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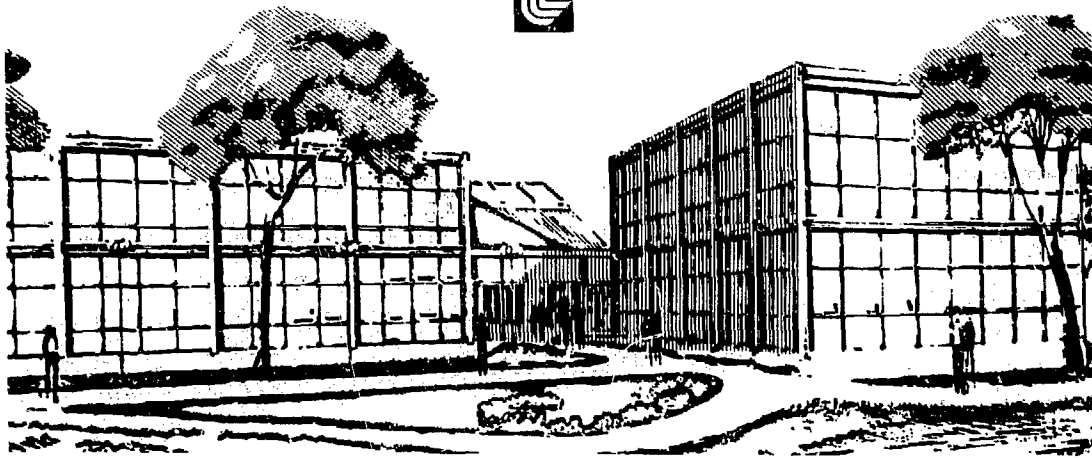
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This paper is a summary of the talk presented at the workshop on Electron- and Photon-Molecule Interactions, held in August 1978, at Asilomar, California.

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Stieltjes-Moment-Theory Technique for Calculating Resonance Widths*

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1. Introduction

Resonant autoionizing states of molecules and autodetaching states of molecular negative ions play important roles in many collision phenomena involving low energy electrons, e.g. dissociative attachment, associative and Penning ionization, dissociative recombination, etc.^{1,2} Although the formal theory³ of resonant scattering of electrons from molecules has been developed during the past 15 years, there have been very few quantitative studies of resonant phenomena even in diatomic molecules. The main reason for this has been the lack of practical methods for calculating the width of molecular resonances within the Born-Oppenheimer approximation.⁴ This situation has prevailed for quite some time, even though methods for calculating the resonance parameters of atoms⁵ and the potential energy curves of molecular resonances⁶ have been available.

In this talk, I will review a recently developed method⁷ for calculating the widths of atomic and molecular resonances. The method is based on the golden-rule definition of the resonance width, $\Gamma(E)$.⁸ The method uses only square-integrable, L^2 , basis functions to describe both the resonant and the non-resonant parts of the scattering wavefunction. It employs Stieltjes-moment-theory techniques⁹ to extract a continuous approximation for the width $\Gamma(E)$ from a discrete representation of the background continuum. Since the method utilizes L^2 basis functions exclusively, it has several advantages. Its

implementation requires only existing atomic and molecular structure codes. Many electron effects, such as correlation and polarization, are easily incorporated into the calculation of the width via configuration interaction techniques. Once the width, $\Gamma(E)$, has been determined, the energy shift⁸ can be computed by a straightforward evaluation of the required principal value integral. The main disadvantage of the method is that it provides only the total width of a resonance which decays into more than one channel in a multi-channel problem.

The remainder of the talk will be divided into two parts: a review of the various aspects of the theory (Section II) and a discussion of representative results which have been obtained with this method for several atomic and molecular resonances (Section III). Finally, I will give a brief summary (Section IV).

II. Theory

A. General Remarks

In Feshbach's theory of resonances⁸, the width of an isolated resonance which decays into a single open channel is defined according to the "golden-rule" formula:

$$\Gamma(E) = 2\pi |\langle \phi_r (H - E) \psi_E^+ \rangle|^2 \quad (1)$$

Here ϕ_r is a localized, L^2 function describing the resonance state. The function ψ_E^+ is an energy-normalized scattering function which represents the non-resonant, background continuum at energy E . The operator H is the full, many-electron Hamiltonian. For narrow resonances, the physical width is $\Gamma(E_r)$, where E_r is the resonance energy.

For molecular resonances, the resonance wavefunction ϕ_r can be computed using well-known techniques, e.g., the stabilization method⁶, which require only standard electronic structure codes. The calculation of the non-resonant wavefunction ψ_E^+ , however, is very difficult for molecules because of the non-spherical and non-local nature of the electron-molecule interaction potential. As a result, previous ab initio calculations of molecular resonance widths utilized very simple approximations for ψ_E^+ , e.g., uncoupled, undistorted Coulomb waves in the case of autoionizing states of neutral molecules like H_2^{10} and HeH .¹¹

One of the major advantages of the present method is that it allows for a more accurate description of the background continuum without sacrificing the computational simplicity inherent in the exclusive use of electronic structure codes. The method accomplishes this through the following essential features.

