Linear algebraic approach to electronic excitation of atoms and molecules by electron impact

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A linear algebraic method, based on an integral equations formulation, is applied to the excitation of atoms and molecules by electron impact. Various schemes are devised for treating the one-electron terms that sometimes cause instabilities when directly incorporated into the solution matrix. These include introducing Lagrange undetermined multipliers and correlation terms. Good agreement between the method and other computational techniques is obtained for electron scattering for hydrogenic and Li-like atomic ions and for H_2^+ in two- to five-state close-coupling calculations.

I. INTRODUCTION

In a recent set of papers,[1–3] we have developed a linear algebraic (LA) method, based on the integral equations formulation, for solving the large sets of coupled integro-differential equations that commonly arise in the description of electron collisions with atoms and molecules. The basic idea underlying the LA approach is the conversion of a set of coupled integral equations to a set of LA equations by imposing a discrete quadrature on the integrals. The resulting set of *matrix* equations can then be handled by standard linear systems methods. The advantages of such an approach arise from its numerical stability, its simplicity and efficiency in incorporating nonlocal terms, and its compatability with the design strategy of the new vector computers. We have applied the technique[1,2] at the static-exchange (SE) level to a number of molecular systems, including H_2, N_2, CO_2, LiH, and LiF, employing both conventional and separable forms of the exchange terms. In addition, the method has been extended by means of an effective optical potential[3] to treat polarization effects in low-energy e-H_2 collisions. In this paper, we further explore the LA method by investigating electronic excitations of atoms and molecules. We develop the method along traditional lines in terms of a single-center coupled-states expansion. In this prescription, a set of coupled integro-differential equations for the scattering electron are derived by expanding the total system wave function in terms of a complete set of target states. The close-coupling (CC) approximation, by which the expansion is truncated at a finite number of terms, is invoked to yield a set of equations of finite order.

As a first test of the LA method for excitation processes, we apply it to electron collisions with hydrogenic and Li-like ions. This choice is particularly appropriate since numerous test cases[4–12] exist with which to compare and since the bound atomic wave functions are accurately known, so that discrepancies that may arise between the computational methods can be attributed to the collisional calculations, and not to differences in the bound basis. The literature on electron-atom collisions is massive and has been effectively reviewed by several authors.[4–8] We wish to emphasize here the other CC methods which have been applied to the electron-impact phenomenon. The four principal approaches are (1) the atomic R-matrix method,[9] (2) a linear algebraic approach (IMPACT) based on the differential equation,[10] (3) a noniterative integral equations method (NIEM),[11] and (4) a matrix variational scheme.[12] The second approach[10] is similar to the one developed here; the differences arise primarily from the choice of the form (integral or differential) of the scattering equations. In Sec. III, we make comparisons between the integral LA approach and those above-mentioned schemes for specific atomic systems.

For molecular excitation by electron impact the literature is much less extensive.[13–16] Until quite recently, the principal source for theoretical excitation cross sections was the Born approximation,[17] although very-low-energy collisions with H_2^+ had been investigated by the polarized-orbital method.[18(a)] Over the past few years, an impact-parameter method[18(b)] as well as a distorted-wave method[19] have been applied to several molecular systems including H_2, N_2, F_2, and CO. In addition, noniterative[20] and iterative[21] close-coupling procedures have been developed along with a multichannel variational scheme.[22] Still, the systems for which CC techniques have been applied are limited to H_2^+, H_2, and N_2. We apply the LA method to electron collisions with H_2^+ and examine the resonant structure below the $1\sigma_u$ threshold as well

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as the excitation cross section in both two- and four-state CC schemes.

We organize the paper along the following lines: Section II is devoted to the formulation of the excitation problem, Sec. III contains the results of calculations for e-atom and -molecule collisions as well as a discussion of these results, and Sec. IV gives a brief summary of our findings.

II. FORMULATION

In this section, we develop the basic formalism for describing electronic excitations of atoms and molecules by electron impact. We attempt to keep the presentation general and relegate to the Appendix the details of the specific forms of the scattering equations. We also draw extensively from our earlier paper[2] (referred to as paper I) on SE collisions and refer the reader, where appropriate, to more detailed discussions of the numerical procedures presented there.

A. Scattering equations

The Schrödinger equation, which describes the collision of an electron with an N-electron target system, has the form

$$(H_e+H_T-E)\Psi(\vec{r}_1,\ldots,\vec{r}_{N+1})=0\ , \tag{1}$$

where

$$H_e=h(N+1)+\sum_{i=1}^{N} g_{iN+1}\ , \tag{2a}$$

$$h(i)=-\tfrac{1}{2}\nabla_i^2-\sum_{a=1} Z_a g_{ia}\ , \tag{2b}$$

and

$$H_T=\sum_{i=1}^{N} h(i)+\sum_{i>j}^{N} g_{ij} \tag{2c}$$

with $g_{ij}=|\vec{r}_i-\vec{r}_j|^{-1}$ and with the sum in Eq. (2b) running over the number of nuclei. The first term H_e contains the kinetic energy operator for the incident electron and the electrostatic interaction of the incident electron with the target. The second term H_T represents the Hamiltonian for the target which possesses an eigenvalue spectrum $\{E_\alpha\}$ with eigenfunctions $\{\Phi_\alpha\}$ satisfying

$$(H_T-E_\alpha)\Phi_\alpha(\vec{r}_i,\ldots,\vec{r}_N)=0\ , \tag{3}$$

where α represents a set of target quantum numbers. The states (α) for atoms are usually labeled by a principal quantum number n, an orbital angular momentum quantum number p_α, and a spin s_α $(\alpha=np_\alpha s_\alpha)$, while for a linear molecule they are designated by the projection μ_α of the total orbital angular momentum on the internuclear axis, the parity ρ_α of the state, and a spin s_α $(\alpha=\mu_\alpha\rho_\alpha s_\alpha)$.

