Equivalent-local calculation of the continuum contributions to electron and positron reactions on atoms

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The target continuum has a large effect on electron and positron scattering to low-lying states of atoms. In addition to ionization the continuum of positron scattering includes positronium-formation channels. The equivalent-local coupled-channel-optical method is a numerically simple way of including the continuum in a coupled-channel calculation. Here it is tested by its prediction of total cross sections for continuum and discrete excitations on inert-gas targets.

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I. INTRODUCTION

The study of electron scattering to low-lying states of atoms has now reached the level of detail where all reaction channels must be taken into account in a calculation in order to achieve agreement with experiment. For a long time it has been possible to treat discrete channels to convergence by solving the corresponding coupled differential or integral equations or by the R-matrix method. Inclusion of continuum channels requires developments in methods.

The coupled-channel-optical (CCO) method [1] solves coupled integral equations for discrete channels (P space) to convergence using a coupling potential that includes an *ab initio* polarization part describing the excitation of the continuum. With different levels of detail the method has had broad success for atoms whose structure can be described by one or two active electrons, for example hydrogen, alkali-metal elements, helium, and magnesium. The convergent-close-coupling method [2] constructs a convergent discrete representation of the whole target space and solves the corresponding coupled integral equations. It has been applied to hydrogen, as have various basis-dependent pseudostate methods [3], and to sodium [4].

The implementation of the coupled-channel-optical method that has the widest applicability at this stage makes equivalent-local approximations [5] to the matrix elements of the polarization potential for computational feasibility. A first check on the validity of the method for a particular target is to calculate the total cross section for the target continuum. For electron projectiles this is the total ionization cross section. For positron projectiles we have in addition the total cross section for positronium formation.

The polarization potential matrix element describing excitation of the continuum contains amplitudes for excitation of a particular continuum state from each of the P-space states, integrated over the kinematic variables of the continuum. In the equivalent-local implementation this integration is performed by a multidimensional method [6] using Cartesian momentum variables. The excitation amplitudes must be approximated by analytic forms in order to calculate the integrand at several hundred thousand points. The total cross section for ionization or positronium formation is calculated by including the relevant polarization potential in a coupled-channel calculation

In the present work we check the equivalent-local polarization potential by comparing calculations of total ionization and positronium formation cross sections with experiment and other calculations. The primary objective is to obtain a polarization potential that has credibility in a coupled-channel-optical calculation, rather than to obtain the greatest possible refinement in calculating the continuum cross sections. However, an early form of the method [7] compared quite well with the distorted-wave Born approximation for total ionization cross sections in electron collisions with atoms or ions. It is interesting to see if good agreement with experiment can be obtained with the present method, which emphasizes detailed treatment of the coupling of important low-lying channels at the expense of the more approximate analytic treatment of the distorted-wave channel state.

II. DETAILS OF THE CALCULATION

The total cross section for excitation of the target continuum is calculated by solving the CCO equations [1]:

$$\langle \mathbf{k}i|T|0\mathbf{k}_0\rangle = \langle \mathbf{k}i|V^{(Q)}|0\mathbf{k}_0\rangle + \sum_{j\in P}\int d^3k' \langle \mathbf{k}i|V^{(Q)}|j\mathbf{k}'\rangle \frac{1}{E^{(+)}-\epsilon_j-\frac{1}{2}k'^2}\langle \mathbf{k}'j|T|0\mathbf{k}_0\rangle \ , \quad i\in P \ . \tag{1}$$

Here the space of target states has been split into two parts. The P space consists of all the discrete states $|i\rangle$ including the ground state $|0\rangle$. The Q space is the continuum. Sufficient P-space states are included for convergence at about the 1% level in the total cross section. The total cross section is calculated by the optical theorem, and the Q-space cross section is obtained by subtracting the integrated cross sections for the P space.

The optical potential $V^{(Q)}$ is the channel-coupling potential V plus a polarization potential $W^{(Q)}$ that describes the excitation of the part of the continuum being investigated.