- (i) The scattering wavefunction is divided into resonant and non-resonant parts using appropriately defined projection operators Q_0 and P_0 .
- (ii) The resonance state is obtained as a discrete eigenstate of $Q_0 H Q_0$ in the usual way.
- (iii) The non-resonant scattering functions are expanded in terms of L^2 , many-electron basis functions.
- (IV) The width matrix-elements are calculated from the "golden-rule" formula.
- (V) Stieltjes-moment-theory techniques⁹ are employed to extract correctly normalized widths from the discrete representation of the background continuum.

B. Calculation of the Resonant and Non-resonant Wave Functions

For a given problem, one starts by selecting a suitable, orthonormal set of one electron basis functions. The choice of the one-electron orbitals is governed by the electronic structure of the target, the expected nature of the resonance under consideration, and the symmetry of the open-channel into which the resonance decays. (The optimization of the basis in stabilization calculations have been discussed previously.⁶) From the one-electron basis, one constructs all the many-electron configurations which will be eventually included in the total wavefunction. This set defines the total space $P_0 + Q_0$,

which, of course, must be incomplete in practice. Hopefully, the space $P_0 + Q_0$ is adequate to describe all the essential physics: the structure of the resonance, its energy and decay lifetime.

The projection operator P_0 is constructed from those configurations which provide a reasonably good approximation for the decay channel, i.e. the target + scattered electron. All the other configurations are included in the subspace Q_0 . This procedure is illustrated with a specific example in Table I, which shows the choice of configurations, and of the subspaces P_0 and Q_0 , for the $(1s\ 2s^2)^2S$ resonance of He^- . This resonance decays to the ground state of He, i.e., $\text{He}^- ({}^2S) \rightarrow \text{He} ({}^1S) + e (ks)$, and a large set of s-type functions must be used in order to accurately represent the scattered, s-wave electron. In this particular case, the SCF function $(1s^2)1S$ provides a sufficiently reasonable approximation for the target state so that only the "static-exchange-like" configurations $(1s^2s_n)$, $n = 1, 2, \dots$ need to be included in subspace P_0 . The resonance wave function ϕ_r , and the corresponding (unshifted) energy ϵ_r , are obtained by diagonalizing $Q_0 H Q_0$. For the choice of subspaces P_0 and Q_0 given in Table I, the $(1s\ 2s^2) \text{He}^-$ resonance corresponds to the lowest eigenvalue of $Q_0 H Q_0$, and the function ϕ_r includes electron correlation effects in the resonance state. However, it should be recognized that in other cases it may be necessary to include configurations constructed from more than one target configuration in the subspace P_0 .

In order to obtain an accurate representation of the non-resonant continuum in many-electron targets, two new projection operators P and Q are defined as

$$Q = \sum_i \phi_{ri} \langle \phi_{ri}$$

and

$$P = 1 - Q = P_0 + (Q_0 - Q)$$

The index i runs over all the resonances of a given symmetry under consideration, e.g., $2s2p$, $2s3p$, $3s2p$ $^1P^0$ in $e + He^+$, or $(1s2s^2)^2S$ in He^- , etc. It is important to note that P space contains not only those configurations which approximate the decay channel (originally in space P_0) but also the higher, non-resonant solutions of Q_0HQ_0 . I have found that this repartitioning of the spaces is essential to incorporate, as fully as possible, many electron correlation and polarization effects in the description of the non-resonant continuum. In the case of many-electron targets, such effects must be accounted for if accurate widths are to be obtained. For example, in the case of the 2S resonance of He^- , if one used only the original subspace P_0 (see Table I) to approximate the background continuum, one would neglect correlation in the $(1s^2)^1S$ target state and would treat the ejected electron only within the static-exchange approximation. In practice, such a procedure yields a width of about 14 meV compared to a more accurate value of 11.5 - 12 meV.^{7,12}

Once the projection operator P is defined, the discrete representation of the non-resonant continuum is obtained by diagonalizing PHP in the basis of all L^2 configurations which make-up the total space $P_0 + Q_0$. The resulting eigenfunctions satisfy

$$\langle \chi_n | PHP | \chi_m \rangle = \delta_{nm} \epsilon_n \quad (2)$$

and

$$\langle \chi_n | \chi_m \rangle = \delta_{nm} \quad (3)$$

All the solutions with non-zero eigenvalues are orthogonal to the resonance functions $\{\phi_{rj}\}$ by construction.