We reduce this many-particle equation to one involving only the continuum electron by (1) expanding the total system wave function in a complete set of target states $\{\Phi_\alpha\}$ as

$$\Psi(\vec{r}_1,\ldots,\vec{r}_{N+1})=A\sum_\alpha F_\alpha(\vec{r}_{N+1})\times\Phi_\alpha(\vec{r}_1,\ldots,\vec{r}_N)\ , \tag{4}$$

and (2) integrating over the coordinates of the target $d\vec{r}_1,\ldots,d\vec{r}_N$. In Eq. (4), F_α represents the continuum orbital, and the symbol A signifies that the total wave function is antisymmetric with respect to pair interchanges. The resulting set of coupled equations, whose solution is F_α, has the form

$$[h(\vec{R})-k_\alpha^2/2]F_\alpha(\vec{R})=\sum_{\alpha'}\int \hat{V}_{\alpha\alpha'}(\vec{R}\,|\,\vec{R}\,')F_{\alpha'}(\vec{R}\,')d\vec{R}\,'\ , \tag{5}$$

where $k_\alpha^2=2(E-E_\alpha)$ and

$$\hat{V}_{\alpha\alpha'}(\vec{R}\,|\,\vec{R}\,')=V_{\alpha\alpha'}(\vec{R})\delta(\vec{R}-\vec{R}\,')+W_{\alpha\alpha'}^{(2)}(\vec{R}\,|\,\vec{R}\,')+W_{\alpha\alpha'}^{(1)}(\vec{R}\,|\,\vec{R}\,')\ . \tag{6}$$

The general form of the terms in Eq. (6) are as follows:

$$V_{\alpha\alpha'}(\vec{R})\propto\int\Phi_\alpha(\vec{r})g_{12}\Phi_{\alpha'}(\vec{r})d\vec{r}\ , \tag{7a}$$

$$W_{\alpha\alpha'}^{(2)}(\vec{R}\,|\,\vec{R}\,')\propto\Phi_{\alpha'}(\vec{R})\Phi_\alpha(\vec{R}\,')g_{12}\ , \tag{7b}$$

$$W_{\alpha\alpha'}^{(1)}(\vec{R}\,|\,\vec{R}\,')\propto(E-E_\alpha-E_{\alpha'})\Phi_{\alpha'}(\vec{R})\Phi_\alpha(\vec{R}\,')\ , \tag{7c}$$

where $g_{12}=|\vec{R}-\vec{R}\,'|^{-1}$. The first term represents the static or direct interaction and depends only on the target-state wave functions. The second two terms, with the integral in Eq. (5) implicitly assumed, represent two- and one-electron exchange terms, respectively. In Eq. (7), the symbol $\vec{r}$ or $\vec{R}$, when associated with a bound orbital, represents all coordinates of the target system $(\vec{r}\equiv\vec{r}_1,\ldots,\vec{r}_N)$.

We now convert Eq. (5) to a set of coupled, radial integro-differential equations by (1) expanding the bound and continuum orbitals in a single-center expansion as

$$F_\alpha(\vec{R})=\sum_{l_\alpha} f_{\alpha l_\alpha m_\alpha}(R)Y_{l_\alpha m_\alpha}(\hat{R})R^{-1}\ , \tag{8a}$$

and

$$\Phi_\alpha(\vec{r})=\sum_{p_\alpha}\phi_{\alpha p_\alpha\mu_\alpha}(r)Y_{p_\alpha\mu_\alpha}(\hat{r})r^{-1}\ , \tag{8b}$$

and (2) integrating over the angular coordinates of the continuum electron $d\hat{R}$. The resulting set of

coupled equations has the form

$$L_\gamma f_{\gamma\gamma_0}(R)=\sum_{\gamma'}\int \hat{V}_{\gamma\gamma'}(R\mid R')f_{\gamma'\gamma_0}(R')dR' , \tag{9}$$

where

$$L_\gamma=d^2/dR^2-\frac{l_\alpha(l_\alpha+1)}{R^2}+k^2 , \tag{9'}$$

$$\hat{V}_{\gamma\gamma'}(R\mid R')=V_{\gamma\gamma'}(R)\delta(R-R')+W^{(2)}_{\gamma\gamma'}(R\mid R')+W^{(1)}_{\gamma\gamma'}(R\mid R') , \tag{9''}$$

and γ is a channel label of the form $\gamma=(\alpha,l_\alpha,m_\alpha)$, where l_α is the orbital angular momentum of the incident electron and m_α is the projection of total orbital angular momentum of the incident electron on the internuclear axis; the extra label γ_0 on f designates a specific linearly independent solution. The particular forms of V, $W^{(2)}$, and $W^{(1)}$ are given by Percival and Seaton[23] for hydrogenic ions, by Burke and Taylor[24] for Li-like ions, and in the Appendix for $H_2{}^+$. While the sums in Eqs. (4) and (8) run to infinity, this is not a practical limit for calculations. We, thus, invoke the close-coupling (CC) approximation and truncate Eq. (8a) at n_c terms, Eq. (8b) at n_b terms, and Eq. (4) at n_s states. The total number of channels N_c included in Eq. (9) is therefore given by $n_s\times n_c$. One more point is in order— Eq. (9) is referred to the body-fixed frame and derived within the fixed-nuclei approximation[18] for the molecular case.

Since our primary purpose to this juncture has been a general description of the excitation process, we have been somewhat insouciant about invoking symmetry constraints on the system wave function. While we can proceed with the solution of Eq. (9) without using symmetry, we would be rather foolish to ignore constraints that can simplify the computation. In the atomic cases we are considering, the total orbital L and spin S angular momenta the system are good quantum numbers. They are formed by vector coupling the orbital and spin angular momenta of the target $(\vec{p},\vec{s})$ and the continuum electron $(\vec{l},\vec{s}_c)$ as

$$\vec{L}=\vec{l}+\vec{p} ,$$

$$\vec{S}=\vec{s}+\vec{s}_c .$$

If we expand Ψ in a basis of eigenfunctions of L^2, L_z, S^2, and S_z, then the coupled equations (9) will be block diagonal in L and S. The appropriate basis is usually constructed from products of the target eigenfunctions and the angular and spin components of the continuum function F_α. In the molecular case, S is still a good quantum number as is the projection of $\vec{L}$ on the internuclear axis $\Lambda=m_\alpha+\mu_\alpha$. Again, the close-coupled equations (9) are block diagonal in a basis which consists of eigenfunctions of S^2, S_z, and L_z.

