule Scattering Considerations

4a The Methods

The most important and most difficult effects to be allowed for in the interaction of an electron with an N-electron atom are electron-electron exchange and correlation. For the total (N + 1) electrons these occurs within the effective radius a of the charge distribution of the N-electrons. Outside this radius the scattered electron experiences only Coulomb and/or multipole moment and centrifugal terms in the interaction. Since these are reasonably weak and well behaved, solutions for $r \geq a$ can easily be obtained at most incident electron energies.

In the internal region, from what has been said above, we ideally should use bound-state configuration interaction type wave functions to deal with electron-electron exchange and correlation. Generalizing our earlier discussion of potential scattering we define a basis set of functions within each πLS of the (N + 1) electron system as

$$\Psi_k = \mathcal{A} \sum_{i\lambda} a_{i\lambda k}\, \Phi_i\, V_\lambda^0(r) + \sum_j b_{jk}\, \chi_j \tag{4.1}$$

where the Φ_i are functions representing the real- or pseudo-target states of interest coupled with functions representing the spin and angular motion of the scattered electron. The target states themselves may be represented by C.I. functions constructed from a bound orbital basis. The V_λ^0 are solutions of Eq. (3.1) with some appropriate zero-order potential, usually the static potential of the target ground state. They represent the radial motion of the scattered electron for $0 \leq r \leq a$, and are generated to be orthogonal to the bound orbitals of the same orbital angular momentum. $\mathcal{A}$ is the antisymmetrization operator which properly antisymmetrizes the (N + 1)-electron orbitals. The functions χ_j are (N + 1)-electron functions constructed from the bound orbital basis alone. They are included to complete the function space omitted by orbital orthogonality in the first term of Eq. (4.1), and to allow for further electron-electron correlation.

Since the basis orbitals satisfy the boundary conditions (2.4) they form a complete discrete set of functions, along with the bound orbitals, for each channel angular momentum ℓ. The functions Ψ_k are therefore a complete set of (N + 1)-electron functions and we may expand the wave function at any energy E as

$$\Psi_E = \sum_k A_{Ek}\, \Psi_k \tag{4.2}$$

We obtain the A_{Ek} by substituting Ψ_E into the Schroedinger equation

$$(H^{N+1} - E)\ \Psi_E = 0 \tag{4.3}$$

and writing a Greens equation s' lar to Eq. (2.6). Use of the boundary condition (2.4) and the fact that all relevant integrals reduce to those in the r_{N+1}th coordinate (since this is the only coordinate with finite surface terms) yields the multichannel forms of Eqs. (2.10) and (2.11) i.e.,

$$R_{ij}(E) = \frac{1}{2a} \sum_k \frac{W_{ik}(a)\ W_{jk}(a)}{E_k - E} \tag{4.4}$$

and

$$F_{ij}(E,a) = \sum_n R_{in}(E) \left(a \frac{dF_{nj}(E,r)}{dr} - b_n\ F_{nj}(E,r) \right)_{r=a} \tag{4.5}$$

where

$$W_{ik}(a) = \sum_\lambda a_{i\lambda k}\ V^0_\lambda(a) \tag{4.6}$$

The main problem remaining is the calculation of the Ψ_k and E_k. These quantities allow us to define the R-matrix by Eq. (4.4) and from Eq. (4.5) we obtain the multichannel K-matrix given by the wave function in the external region. Methods for determining this wave function have been adequately discussed [17] and programmed [18] by Norcross.

Two approaches have principally been used in atomic physics to obtain Ψ_k and E_k. In the first, adopted by Burke et al. [3] the Hamiltonian is divided into two parts

$$H^{N+1} = H_0 + H_{int} \tag{4.7}$$

where H_0 defines a zero-order potential problem in each channel, as per equation (2.1), which can be used to determine the orbitals $V_j^0(r)$. The coefficients a_{jkk} and b_{jk}, and eigenvalues E_k are determined by diagonalizing the Hamiltonian matrix

$$(\Psi_j | H^{N+1} | \Psi_k) = E_k \delta_{kk}. \tag{4.8}$$

Important advantages of this method are (a) that a single matrix diagonalization [illegible] (b) [illegible] be used to [illegible] R-matrix elements.