C. Calculation of the Resonance Widths

It is now recognized that the eigenvalues and the eigenfunctions which result from diagonalizing the Hamiltonian for a scattering problem in an L^2 basis will form a discrete representation of the scattering continuum. For sufficiently large basis sets, each solution χ_n approximates ψ_E^+ with $E = \epsilon_n$ in a region near the nuclei, except for an overall normalization factor. Since the "golden-rule" formula in Equation (1) contains the bound function ϕ_r localized near the nuclei,

the matrix element has no significant contribution from the asymptotic region where x_n fails to approximate ψ_E^+ .¹³ Consequently, it is possible¹⁴ to use $\{x_n\}$ to calculate the width matrix-elements:

$$\gamma_n = 2\pi |\langle \phi_r | H | x_n \rangle|^2 \quad (4)$$

However, x_n cannot be used directly to approximate $\Gamma(E = \epsilon_n)$ because x_n is unit-normalized [Equation (3)], whereas ψ_E^+ is energy normalized. To calculate the width, some way must be found to determine the normalization constant relating x_n and $\psi_{\epsilon_n}^+$.

The same problem occurs when one employs L^2 basis function to calculate continuum oscillator strengths or photoionization cross sections which describe transitions from bound initial states to continuum final states. In that case the work of Langhoff and coworkers have shown that accurate photoionization cross sections can be computed from variationally constructed, discrete pseudospectra employing Stieltjes moment theory.⁹ In the present context, the same technique is used to extract appropriately normalized resonance widths from the pseudospectrum $\{\gamma_n \epsilon_n\}$ defined in Equations (2)-(4).

It is useful to consider the so-called cumulative function $F(E)$ defined according to the equations:

$$F(E) = \int dE' \Gamma(E') \quad (5a)$$

$$\Gamma(E) = \frac{dF}{dE} \quad (5b)$$

The pseudospectrum $\{\gamma_n \epsilon_n\}$ associated with the non-resonant solutions of PHP defines a histogram approximation to $F(E)$:

$$\tilde{F}(E) = 0, \quad 0 \leq E \leq \epsilon_1 \quad (6a)$$

$$\tilde{F}(E) = \sum_{n=1}^k \gamma_n = \sum_{n=1}^k 2\pi |\langle \phi_r | H | \chi_n \rangle|^2, \quad \epsilon_k < E < \epsilon_{k+1} \quad (6b)$$

At the rise points, $E = \epsilon_k$, the cumulative function is approximated by

$$\begin{aligned} \tilde{F}(E) &= \frac{1}{2} [\tilde{F}(\epsilon_k^-) + \tilde{F}(\epsilon_k^+)] \\ &= \sum_{n=1}^{k-1} \gamma_n + \frac{1}{2} \gamma_k, \quad E = \epsilon_k \end{aligned} \quad (7)$$

It is interesting to compare the expression in Equation (6b) to the result that one would obtain by evaluating the integral in Equation (5a) using numerical quadrature, i.e.,

$$F(E) \approx 2\pi \sum_n \omega_n |\langle \phi_r | H | \psi_{E_n}^+ \rangle|^2 \quad (8)$$

where, E_n and ω_n are the quadrature points and weights. It is clear that in the Stieltjes development the non-resonant eigenvalues $\{\epsilon_n\}$ are used as the points associated with an equivalent quadrature.¹⁵ Furthermore, the normalization constants relating χ_n and $\psi_{\epsilon_n}^+$, $n = 1, 2, \dots$ determine implicitly the quadrature weights, ω_n .

The Stieltjes derivative of the histogram approximation to $F(E)$ is obtained as the slope of a straight line connecting the values of F at two neighboring rise points [Equation (7)]. The resulting histogram approximation for $\Gamma(E)$ has the form

$$\tilde{\Gamma}(E_k) = \frac{\gamma_k + \gamma_{k+1}}{2(\epsilon_{k+1} - \epsilon_k)} \quad k = 1, 2, \dots \quad (9)$$

where E_k are the half-way points $E_k = \frac{1}{2}(\epsilon_k + \epsilon_{k+1})$. The result in Equation (9) shows that the "correct" normalization constants associated with the discrete, non-resonant eigenfunctions χ_n are determined by the density of eigenvalues representing the continuous spectrum of PHP.

In actual computations employing Stieltjes imaging, one does not work, directly with the pseudospectrum

$$\{\gamma_n, \epsilon_n, n = 1 \dots N\}$$

Instead, one performs a moment analysis to obtain a "smoothed" spectrum

$$\{\bar{\gamma}_n^{(M)}, \bar{\epsilon}_n^{(M)}, n = 1 \dots M\}$$

whose elements are uniquely determined by the first $2M$, inverse power moments of the original pseudospectrum provided $M \leq N$. Usually, the calculations must be repeated for several values of M , ($M \ll N$) until mutually consistent results are obtained. The details of the moment analysis have already been discussed at this workshop by Peter Langhoff, so I will not discuss them further.

It should be noted, however, that to calculate the physical width of the resonance, $\Gamma(E_r)$, some interpolation of the Stieltjes values given in Equation (9) seems to be required. In the present work the approximate cumulative function given by Equation (7) was fitted to an appropriate analytic function of E which could be differentiated at any energy to yield $\Gamma(E)$.