B. Linear algebraic method

We convert Eq. (9) to an integral equation by using the free-particle Green's function $G^0_\gamma(R\mid R')$ to obtain

$$f_{\gamma\gamma_0}(R)=\hat{j}_{l_\alpha}(k_\alpha R)+\sum_{\gamma}\int G^0_\gamma(R\mid\bar{R})\int \hat{V}_{\gamma\gamma'}(\bar{R}\mid R')f_{\gamma'\gamma_0}(R')\times dR'd\bar{R} , \tag{10}$$

where $\hat{j}_{l_\alpha}(\hat{n}_{l_\alpha})$ is the Ricatti-Bessel (-Neumann) function of order l_α for neutral targets and the regular (irregular) Coulomb function for ions. We introduce a quadrature of N_p points for the integrals, place the functions on a discrete mesh, and rearrange Eq. (10) to give

$$\sum_{\gamma' k}(\delta_{ik}\delta_{\gamma\gamma'}-M_{\gamma i,\gamma' k})f_{\gamma'\gamma_0}(k)=\hat{j}_\gamma(i)\delta_{\gamma\gamma_0} \tag{11a}$$

such that

$$M_{\gamma i,\gamma' k}=\sum_j G^0_\gamma(i\mid j)\hat{V}_{\gamma\gamma'}(j\mid k)w_j w_k , \tag{11b}$$

with (R_i,w_i) representing the set of points and weights for the quadratures, and $A(i)\equiv A(R_i)$. Equation (11) is just a matrix equation that can be written in the following compact notation:

$$\underline{M}\,\underline{f}=\underline{\hat{j}} , \tag{12}$$

where $\underline{M}$ is a matrix of order $N_p\times N_c$ $(=O_m)$, and $\underline{f}$ and $\underline{G}^1$ are matrices of size $O_m\times N_p$. We solve for $\underline{f}$ by standard linear systems routines. In fact, Eq. (11) remarkably resembles Eq. (I.10) with l replaced by γ. All of the powerful procedures and arcane lore developed in the context of the SE equations can be transferred directly to the solution of Eq. (12).

As noted in paper I, a more judicious choice of solution to Eq. (11) is the general R matrix $g_{\gamma\bar{\gamma}}(R\mid R_a)$ defined by

$$f_{\gamma\gamma_0}(R)=\sum_{\bar{\gamma}}g_{\gamma\bar{\gamma}}(R\mid R_a)\frac{\partial f_{\bar{\gamma}\gamma_0}}{\partial R}\bigg|_{R_a} \tag{13}$$

and determined by applying logarithmic boundary conditions on the solution at R_a. The advantage of this approach is that radial space can be divided into two regions. In the inner region $(R\le R_a)$, where exchange and static interactions are strong, the LA ap-

proach is used, while in the outer region ($R \geq R_a$), where the potential is weak and local (usually just a multipolar form), we use a standard propagation scheme such as the R-matrix propagator.[25]

From the solution in the asymptotic region, we can extract the K or T matrix, and from either construct the cross section. Asymptotically, the solution of Eq. (11) must become

$$f^{MS}_{\gamma\gamma_0}(R) \underset{R\to\infty}{\sim} \hat{j}_{l_\alpha}(k_\alpha R)\delta_{\gamma\gamma_0} + \left[\frac{k_{\alpha_0}}{k_\alpha}\right]^{1/2} \hat{n}_{l_\alpha}(k_\alpha R) K^{MS}_{\gamma\gamma_0} , \quad (14)$$

where $M = L$ (atoms) or Λ (molecules). At some very large distance from the target (R_m), we match the solution of Eq. (11) to this form and extract the K matrix. The cross section for excitation from state α to α' for an electron scattering from a target with a single electron in the valence orbital is given by

$$Q_{\alpha\alpha'} = \sum_{LS} Q^{LS}_{\alpha\alpha'} \quad (15a)$$

for atoms and

$$Q_{\alpha\alpha'} = \sum_{|\Lambda|=0} \sum_{S} (2-\delta_{\Lambda 0}) Q^{\Lambda S}_{\alpha\alpha'} \quad (15b)$$

for molecules, where

$$Q^{LS}_{\alpha\alpha'} = \tfrac{1}{4}\pi \sum_{l_\alpha l_{\alpha'}} \frac{(2L+1)(2S+1)}{(2p_\alpha+1)} |T_{\gamma\gamma'}|^2 ,$$

$$Q^{|\Lambda| S}_{\alpha\alpha'} = \tfrac{1}{4}\pi \sum_{l_\alpha l_{\alpha'}} (2S+1) |T_{\gamma\gamma'}|^2 ,$$

where p_α is the orbital angular momentum associated with the atomic state α.

C. One-electron terms

In examining the form of the two types of exchange terms in Eq. (9), one might be tempted to suspect that the two-electron terms $W^{(2)}$ would be the most difficult to handle numerically. Actually, these terms can be treated quite accurately and efficiently through conventional[1] or separable[1,2,26] procedures. Curiously, it is the one-electron terms $W^{(1)}$ that pose the most difficulty to obtaining an accurate, stable solution to Eq. (11).[4,27] To understand this, we must investigate the form of the one-electron terms in more detail. In order to accomplish this, we rearrange Eq. (11) by transferring to the left-hand side (lhs) all terms except the ones involving $W^{(1)}$ and defining the new lhs as $L_{\gamma\gamma'} f_{\gamma'}$. The resulting equation has the form

$$\sum_{\gamma'} L_{\gamma\gamma'} f_{\gamma'\gamma_0}(R) = \sum_{\gamma'} \int W^{(1)}_{\gamma\gamma'}(R \mid R') \times f_{\gamma'\gamma_0}(R') dR' .$$

We now consider a representative form for $W^{(1)}$ (see, e.g., the Appendix) and perform the integral over dR' to obtain

$$\sum_{\gamma'} L_{\gamma\gamma'} f_{\gamma'\gamma_0}(R) = \sum_{\alpha' l'_\alpha} C_{\alpha\alpha'} \Phi_{\alpha' l_\alpha}(R) \times \Delta(\Phi_{\alpha l'_\alpha} f_{\alpha' l'_\alpha}) , \quad (16)$$

where we have dropped the symmetry labels μ and m for convenience. In Eq. (16), $C_{\alpha\alpha'}$ is a constant, usually depending on energy, and

$$\Delta(AB) = \int A(r) B(r) dr .$$

There are four possible approaches to evaluating the effects of these one-electron terms on the solution: (1) delete them entirely, (2) include them directly in $\underline{M}$ [as in Eq. (11)], (3) replace them with Lagrange undetermined multipliers (LUM), or (4) replace them with correlation terms.