The [illegible] molecule [illegible] analytic [illegible] Bloch [illegible]

$$L_b = \frac{1}{2} \sum_i [illegible] \left(\frac{1}{[illegible]} - \frac{b}{[illegible]} \right) [illegible] \tag{4.9}$$

which [illegible] a Hermitian operator [illegible] prolate [illegible] STO basis on the nucleus and the center of mass of the target. The main advantage of these approaches is that analytic integrals can be performed rapidly, however, it is not clear as yet that in problems which involve several electronic states and/or significant electronic interchannel coupling, that such arbitrarily chosen bases will have satisfactory convergence and linear-independence properties.

Two other methods have been applied to limited cases in atomic physics. Fano and Lee [11] and Lee [14] have used an

eigenchannel approach to study the $e^- + Ar^+$ interaction in the photoionization of Ar. This method essentially adjusts the boundary conditions (2.4) in each channel so that an eigenvalue E_k falls at the energy E of interest. Shimamura [24] has indicated how this approach might be extended to problems with long-range potentials. Oberoi and Nesbet [19] have used another approach which essentially rewrites the equation for the A_{kk} as a set of linear equations at each energy E. Since the solution of a set of linear equations is much more rapid than the diagonalization of a matrix of equivalent dimension, this method may be much more rapid if only a few energies are required.

Further ideas for improvements in weaknesses in the above methods have been discussed in the literature. Shimamura [5] has shown how to obtain a continuous wave function at the R-matrix boundary from quantities currently evaluated in the theory, and Zvejnieks et al [20] have shown how to variationally correct the lower eigenvalues E_k of Eq. (4.5) for the effect of the highly nonlinear poles neglected in the finite matrix diagonalization.

4b Computational Aspects of the Methods

The major computational task in R-matrix methods is the calculation and diagonalization of a Hamiltonian matrix. This is equivalent to the problem of configuration interaction for bound states, and so the same well-tried analytic and numerical procedures and computer codes [11, 21] can be used. The methods are also remarkably free of numerical errors which can occur in direct numerical integration of the close-coupling equations, since they deal with integrals of basis functions which can be evaluated with high precision. Further we may easily add spin-orbit terms and other relativistic terms to the Hamiltonian since only a few additional integrals need be calculated.

Some comments about the practical aspects of using the orthogonal and arbitrary basis set methods are required. The

arbitrary basis method does not build any of the physics of the problem into the basis a priori. Rather it relies on using the simultaneous diagonalization and application of the Bloch operator to obtain accurate R-matrix eigensolutions, which may not however be sequential.

In contrast the orthogonal basis method builds essential physics into the potential V_0 and adds on eigensolutions sequentially. The methods therefore are analogous in character to the Multi-Configurational Hartree-Fock and Superposition of Configuration methods of bound state calculations, and it is to be expected that the arbitrary basis set should provide better lower eigensolutions than the equivalent sized orthogonal basis set. However there is danger of redundancy, linear dependence and omission of significant parts of function space in the arbitrary basis method which is not present in the orthogonal basis method.

5 Results from R-matrix Calculations

R-matrix methods have been used in atomic physics to calculate electron scattering cross-sections, dipole polarizabilities, photoionization cross sections, Van der Waals coefficients, free-free bremsstrahlung and optical harmonic coefficients. A review of this work has been given by Reed [5]. To facilitate quantitative illustration of some of the computational points discussed in the previous sections, we will restrict ourselves to these examples.