In closing this discussion of the Stieltjes technique, I wish to point out that Hickman, Isaacson and Miller¹⁴ were the first to calculate resonance widths using L^2 approximations for the non-resonant wavefunction in the "golden-rule" formula. However, in their work, Hickman et al had to re-diagonalize PHP in different basis sets until one of the background eigenvalues ϵ_n came close to the resonance energy E_r . In addition, they used a "box-normalization" idea¹⁶ to normalize correctly the L^2 approximations to ψ_E^+ . In contrast, the Stieltjes-moment theory procedure provides both the required renormalization of the discrete eigenfunctions and the entire

non-resonant continuum in a single diagonalization of PHP. The latter feature makes the method practical even when very large CI matrices must be diagonalized to obtain accurate results for molecular resonances.

D. Calculation of Resonance Shifts

In Feshbach's theory of resonances⁸, the energy shift, $\Delta(E)$ of an isolated resonance is given by the principal value integral:

$$\Delta(E) = (2\pi)^{-1} P \int \frac{\Gamma(E')dE'}{E - E'} \quad (10)$$

For narrow resonances, the resonance energy E_r satisfies the equation:

$$E_r = \epsilon_r + \Delta(E_r)$$

where ϵ_r is the eigenvalue of $Q_0 H Q_0$.

The Stieltjes-moment-theory technique allows for calculating the shift, $\Delta(E)$, since it provides an approximation for not only the physical width, but also the width as a function of energy, i.e., $\Gamma(E)$. To obtain the results which I will show shortly for the ${}^2\Pi_g$ shape-resonance of N_2^- , $\Delta(E)$ was evaluated by using the histogram representation of $\Gamma(E)$ to approximate the integrand in Equation (10). In terms of the pseudospectrum $\{\gamma_n \epsilon_n\}$ representing the non-resonant continuum, this approximation yields the result:¹⁷

$$\tilde{\Delta}(E) = (2\pi)^{-1} \sum_{k=1}^M \tilde{\Gamma}(E_k) \omega_k \left| \frac{\epsilon_k - E}{\epsilon_{k+1} - E} \right| \quad (11)$$

where $\tilde{\Gamma}(E_k)$, $k = 1, 2, \dots$ are the Stieltjes values given by Equation (9).

III. Results

A. Atomic Resonances

The method which I have just described has been applied to several, well-known resonances in He, He⁻ and Mg for which previous calculations are available for comparison. Table II summarizes⁷ the computed resonance energies and widths. In these cases, moderately sized basis sets of 130-260 configurations were used to define the total space $P_0 + Q_0$. As the results for He and He⁻ show, the method is quite successful for core-excited, or Feshbach-type resonances. Accurate widths are obtained even for cases which involve many-electron targets e.g., He⁻ ²S, because polarization and correlation effects are included in the description of the non-resonant, background continuum. The method is applicable to higher resonances of a given symmetry; for example, accurate resonance parameters were obtained for the third lowest ¹P resonance below the $n = 3$ threshold in e + He⁺. The method can also be used for shape-resonances, although the definition of the projection operators P_0 and Q_0 are not as straightforward as in the case of

core-excited resonances. The width calculated for the $2p$ shape-resonance of Mg^- is quite encouraging since this is a very broad resonance close to threshold.

In closing, I wish to emphasize that the Stieltjes-moment-theory procedure is not designed to provide very precise widths for atomic resonances but it is intended for molecular problems where the implementation of other methods becomes prohibitively difficult.

B. 2_{Π_g} Shape-Resonance of N_2^-

The first molecular application of the method that I wish to discuss is the well-known, low-energy shape-resonance of N_2^- . This resonance has been studied extensively, and there are several recent static-exchange calculations²²⁻²⁵ from which the resonance parameters have been determined. The objective of the present calculations was not to obtain definitive results for N_2^- , but to test the Stieltjes-imaging procedure on a well-defined model for which several different methods have been used to determine r .

The present calculations were carried out in the static-exchange model, where the bound orbitals were taken from an SCF calculation of the $1_{\Sigma_g^+}$ ground state of N_2 . The one-electron, GTO basis set was augmented with up to 20 π_g orbitals to describe both the resonance and the non-resonant background. The calculations were repeated for several internuclear distances between 1.744 and 2.3916 bohr.