The first method is certainly the simplest, if perhaps not the wisest. We can demonstrate its shortcomings by considering e-H collisions at the SE level. For ^3S scattering, the bound and continuum electrons have their spins aligned. Therefore, the Pauli principle demands that the electrons occupy different spatial regions, and $\Delta(\Phi F)$ is formally zero. Dropping the one-electron term for ^3S scattering does not change the solution of the differential equations. However, for ^1S scattering, there is no such orthogonality restriction on $\Delta(\Phi F)$. In fact, the one-electron term must be retained in order to obtain the correct solution as has been demonstrated by Rescigno.[27(b)] Although dropping the one-electron terms entirely would be the simplest cure, it would lead to scattering equations of the wrong form. Thus we must continue our search for a method to treat these terms and embrace Hume's dictum that one must endeavor to palliate what he cannot cure.[28]

The second method, to include the one-electron terms directly in $\underline{M}$, is quite attractive since it involves introducing no new formalism. In fact, this procedure works quite well for electron-atom and -ion collisions. However, for e-molecule scattering in some symmetries, we observe an erratic behavior in the convergence of the cross section with number of channels. By including a large number of channels, this behavior can be damped, and convergence to the correct result observed. However, sometimes, more channels must be included to guarantee this damping than are actually needed to converge the

cross section by other prescriptions. Thus we must seek a more general procedure for handling these terms.

In the third method, which we use to produce most of the e-H_2^+ results, we replace the one-electron terms by LUM's. We rewrite Eq. (16) in the following form:

$$\sum_{\gamma'} L_{\gamma\gamma'} f_{\gamma'\gamma_0}(R) = \sum_{\alpha'} C_{\alpha\alpha'} \Phi_{\alpha' l_\alpha}(R) \lambda_{\gamma_0}^{\alpha\alpha'} , \tag{17a}$$

where

$$\lambda_{\gamma_0}^{\alpha\alpha'} = \sum_{l'_\alpha} \Delta(\phi_{\alpha l'_\alpha} f_{\alpha' l'_\alpha \gamma_0}) . \tag{17b}$$

We can readily demonstrate that Eq. (17a) is solved by a solution of the form

$$f_{\gamma\gamma_0}(R) = f^0_{\gamma\gamma_0}(R) + \sum_{\alpha''} P_\gamma^{\alpha''}(R) \lambda_{\gamma_0}^{\alpha\alpha''} , \tag{18a}$$

such that

$$\sum_{\gamma'} L_{\gamma\gamma'} f^0_{\gamma'\gamma_0}(R) = 0 \tag{18b}$$

and

$$\sum_{\gamma'} L_{\gamma\gamma'} P_{\gamma'}^{\alpha''} = C_{\alpha\alpha''} \Phi_{\alpha'' l_\alpha} . \tag{18c}$$

The LUM can be determined by substituting Eq. (18a) into (17b) to find

$$\sum_{\alpha''} (\delta_{\alpha'\alpha''} - D_{\alpha''}^{\alpha\alpha'}) \lambda_{\gamma_0}^{\alpha'\alpha''} = D_{\gamma_0}^{\alpha\alpha'} , \tag{19}$$

where

$$D_{\gamma_0}^{\alpha\alpha'} = \sum_{l'} \Delta(\phi_{\alpha l'} f^0_{\gamma'\gamma_0}) ,$$

$$D_{\alpha''}^{\alpha\alpha'} = \sum_{l'} \Delta(\phi_{\alpha l'} P_{\gamma'}^{\alpha''}) .$$

Equation (19) can then be solved simultaneously for the λ terms, and the new solution determined by Eq. (18a). This procedure is quite similar to ones developed in the context of an iterative method by Robb and Collins[29] at the SE level and by Robb[21] for excitation. Difficulties in this procedure can arise when several of the multipliers are equal. In this case the matrix in Eq. (19) can be singular, and no solution is found. To correct this, we simply solve for only the unique λ terms. Such cases are rather easy to spot for e-H_2^+, but may prove more subtle to detect for more complex systems.

The fourth method, to employ correlation terms instead of $W^{(1)}$, is the usual procedure employed in most e-atom collisional codes.[4] We start with the supposition that the bound and continuum orbitals are orthogonal. In the standard electron-ion collision codes,[9–12] this constraint is enforced by the introduction of Lagrangian undetermined multipliers much as in the previous discussion. For those scattering symmetries for which this is not true (e.g., e-H ^1S), we must augment the total system wave function with a correlation term that represents this omitted case. The form of the total system wave function then becomes [see Eq. (4)]

$$\Psi(\vec{r}_1, \ldots, \vec{r}_{N+1}) = A \sum_\alpha F_\alpha(\vec{r}_{N+1}) \Phi_\alpha(\vec{r}_1, .., \vec{r}_N) + \sum_n C_n \chi_n(\vec{r}_1, \ldots, \vec{r}_{N+1}) , \tag{20}$$

where $\Delta(\Phi_\alpha F_\alpha) = 0$ for all α, and χ_n is an antisymmetric $N+1$ electron function composed of the N-*electron* target functions $\Phi_\alpha(\Delta(\chi_n \chi_{n'}) = \delta_{nn'})$. For ^1S e-H scattering in the SE approximation, Ψ would have the form

$$\Psi(12) = \frac{1}{\sqrt{2}} [F(1)\phi_{1S}(2) + F(2)\phi_{1S}(1)] + C\phi_{1S}(1)\phi_{1S}(2) .$$

We have two basic unknowns—the continuum orbital F_α and the constants C_n multiplying the correlation functions. We derive a set of simultaneous equations for F_α and C_n by (1) multiplying Eq. (1) with Ψ given by Eq. (20) by $\Phi_\alpha^\dagger$, and integrating over the target coordinates, and (2) by multiplying Eq. (1) by $\chi_n^\dagger$ and integrating over *all* coordinates. The resulting set of coupled equations for e-H_2^+ collisions can be expressed as

$$[h(\vec{R}) - k_\alpha^2/2] F_\alpha(\vec{R}) - \sum_{\alpha'} \int \hat{V}'_{\alpha\alpha'}(\vec{R} \mid \vec{R}') F_{\alpha'}(\vec{R}') d\vec{R}' + \sum_n U_{\alpha n}(E_n \mid \vec{R}) C_n = 0 \tag{21a}$$

$$\sum_{\alpha'} \int U_{\alpha' n}(0 \mid \vec{R}') F_{\alpha'}(\vec{R}') d\vec{R}' + \sum_{n'} H_{nn'} C_{n'} = 0 , \tag{21b}$$

where

$$U_{\alpha n}(E_n \mid \vec{R}) \propto [E_n \delta_{\alpha n} + V_{\alpha n}(\vec{R})] \Phi_n(\vec{R}) , \tag{22a}$$

$$H_{nn'} \propto E_n \delta_{nn'} + \int \Phi_n^\dagger(\vec{R}) V_{nn'}(\vec{R}) \Phi_{n'}(\vec{R}) d\vec{R} , \tag{22b}$$

$\hat{V}_{\alpha\alpha'}$ is given by Eq. (6) with $W^{(1)} = 0$,

$$\chi_n(12) \propto [\phi_\beta(1)\phi_{\beta'}(2) + (-1)^S \phi_\beta(2)\phi_{B'}(1)] ,$$

and $E_n = (E_\beta + E_{\beta'} - E)$. The standard procedure for solving this set of equations is to eliminate C_n from Eq. (21a) by using Eq. (21b). We note that

both terms in Eq. (22) depend on known functions—the energy, the target eigenfunctions, and the interaction potential.