5a Elastic Scattering of Electron by Atomic Helium

Absolute values of elastic scattering phase shifts for atomic helium are required to serve as a measurement standard for future experiments. Berrington, et al. [1] have recently performed an R matrix calculation for electron-helium scattering in which they claim maximum errors of 1½% in the s-wave phase shift,

6% in the [illegible] phase shift, much less than [illegible] in higher partial wave phase shifts, and [illegible] in the total and momentum transfer cross-sections at [illegible] from [illegible] eV. To obtain these results

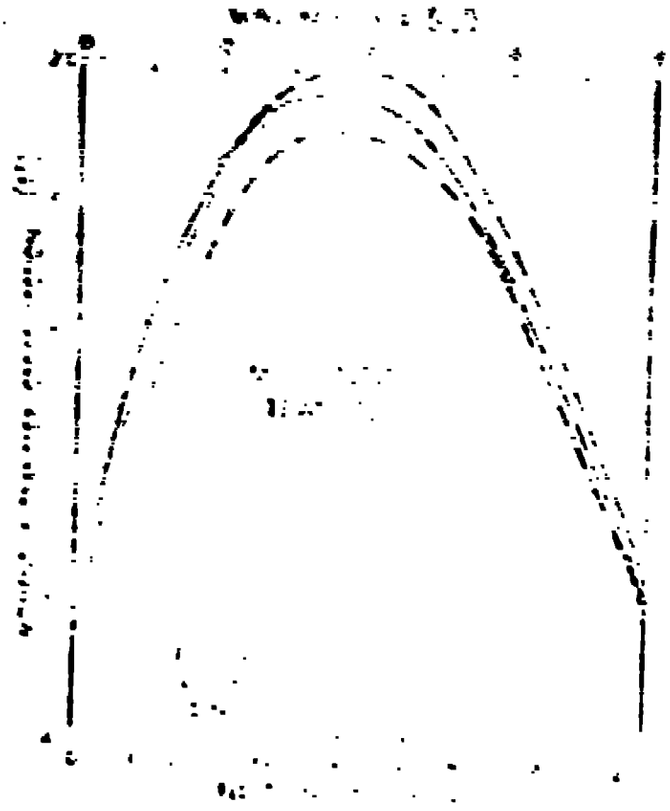

Fig. 3. [illegible] cross-sections for electron-helium scattering. The present results are those of [illegible] et al. [1], [illegible] of [illegible] lation [illegible] and [illegible] using less accurate target wave functions.

they used a ground state wave function which gave 98% of the ground state correlation energy, together with 2 ^1P and 3 ^1D pseudostates which gave the exact ground state dipole and quadrupole polarizabilities. In addition they added 10% and 10% of the three electron χ_j functions of Eq. (4.1) in the ^2S and $^2P^o$ symmetries, respectively, to allow as completely as possible for higher

channel couplings. Further, they adjusted the logarithmic derivative b_i in each channel to give most rapid convergence of the R-matrix basis set. Using the minimum principle discussed above and fitting of the phase shifts to effective range formulae, they are able to make estimates of both the magnitude and sign of the error in phase shifts and cross sections. We show a plot of the momentum tranfer cross section in Fig. 3. At all the energies here they provide their theoretical error estimate they obtain the correct sign, and at all energies they lie well within the ±2% experimental error bars.

5b Attachment Energies

An important development in the use of R-matrix theory has been the determination of bound state energies and wave functions for the (N + 1)-electron system. In this case we run the code as a collision problem with all channels closed, and look for the eigenvalues which give a continuous wave function at the R-matrix boundary. Some of the impressive results obtained by LeBourneuf [12] with this method are given in Table I for C^-, N^-, and O^-.

TABLE I

Attachment Energies (in eV) of Cargon, Nitrogen and Oxygen Atoms

	C^-		N^-	O^-
	$^4S^o$	$^2D^o$	$^3P^e$	$^2P^o$
Experiment	1.262	.035	-.050±.050?	1.462
R-matrix	1.228	.001	0.004	1.412
H.F	.550		-2.150	-0.542
B.G.	1.211	-.275	-0.582	0.963
S.O.C.	1.11		-0.52	1.13

This table clearly shows the limitations of the standard structure methods, such as Hartree-Fock (H.F.) [8], Bethe-Goldstone (B.G.) [16] and Superposition of Configurations (S.O.C.) For

example, the most extensive S.O.C. calculations of Sasaki and Yoshimine [22], which includes as many as 2649 configurations for O^-, has an error of 0.33 eV for O^- and nearly 0.5 eV for S^-. The R-matrix method, which is basically a collisional approach, concentrates directly on the energy difference between the target ground state and negative ion ground state, and in all cases is in reasonable agreement with experiment.