The computed resonance energies and widths are plotted as a function of internuclear distance in Figure 1. As I have mentioned before, in this case the energy shift, $\Delta(E)$, was computed utilizing the histogram approximation for $\Gamma(E)$ to evaluate the required principal value integral. The shift varied between -0.25 and -0.40 eV for the internuclear distances considered. The present resonance energies are somewhat higher than those obtained by Levin and McKoy²⁴ from the T-matrix calculations, except at $R = 2.3916$ bohr. At the equilibrium geometry, ($R = 2.068$ bohr) all the calculated widths, ≈ 1.2 eV, agree very well except the static-exchange result of Buckley and Burke.²² This discrepancy has been attributed²⁵ to the neglect of exchange with the $1\sigma_g$ and $1\sigma_u$ occupied orbitals in their calculations. The width obtained with the Stieltjes-imaging procedure increases smoothly with decreasing internuclear distance. However, significant discrepancies between the present widths and those Levin and McKoy²⁴ are observed for internuclear distances less than 2.068 bohr. The source of this discrepancy is not understood at this time. It should be recognized, however, that in the static-exchange model, the $2\Pi_g^-$ resonance of N_2^- is very broad and rather large uncertainties may be associated with the computed resonance parameters. In addition, for such broad resonances it is not trivial to extract unique E_r and Γ from the computed energy dependence of the eigenphase sums, as required in scattering calculations.

C. Core Excited Resonances of H_2

The Stieltjes technique for calculating resonance widths has been also applied to the lowest ${}^1\Pi_u$ and ${}^1\Sigma_u^+$ doubly-excited states of H_2 which are core-excited resonances associated with the repulsive, ${}^2\Sigma_u^+$ state of H_2^+ .

The $(1\sigma_u 1\pi_g) {}^1\Pi_u$ resonance decays to the ${}^2\Sigma_g^+$ ground state of H_2^+ and an ejected $k\pi_u$ electron. In this case, the total space $(P_0 + Q_0)$ included all 2-electron configurations constructed from a basis of $5\sigma_g$, $5\sigma_u$, $8\pi_g$ and $22\pi_u$ orbitals. The very large π_u basis set was required to describe accurately the non-resonant $1\sigma_g k\pi_u$ continuum. Since this ${}^1\Pi_u$ resonance decays into both the $p\pi_u$ ($\ell = 1$) and $f\pi_u$ ($\ell = 3$) components of the open channel, the present calculations were performed with two different π_u basis sets. In one case, the $f\pi_u$ molecular orbitals were constructed as linear combinations of $d\pi$ -GTO's centered on the two nuclei (basis 2c-d π); in the other case, they were chosen as $f\pi$ -GTO's on the center of the molecule (basis 1c-f π). The results of these calculations for $R = 2.0$ bohr are shown in Table III. The computed resonance energy agrees well with that obtained by Robb (private communication) in a 2-state close-coupling calculation. The present widths, 11-12 meV, are somewhat higher than his value of 8.0 meV. In order to test whether any of this difference is due to truncating the expansion to the lowest two states of H_2^+ ($1\sigma_g$ and $1\sigma_u$), we have repeated our calculations with only these sigma orbitals. As Table III shows the computed width decreased to 10.5 meV.

The current results for this particular resonance of H_2 shed some light on channel-coupling as it affects Stieltjes calculations of molecular continuum processes - an interesting question raised earlier by Hugh Kelly. As I already mentioned, the $(1\sigma_u 1\pi_g)^1\Pi_u$ resonance decays into both the $p\pi_u$ and $f\pi_u$ components of the open $(1\sigma_g k\pi_u)$ channel but with most of the flux going into the latter. Since our π_u basis contained both components, the resulting pseudo spectra $\{\gamma_n \epsilon_n\}$ consisted of successive pairs of one large and one small width-matrix elements, γ_n , in this case. The resulting cumulative function for orders 3-12 and the best analytic fit are shown in Figure 2. The data points, which correspond to Equation (7), clearly show oscillations which are due to alternating $p\pi$ and $f\pi$ non-resonant eigenfunctions in the spectrum of PHP. In such a case, one may use two procedures to obtain meaningful results. First, one can use only those Stieltjes values which are derived by solving the inverse moment problem for low orders. this procedure tends to smooth out the oscillations in the cumulative function, as illustrated in Figure 3, where only points from orders 3-7 are plotted. The widths given in the third column of Table III were obtained in this way. A second procedure is possible when each non-resonant eigenfunction can be uniquely associated with each of the channel components. In the present case, we divided the pseudospectrum into $p\pi$ and $f\pi$ components by inspecting each of the eigenfunctions, χ_n . Then, the two subspectra were imaged separately to yield the "partial" widths shown in the last column of Table III. The fact that the width

calculated with the first procedure (column 3) is consistent with the sum of the two "partial" widths (column 4) for each calculation is very encouraging and gives us confidence in the results.