We have implemented this procedure for e-H_2^+ collisions and found results in excellent agreement with the LUM approach. In its present form, the only drawback of the correlation-function technique is its computational inefficiency. Most of these difficulties can be circumvented by incorporating these terms into the separable optical-potential method we have already developed for treating exchange and polarization.[3] Since the offending terms all involve bound-state orbitals, they are of finite range and can be calculated with well-developed techniques from quantum chemistry.

III. RESULTS AND DISCUSSION

Before proceeding to an exposition of our results for electron scattering from several atomic and molecular systems, we collect the relevant nomenclature introduced in Sec. II. We have made the following definitions:

(1) n_s is the number of states included in the CC expansion [Eq. (4)].

(2) n_c is the number of continuum partial waves per state [Eq. (8a)].

(3) n_b is the number of bound partial waves per state [Eq. (8b)].

(4) n_e is the number of continuum partial waves per state included in the exchange term.

(5) R_a is the radius at which the logarithmic boundary conditions are imposed.

(6) R_m is the asymptotic matching radius.

We use the notation n_sCC to designate an n_s-state close-coupling calculation.

In the case of electron scattering from hydrogenic and Li-like ions, some of these parameters are redundant. Since a given atomic state has only one associated particle wave (p_α), we have $n_b=1$. The set of coupled equations is determined by the number of states, the value of L—the total orbital angular momentum, and the value of S—the total spin angular momentum. For a given state and values of L and S, we include all continuum partial waves consistent with the triangular rule $|L-p_\alpha| \le l_\alpha \le |L+p_\alpha|$ and include all of these channels in the evaluation of the exchange term ($n_e=n_c$). For e-molecule collisions, all of these parameters are needed to specify a collisional calculation. The set of coupled equations to be solved are now determined by the number of states, the value of Λ, the projection of the total orbital angular momentum on the internuclear axis, and the value of S. For a given value of n_s, we systematically increase n_c, n_b, and n_e until a converged cross section is obtained. We then increase n_s and repeat the convergence method in partial-wave parameters. This procedure is continued until the cross section converges in n_s, n_c, n_b, and n_e.

A. Electron-atom (-ion) scattering

In order to test the LA method, we have calculated excitation cross sections for electron collisions with hydrogenic and Li-like ions. Our three-state close-coupling calculations ($1s$-$2s$-$2p$) for e-H and He^+ are in excellent agreement with those of other authors.[30,31] For Be^+ scattering, our 2CC ($1s^22s, 1s^22p$) and 5CC ($1s^22s, 2p, 3s, 3p, 3d$) results for the $2s$-$2p$ excitation cross section agreed well with those produced by the atomic R matrix, by IMPACT, and by a direct numerical propagation method.[32] Similarly, for e-O^{5+}, we produce excitation cross sections in excellent agreement with those of Bhadra and Henry[33] for a 5CC case. For the Li-like ions, we have used the Hartree-Fock target wave functions of Weiss.[34]

In order to demonstrate the level of agreement between the results obtained with the present LA method and various other techniques, we present in Table I selected K-matrix elements at $k^2=1.0$ Ry for e-Li collisions in a 2CC approximation. The agreement between the LA results and those of atomic R-matrix code[35] and those of the NIEM[36] approach is quite good. However, in some cases there are quite substantial differences with the K-matrix elements of Burke and Taylor[24] for $L \le 2$. For higher symmetries, all methods produce basically the same results. Norcross has shown that the very-low-energy ($k^2 \le 0.06$ Ry) results in the ^3S symmetry of Burke and Taylor are in error due to the "nonuniqueness" of their scattering solution.[27] We have performed LA calculations at these energies and obtain excellent agreement with Norcross in *all* symmetries including the ^3S. While it is difficult to determine the source of the other discrepancies between Burke and Taylor and the other methods, it is curious that these differences arise in precisely those symmetries that contain one-electron terms. These errors in the low-symmetry results of Burke and Taylor only slightly effect the value of the $2s$-$2p$ excitation cross section. Since this transition is optically allowed, the principal contribution to the cross section comes from higher symmetries. From these examples, we are encouraged to believe that the LA method is quite capable of handling a variety of atomic excitation problems.

TABLE I. Selected K-matrix elements for e-Li scattering at $k^2=1.0$ Ry in the 2 CC $(2s,2p)$ approximation.

LS	$K_{11}(L \mid L)$[a]	$K_{12}(L,L-1)$	$K_{22}(L-1,L-1)$
00	0.0760[b]	0.2944	0.3535
	0.0725[c]	0.2950	0.3630
	0.0753[d]	0.2966	0.3530
	0.0735[e]	0.2949	0.3564
11	1.8029	0.5205	0.1209
	1.8025	0.5183	0.1115
	1.8033	0.5210	0.1208
	1.8310	0.4782	0.1698
21	0.5574	0.3981	3.0730
	0.5563	0.3978	3.0214
	0.5569	0.3992	3.0820
	0.5644	0.5110	4.5137

[a] $|K_{ij}|$ presented; for $L=0$, $L+1$ instead of $L-1$.
[b]LAM, $R_a=20.0a_0$, $R_m=1000.0a_0$; 100-pt. mesh (25 pts. in each region: 0.0–0.1, 0.1–0.5, 0.5–1.5, 1.5–10.0, 10.–20.0a_0).
[c]R matrix (Refs. 35 and 9).
[d]NIEM (Refs. 36 and 11).
[e]NDEM (Ref. 24).