5c Photoionization of Atomic Aluminum

An important consequence of the last section is that for photoionization one can evaluate both the bound and continuum wave functions within the electron-plus-residual-ion framework, with the same basis functions, and thus treat both on the same footing (i.e., with the same correlation effects in both). In this way we can obtain accurate ionization threshold energies, and thus resonance positions, and can include the amount of correlation required to obtain good agreement between the length and velocity forms of the cross section. A particularly sensitive case is the open-shell atom Aluminum. For this case there is considerable configuration interaction in both the N- and (N + 1)-electron systems. In Fig. 4, we show the length photoionization spectrum from the R-matrix calculation of Le Dourneuf, et al. [13] compared with the experimental spectrum of Esteva, et al. [9]. The absolute magnitudes of the cross sections, not compared here, lie within a few percent of one another. It should be noted that the R-matrix calculation accurately represents the $^2D^e$ autoionization spectrum which is strongly perturbed by correlation χ_j functions such as $1s^2\ 2s^2\ 2p^6\ 3s\ 3p^2\ ^2D^e$.

7 Concluding Remarks

We can definitely say that R-matrix methods are an established useful tool for solving atomic scattering problems. However, these methods are still far from their final development. All of the above discussion has involved the solution of

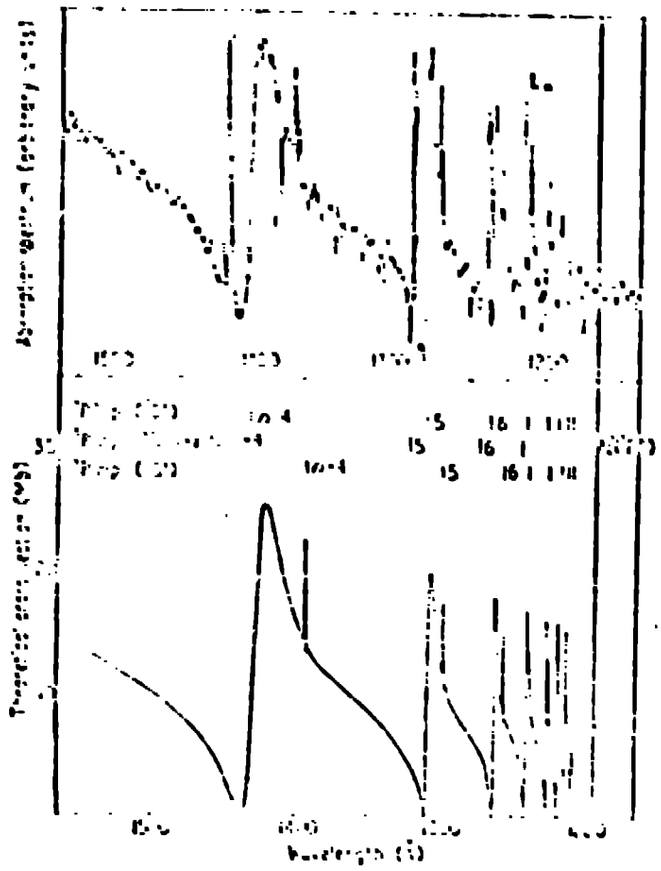

Fig. 4. Comparison of the length photoionization cross-section of Lebourgeois et al. [13] with the experimental results of Estevez et al. [9]. The energy scale has been adjusted so that the theoretical and experimental $Al^+(^1P^o)$ thresholds coincide.

coupled-channel problems in terms of uncoupled-channel bases. Many coupled channel zero-order problems are extremely tractable to solution, e.g., the no-exchange close-coupling equations, and could possibly provide much more rapidly convergent bases than those tried so far.

There is also the problem of two low energy electrons in the continuum. An R-matrix calculation should be particularly appropriate for this problem since the two electrons correlate with

the other electrons only when they are within the residual ion charge cloud, and outside of this region a correlated asymptotic form of their wave function has been discussed by Peterkop [20]. This subject has been discussed further by Fano and Inokuti [10].

Acknowledgements

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