As the last application, I wish to discuss briefly the widths calculated for the $(1\sigma_u 2\sigma_g)^1\Sigma_u^+$ resonance of H_2 . The dependence of the width on internuclear distance is uncertain for this resonance since two previous calculations,^{26,27} both using undistorted Coulomb waves for ψ_E^+ predicted totally different behavior. The Stieltjes calculations utilized all $^1\Sigma_u^+$ configurations constructed from a basis of $5\sigma_g$, $18\sigma_u$, $4\pi_u$ and $4\pi_g$ orbitals. Table IV shows the calculated resonance parameters for internuclear distances between 1.0 and 3.0 bohr. The present results confirm the conclusion of Kirby et al²⁷ that the width of this resonance is an increasing function of internuclear separation. However, the present widths, which were obtained by including both distortion and polarization effects in the description of the non-resonant continuum, are consistently higher than those calculated by Kirby et al using one- and two-center Coulomb waves (columns labelled "a" and "b", respectively) in the "golden-rule" formula. A recent, independent study of autoionizing states in $e + CH^+$ ²⁸ has shown that using undistorted, uncoupled Coulomb waves to describe the background continuum seriously underestimates the widths, at least, in that system.

IV. Summary

In this talk I have attempted to show that Stieltjes-moment-theory provides a practical and a reasonably accurate method for calculating the widths of atomic and molecular resonances. The method seems to possess a number of advantages for molecular applications, since it avoids the explicit construction of continuum wavefunctions. It is very simple to implement the technique for molecular resonances, because it requires only existing bound-state structure codes. Through the use of configuration interaction techniques, many electron correlation and polarization effects can be included in the description of both the resonance and the non-resonant background continuum. However, it is also clear that additional work is required to refine the method and to gain computational experience. In application to shape-resonances, the definition of the projection operators P_0 and Q_0 is somewhat ambiguous. The question of channel coupling and its effect on the computed widths need to be studied further. The criteria for choosing augmented GTO basis sets which can give uniformly accurate widths at several internuclear distances have not yet been established. Finally, the applicability of the method to resonances occurring in electron-polar molecule collisions needs to be investigated.

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Table I

Orbital Basis and Partitioning of Configurations for He (1s 2s²)²S

Orbital Basis: 1s, 2s, s₁, s₂, ... p₁, p₂, ... d₁, d₂, ...

1s: SCF orbital for He (1s²)¹S

2s: first approximation to resonance orbit

s_n, n = 1, 2, ... : adequate to describe both relaxation of
1s, 2s and the continuum orbital ks.

p_n, d_n, n = 1, 2, ... : adequate to describe correlation in target
and in the resonance state.

Configurations:

P ₀ :	1s 1s 2s	1s 1s s _n	n = 1, 2, ...
Q ₀ :	1s 2s 2s	s _n 2s 2s	1s 2s s _n 1s s _n s _n ' etc.
	1s p _n p _n '	2s p _n p _n '	s _n p _n ' p _n "
	1s d _n d _n '	2s d _n d _n '	s _n d _n ' d _n "
	p _n p _n ' d _n "		

Table II

COMPARISON OF COMPUTED RESONANCE PARAMETERS FOR ATOMS

<u>Resonance</u>	<u>Present Method</u>		<u>Previous Calculations</u>	
	<u>E_{res} (eV)</u>	<u>Γ (meV)</u>	<u>E_{res} (eV)</u>	<u>Γ (meV)</u>
He (2s2p) ³ P	58.31	8.3	58.30	8.4 ^a
			58.31	10 ^b
He (2s2p) ¹ P	60.19	36	60.13	38 ^c
			60.13	37 ^b
He (2s3p) ₊ ¹ P	63.67	8.3	63.68	8.0 ^a
He ⁻ (1s2s ²) ² S	19.40	11.5	19.40	12.1 ^a
			19.39	12.1 ^e
Mg ⁻ (3s ² 3p) ² P	--	200	0.15	230 ^f

^aBhatia and Temkin, Ref. 18

^dBain et al, Ref. 21

^bDrake and Dalgarno, Ref. 19

^eJunker and Huang, Ref. 12

^cBhatia et al, Ref. 20

^fRobb (unpublished)

Table III

WIDTH OF $H_2 (1\sigma_u 1\pi_g)^1\Pi_u$ STATE $R = 2.0$ bohr

Calculation	E_{res} (eV)	Γ (meV)	Γ (meV) "decoupled"
$5\sigma_g, 5\sigma_u, 8\pi_g, 22\pi_u (2c - d\pi)$	25.62	12.2 ± 0.5	10.1 2.3
$5\sigma_g, 5\sigma_u, 8\pi_g, 22\pi_u (1c - f\pi)$	25.62	11.1 ± 0.5	8.2 2.8
$1\sigma_g, 1\sigma_u, 3\pi_g, 22\pi_u (2c - d\pi)$	25.64	10.6 ± 0.5	7.7 3.0
$1\sigma_g, 1\sigma_u, 8\pi_g, 22\pi_u (1c - f\pi)$	25.64	10.5 ± 0.5	7.4 3.1
Robb's 2-state close-coupling	25.62	8.0 ± 0.1	6.9 1.1

Table IV

COMPARISON OF CALCULATED WIDTHS FOR $1\Sigma_u^+$ AUTOIONIZING STATE OF H_2

R(au)	E_r (eV)	Γ (eV)		
		Present	Previous Results	
1.0	39.46	0.22	0.17 ^a	0.17 ^b
1.4	30.71	0.40	0.29 ^a	0.29 ^b
1.8	25.54	0.65	0.38 ^a	0.37 ^b
2.0	23.71	0.74	0.43 ^a	0.40 ^b
2.5	20.55	0.88	0.56 ^a	0.48 ^b
3.0	18.67	1.05	0.70 ^a	0.54 ^b

^{a,b}K. Kirby, S. Guberman and A. Dalgarno, J. Chem. Phys., to be published.