B. e-H_2^+ collisions

We have performed calculations for excitation of H_2^+ by electron impact in both two-state $(1\sigma_g,1\sigma_u)$ and four-state $(1\sigma_g,1\sigma_u,1\pi_u^+,1\pi_u^-)$ close-coupling approximations. The target states were represented by the linear combination of atomic orbitals–molecular orbital–self-consistent-field (LCAO-MO-SCF) wave functions determined by Cohen and Bardsley.[37] Each wave function employed a $1s\,2s\,2p$ STO basis with full variation of the linear and exponential coefficients. The energies calculated from this basis agree quite well with those of the exact H_2^+ wave function.[38] This basis gave a threshold energy of 0.868 Ry for excitation of the $1\sigma_u$ state and 1.34 Ry for the $1\pi_u$ state. We found that a Gauss-Legendre quadrature mesh of 45 points, distributed as follows: (1) 5 points, 0.0–0.5; (2) 20 points, 0.5–1.5; (3) 10 points, 1.5–3.0; and (4) 10 points, 3.0–10.0a_0, gave highly converged collisional parameters. We selected $R_a=10.0a_0$ and $R_m=100.0a_0$. At R_m, we matched to regular and irregular Coulomb functions. As noted before, all H_2^+ calculations were performed with the LUM representation of the one-electron terms. In Table II(a), we present a convergence study for the $1\sigma_g-1\sigma_u$ excitation cross section at two energies above the $1\sigma_u$ threshold at the equilibrium distance of 2.0a_0. A similar convergence trend is observed for the resonant parameters below the $1\sigma_u$ threshold. We note, as in the SE case, that the exchange terms converge in fewer partial waves than the solution to the coupled equations. The introduction of the π_u states changes the excitation cross section by less than 10%. However, between the $1\sigma_u$ and $1\pi_u$ thresholds, there will be resonances due to the closed $1\pi_u$ channels. Thus the 10% change at 0.9 Ry due to the π_u states is the enhancement of the background. In addition, we present in Table II(b) the results at a few selected symmetries of employing the correlation-term formulation; the agreement with the LUM results is excellent.

In Table III, we present the values for the positions (E_r) and widths (Γ) of selected resonances below the $1\sigma_u$ threshold. These parameters were determined by fitting a Breit-Wigner plus quadratic background form to the eigenphase sums calculated by the LA method. We compare with the calculations of Hazi,[39] who used a Stieltjes-moment-theory procedure, of Takagi and Nakamura,[22] who used a Kohn variational scheme, and with Bottcher and Docken,[40] who used a projection-operator technique which represents the target by a configuration-interaction (CI) wave function and the incident electron by a Coulomb wave. In general the agreement is quite good. Particularly encouraging are the results for the $^1\pi_u$ resonance, since adding the $1\pi_u$ states brings the width into much better agreement with Hazi. In Figs. 1 and 2 we present the width as a function of internuclear separation R for the $^1\Sigma_g$

TABLE II. (a) Convergence study of the excitation cross section $Q(1\sigma_g, 1\sigma_u)$ as a function of number of states and partial waves at $R_e = 2.0a_0$ for e-H_2^+ collisions. (b) Comparison of the LUM and correlation-term (COR) approaches for 2 CC e-H_2^+ scattering for the excitation cross section $1\sigma_g \rightarrow 1\sigma_u$ at 0.9 Ry.

	$Q^{AS}(1\sigma_g, 1\sigma_u)$ (a_0^2)						
States		2 CC				4 CC	
Channels							
k^2 (Ry)	2	3	4	4(3)	5(3)	2	3
				(a)			
0.90							
$^1\Sigma_g$	0.406	0.432	0.434	0.433	0.434	0.438	0.465
$^3\Sigma_g$	0.002	0.040	0.040	0.040	0.040	0.002	0.040
$^1\Sigma_u$	0.719	0.730	0.731	0.731	0.731	0.709	0.720
$^3\Sigma_u$	0.432	0.454	0.455	0.456	0.456	0.451	0.474
$^1\Pi_g$		0.555				0.499	0.496
2.00							
$^1\Sigma_g$	0.139	0.192	0.202	0.201	0.204	0.147	0.198
$^3\Sigma_g$	0.014	0.124	0.151	0.152	0.159	0.015	0.125
$^1\Sigma_u$	0.309	0.337	0.343	0.343	0.344	0.288	0.316
$^3\Sigma_u$	0.183	0.251	0.265	0.265	0.269	0.178	0.247
$^1\Pi_g$		0.199				0.182	0.191
n_s	2	2	2	2	2	4	4
n_c	2	3	4	4	5	2	3
n_e	2	3	4	3	3	2	3
n_b	2	3	4	3	3	2	3

	Symmetry n_s/n_c	LUM $Q(a_0^2)$	COR Q	H_{11}[a]
		(b)		
$^1\Sigma_g$				
	2/2	0.406	0.410	−0.895
	2/3	0.432	0.440	−0.891
$^3\Sigma_g$				
	2/2	0.0016	0.0016	−0.270
	2/3	0.0397	0.0397	−0.269
$^1\Sigma_u$				
	2/2	0.710	0.712	−0.020
	2/3	0.730	0.729	−0.023
$^3\Sigma_u$				
	2/2	0.432	0.435	−0.269
	2/3	0.454	0.454	−0.269

[a]Equation (22b) with E removed from E_n.

and $^1\Sigma_u$ symmetries, respectively. Again, our results with a 4 CC calculation are in good agreement with those of other CC-like calculations. The greater differences between the LAM and Kohn variational results away from equilibrium can probably be attributed to differences in the representations of the bound H_2^+ states. The differences between the LAM and the Stieltjes method are somewhat more difficult to explain. The Stieltjes approach incorporates more correlation while the LAM includes a better representation of the channel coupling. We are in the process of extending the optical-potential formulation[3] to H_2^+ collisions in hopes of resolving this disparity. We also note that the width changes by as much as 20% between the 2 CC and 4 CC calculations away from equilibrium. The rather stunning disagreement for $^1\Sigma_g$ scattering with the Bottcher and Docken results can probably be attributed to their rather crude approximation to the continuum wave function. Finally, in Table IV

TABLE III. Resonances below the $1\sigma_u$ threshold for e-H_2^+ scattering at $R_e = 2.0a_0$.

	Description	E_{res} (Ry)	Γ (Ry)
$^1\Sigma_g$	a	0.4438	0.102
	b	0.4420	0.104
	c	0.4321	0.114
	d	0.402	0.118
$^1\Sigma_u$	a	0.6245	0.048
	b	0.6255	0.049
	c	0.6228	0.049
	d	0.6273	0.052
	e	0.623	0.054
$^1\Pi_u$	b	0.7590	7.7(−4)
	c	0.758	8.7(−4)
	e	0.759	9.0(−4)
$^1\Pi_g$	c	0.6255	0.038

[a]LAM, $n_s=2$, $n_c=n_e=n_b=3$.
[b]LAM, $n_s=2$, $n_c=n_e=n_b=4$.
[c]LAM, $n_s=4$, $n_c=n_e=n_b=3$.
[d]Takagi and Nakamura (Ref. 22).
[e]Hazi (Ref. 39).

we present the total $1\sigma_g - 1\sigma_u$ excitation cross sections as a function of energy for e-H_2^+ collisions at $R=2.0a_0$. The results from the LA method for excitation of H_2^+ are indeed encouraging and warrant the extension of the method to more complex systems.