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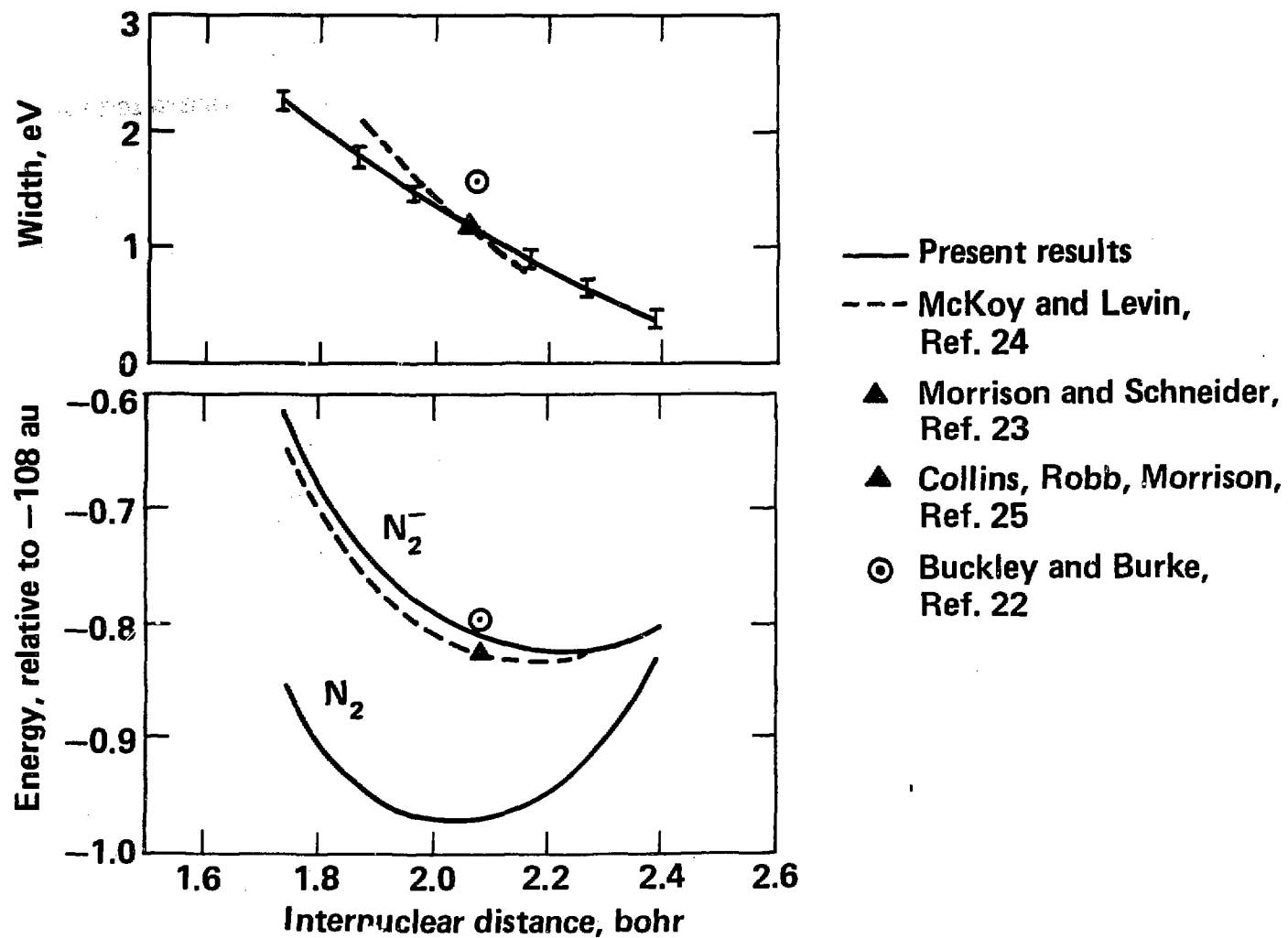


Figure 1

$H_2 (1\sigma_u 1\pi_g)^1 \Pi_u$ $R = 2.0$ bohr

CUMULATIVE FUNCTION FROM ORDERS 3 – N_{\max}

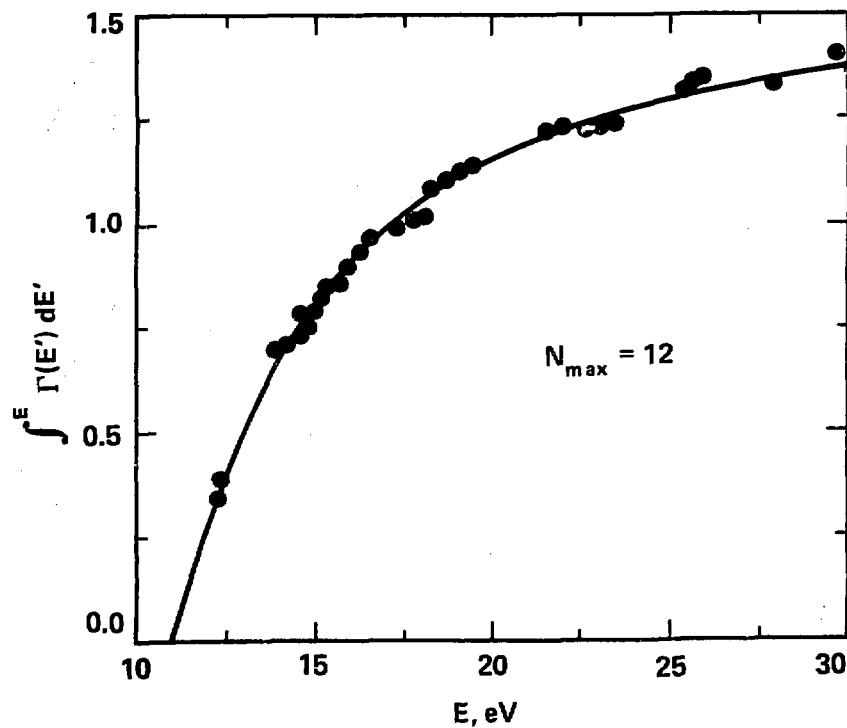
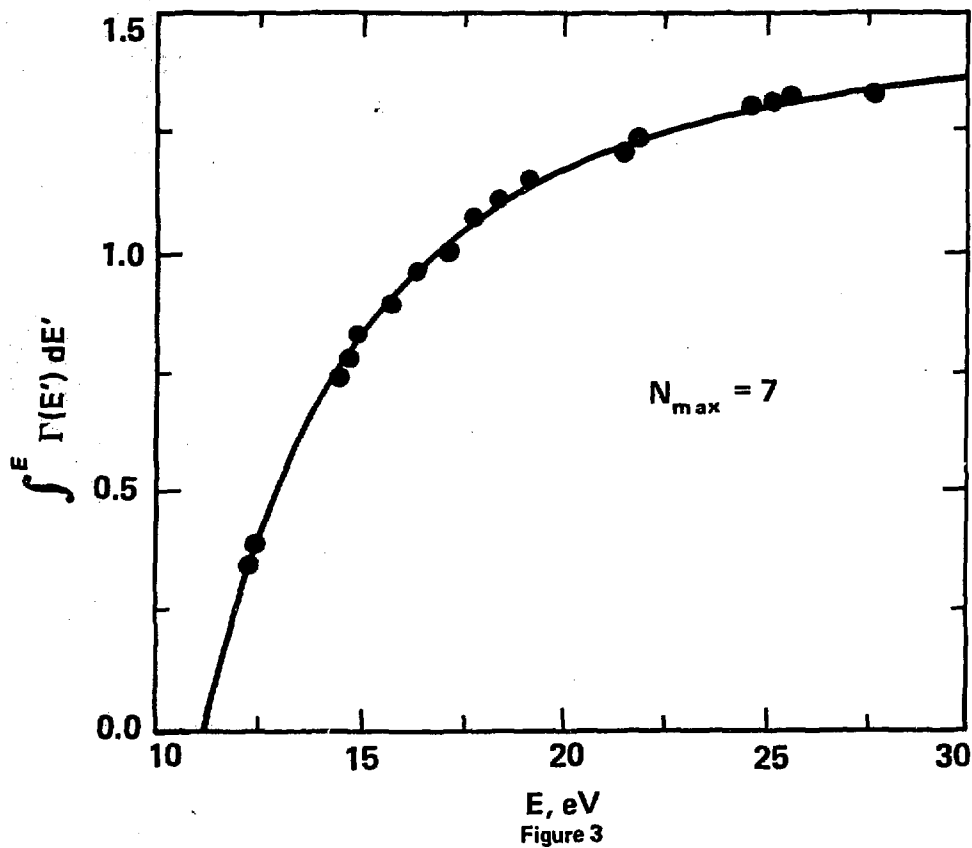


Figure 2

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$H_2 (1\sigma_u 1\pi_g) ^1\Pi_u$ $R = 2.0$ bohr

CUMULATIVE FUNCTION FROM ORDERS 3 - N_{max}



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