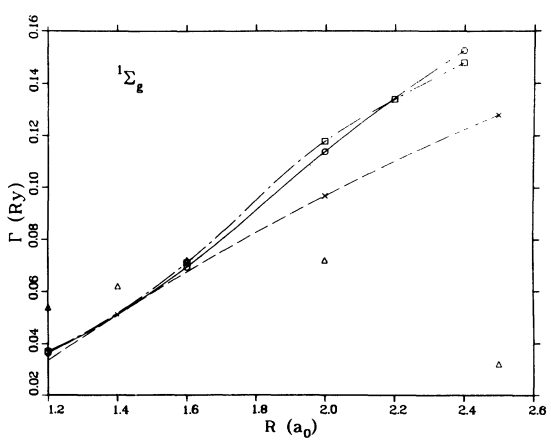

FIG. 1. Resonant width as a function of internuclear distance for the lowest $^1\Sigma_g$ resonance in e-H_2^+ scattering. Curves are labeled as follows: solid line (circle), present results (4 CC); chain dash (square), Kohn variational (Ref. 22); chain dot (cross), Stieltjes moment (Ref. 39); dot (triangle), projection operator (Ref. 40). Symbols represent the calculated points.

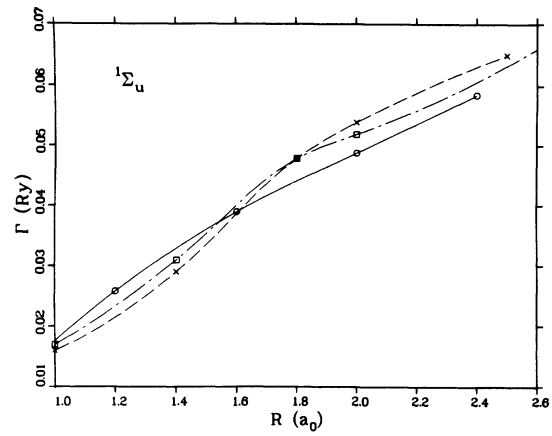

FIG. 2. Resonant width as a function of internuclear distance for lowest $^1\Sigma_u$ resonance in e-H_2^+ scattering. Curves labeled same as in Fig. 1.

IV. SUMMARY

We have extended a LA method to treat excitation of atoms and molecules by electron impact. The development is performed along traditional lines of obtaining a set of radial, coupled integro-differential equations for the scattering electron by making a single-center expansion of the system wave functions in terms of bound target states. This set of coupled equations is converted to an integral form which in turn is transformed to a set of linear algebraic equations whose solution is the continuum orbital at discrete values of the radial variable. This set of matrix equations is solved by standard linear systems routine. The method is particularly efficient in treating the nonlocal exchange terms and is well suited to the new vector computers. We find that we can transfer most of our lore at the SE level, such as choice of quadrature and distribution of meshes, directly to the excitation case. The one-electron terms, which provided no complications at the SE level or for atomic excitation, in certain cases, gave rise to instabilities in the e-molecule exci-

TABLE IV. Total excitation cross section $1\sigma_g \rightarrow 1\sigma_u$ e-H_2^+ scattering.

k^2	$Q(1\sigma_g \rightarrow 1\sigma_u)(a_0^2)$[a]
1.00	4.61
1.20	4.51
1.40	4.23
1.60	3.96
1.80	3.74
2.00	3.56

[a]$n_s=2$, $n_c=4$, $n_e=3$, $n_b=3$, $R_m=100.0$, $\Lambda_{max}=5$.

tation solution. This problem was circumvented by using Lagrange multipliers or correlation terms. Comparisons with some other calculations for excitations of hydrogenic and Li-like ions and of H_2^+ were quite encouraging since they showed remarkably good agreement. We are currently engaged in merging the coupled-states LA method with the effective optical-potential approach. On completion, this composite approach should allow for a systematic scheme for including the effects of high-lying states with little increase in storage in the collisional code.

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APPENDIX: e-H_2^+ SCATTERING EQUATION

We present the details of the form of the scattering equations for e-H_2^+ collisions in the single-center expansion. For e-H_2^+ collisions, we have a two-electron system and therefore the total system wave function must be either singlet or triplet. The form of the wave function in Eq. (4) is

$$\Psi(12)=\frac{1}{\sqrt{2}}\sum_{\alpha}[F_\alpha(1)\Phi_\alpha(2)+(-1)^S F_\alpha(2)\Phi_\alpha(1)]\,, \qquad \text{(A1)}$$

where $S=0$ (1) for singlet (triplet) symmetry. The close-coupling equations (9), then have the form

$$L_\gamma f_\gamma(R)=\sum_{\gamma'}\int[V_{\gamma\gamma'}(R)+W^{(2)}_{\gamma\gamma'}(R\mid R')+W^{(1)}_{\gamma\gamma'}(R\mid R')]f_{\gamma'}(R')dR'\,, \qquad \text{(A2)}$$

where

$$V_{\gamma\gamma'}(R)=[V^n_{\gamma\gamma'}(R)+V^e_{\gamma\gamma'}(R)]\delta(R-R')\,, \qquad \text{(A3)}$$

$$V^n_{\gamma\gamma'}(R)=\sum_{\lambda}C(l'_\alpha\lambda l_\alpha)\delta_{\alpha\alpha'}v^n_\lambda(R)\,,$$

$$v^n_\lambda(R)=-4(\rho_</\rho_>)^\lambda\rho_>^{-1}\,,$$

$$V^e_{\gamma\gamma'}(R)=2\sum_{\lambda\eta}C(l'_\alpha\lambda l_\alpha)v^{\alpha\alpha'}_{\lambda\eta}(R)\,,$$

$$v^{\alpha\alpha'}_{\lambda\eta}(R)=\sum_{P\alpha P\alpha'}C(p_{\alpha'}\lambda p_\alpha)(-1)^\eta y_\lambda(\phi_\alpha\phi_{\alpha'}\mid R)\,,$$

$$W^{(2)}_{\gamma\gamma'}(R\mid R')=2(-1)^S\times\sum_{\lambda\eta}\sum_{P\alpha P\alpha'}C(p_{\alpha'}\lambda l_\alpha)C(l'_\alpha\lambda p_\alpha)\times g_{\alpha\alpha'}(R\mid R')\,, \qquad \text{(A4)}$$

$$g_{\alpha\alpha'}(R\mid R')=\phi_{\alpha'}(R)\phi_\alpha(R')(r_</r_>)^\lambda r_>^{-1}\,,$$

$$W^{(1)}_{\gamma\gamma'}(R\mid R')=2(-1)^{S'}(E_\alpha+E_{\alpha'}-E)\times\phi_{\alpha'}(R)\phi_\alpha(R')\,, \qquad \text{(A5)}$$

with

$$y_\lambda(AB\mid R)=\int A(r)B(r)(r_</r_>)^\lambda r_>^{-1}\,,$$

$$r_<(r_>)=\min(\max)[r,R]\,,$$

$$\rho_<(\rho_>)=\min(\max)[R,R_\alpha].$$

The term C is a product of Clebsch-Gordan coefficients of the form

$$C(l_1l_2l_3)=(2l_1+1/2l_3+1)^{1/2}\times C(l_1l_2l_3\mid m_1m_2m_3)\times C(l_1l_2l_3\mid 000)\,.$$

The term $\gamma=(\alpha l_\alpha m_\alpha)$ labels a channel and $\alpha=(\mu_\alpha\rho_\alpha)$ labels a state. The total symmetry $\Lambda=m_\alpha+\mu_\alpha$ is a constant. The symbol $\phi_\alpha(r)$ is used to represent the radial expansion term $\phi^{u_\alpha}_{\alpha l_\alpha}(r)$ in Eqs. (A2)–(A5).

[1]B. I. Schneider and L. A. Collins, Phys. Rev. A 24, 1264 (1981).
[2]L. A. Collins and B. I. Schneider, Phys. Rev. A 24, 2387 (1981).
[3]B. I. Schneider and L. A. Collins, J. Phys. B 15, L334 (1982).
[4]P. G. Burke and M. J. Seaton, Math. Comput. Phys. 10, 1 (1971).
[5]R. K. Nesket, Adv. At. Mol. Phys. 13, 315 (1977).
[6]R. J. W. Henry, Phys. Rep. 68, 1 (1981).
[7]B. H. Bransden and M. R. C. McDowell, Phys. Rep. 30, 207 (1977).
[8]M. Rudge, Adv. At. Mol. Phys. 9, 48 (1973).
[9]K. A. Berrington, P. G. Burke, M. LeDeurneuf, W. D.

Robb, K. T. Taylor, and Vo Ky Lan, Comput. Phys. Commun. 14, 367 (1978).
[10]M. J. Seaton, J. Phys. B 7, 1817 (1974).
[11]E. R. Smith and R. J. W. Henry, Phys. Rev. A 7, 1585 (1973).
[12]R. K. Nesbet, Quant. Chem. 9, 215 (1978).
[13]N. F. Lane, Rev. Mod. Phys. 52, 29 (1980).
[14]P. G. Burke, Adv. At. Mol. Phys. 15, 471 (1979).
[15]B. D. Buckley, P. G. Burke, and C. J. Noble, Electron-Molecule Collisions (Plenum, New York) (in press).
[16]D. W. Norcross and L. A. Collins, Adv. At. Mol. Phys. (in press).
[17]S. Chung and C. C. Lin, Phys. Rev. A 6, 988 (1972); S. Chung, C. C. Lin, and E. T. P. Lee, *ibid.* 12, 1052 (1975); D. C. Cartwright, *ibid.* 5, 1331 (1972); S. P. Khare, Phys. Rev. 157, 107 (1967).
[18](a) A. Temkin and K. V. Vasavada, Phys. Rev. 160, 109 (1967); A. Temkin, K. V. Vasavada, E. S. Chang, and A. Silver, *ibid.* 186, 57 (1969); (b) A. Hazi, Phys. Rev. A 23, 2232 (1981).
[19]A. W. Fliflet and V. McKoy, Phys. Rev. A 21, 1863 (1980); A. W. Fliflet, V. McKoy, and T. N. Rescigno, J. Phys. B 12, 3281 (1979); L. Mu-Tao and V. McKoy, *ibid.* (in press).
[20]S. Chung and C. C. Lin, Phys. Rev. 17, 1874 (1978); T. M. Holley, S. Chung, C. C. Lin, and E. T. P. Lee, Phys. Rev. A 24, 2946 (1981).
[21]W. D. Robb (private communication).
[22]H. Takagi and H. Nakamura, J. Phys. B 13, 2619 (1980); *Proceedings of the Physics of Electronic and Atomic Collisions,* edited by S. Datz (ICPEAC, Gatlinburg, 1981), p. 457.
[23]I. C. Percival and M. J. Seaton, Proc. Cambridge, Philos. Soc. 53, 654 (1957).
[24]P. G. Burke and A. J. Taylor, J. Phys. B 2, 869 (1969).
[25]J. C. Light and R. B. Walker, J. Chem. Phys. 65, 4272 (1976).
[26]T. N. Rescigno and A. E. Orel, Phys. Rev. A 24, 1267 (1981).
[27](a) D. W. Norcross, J. Phys. B 4, 1458 (1981); 2, 1300 (1969); (b) T. N. Rescigno, J. Chem. Phys. 66, 5255 (1977).
[28]D. Hume, *Essays* (Longmans, London, 1875).
[29]W. D. Robb and L. A. Collins, Phys. Rev. A 22, 2474 (1980).
[30]P. G. Burke, H. M. Shey, and K. Smith, Phys. Rev. 129, 1258 (1963).
[31]P. G. Burke, D. D. McVicar, and K. Smith, Proc. Phys. Soc. London 83, 379 (1964).
[32]M. A. Hayes, D. W. Norcross, J. B. Mann, and W. D. Robb, J. Phys. B 10, L429 (1977).
[33]K. Bhadra and R. J. W. Henry, Phys. Rev. A (in press).
[34]A. W. Weiss, Astrophys. J. 138, 1262 (1963).
[35]W. D. Robb, local Los Alamos National Laboratory version of Ref. 9.
[36]R. J. W. Henry (private communication).
[37]J. S. Cohen and N. Bardsley (private communication).
[38]D. R. Bates, K. Ledsham, and A. L. Stewart, Proc. R. Soc. London 246, 28 (1953).
[39]A. Hazi, *Electron- and Photon-Molecule Collisions,* edited by T. Rescigno, V. McCoy, and B. Schneider (Plenum, New York, 1979), p. 281.
[40]C. Bottcher and K. Docken, J. Phys. B 7, L5 (1974).