The form used here for the matrix element of the polarization potential is

$$\langle \mathbf{k}'i|W^{(Q)}|j\mathbf{k}\rangle = \sum_{n\in Q}\langle \mathbf{k}'i|V|\Psi_n^{(-)}\rangle \frac{1}{E^{(+)}-E_n}\langle \Psi_n^{(-)}|V|j\mathbf{k}\rangle , \quad (2)$$

where $|\Psi_n^{(-)}\rangle$ represents the time reverse of the exact state vector for a reaction starting in channel n. The notation n is a discrete notation for the three-body ionization continuum or the two-body positronium rearrangement channels. Spin dependence is implicit in the notation. We use the LS-coupling representation for that which is due only to electron exchange.

The exact state vectors cannot be calculated. For ionization the model used is

$$|\Psi_n^{(-)}\rangle = |c\psi^{(-)}(\mathbf{q}_<)\mathbf{q}_>\rangle , \quad (3)$$

where $q_>$ and $q_<$ are the greater and lesser, respectively, of the absolute momenta of the outgoing particles. Ionization is described in the independent-particle model, where c is the remaining core and $\langle \mathbf{r}|\psi^{(-)}(\mathbf{q}_<)\rangle$ is a Coulomb wave orthogonalized to the orbital from which the electron is removed. If the slow particle is a positron there is no corresponding orbital, and the appropriate Coulomb wave is used. $\langle \mathbf{r}|\mathbf{q}_>\rangle$ is a plane wave. In this model there is an analytic form [8] for the direct potential matrix element. The exchange matrix element for the case of an incident electron has a similar analytic form in the equivalent-local approximation.

The model used for positronium formation is

$$|\Psi_n^{(-)}\rangle = |c\phi_\mu \mathbf{Q}\rangle , \quad (4)$$

where ϕ_μ is the state of positronium, and $\mathbf{Q}$ is the momentum of the positronium center of mass. The plane wave $\langle \mathbf{R}|\mathbf{Q}\rangle$ represents the motion of positronium quite well, since only short-range terms in the positronium-ion potential survive.

In addition to the equivalent-local approximation for the exchange amplitudes for an incident electron, a half-on-shell equivalent-local approximation is made for the whole polarization potential. This is necessary for computational feasibility. The polarization potential matrix element is calculated only at about ten points in the variable K, where

$$K = |\mathbf{k}-\mathbf{k}'| , \quad \tfrac{1}{2}k^2 = E-\epsilon_0 . \quad (5)$$

This is achieved by an angular-momentum projection

$$\langle \mathbf{k}'i|W^{(Q)}|j\mathbf{k}\rangle = \sum_{l''m''} C_{l'l''l}^{m'm''m} U_{l'l''l}(K) Y_{l''m''}(\hat{\mathbf{K}}) . \quad (6)$$

The calculation is done for the complex one-dimensional functions

$$U_{l'l''l}(K) = \sum_{m'm''} C_{l'l''l}^{m'm''m} \times \int d\hat{\mathbf{k}}\langle \mathbf{k}'i|W^{(Q)}|j\mathbf{k}\rangle i^{-l''} Y^*_{l''m''}(\hat{\mathbf{K}}) . \quad (7)$$

Cubic spline interpolation is used for general values of K.

A simple estimate [1] of the total cross section for exciting states of Q space is given, instead of including all the states of P space in solving the equations (1), by approximating the entrance-channel T-matrix element of (1) by its driving term. This results in

$$\sigma_Q = (2/k)(2\pi)^3 \mathrm{Im}\langle \mathbf{k}0|W^{(Q)}|0\mathbf{k}\rangle . \quad (8)$$

III. EFFECT OF DISCRETE INELASTIC CHANNELS ON CONTINUUM CALCULATIONS

In order to use the predictions of total cross sections σ_Q for different parts of Q space to test the validity of the corresponding optical potential, it may be consistent with the rough validity of all the approximations to calculation σ_Q by the estimate (8) rather than the full solution of (1).

We compare the two methods for the case of positron scattering on helium, where P space includes the lowest ten states. They are $1,2,3\,^1S$; $2,3\,^1P$; $3\,^1D$, $2,3\,^3S$; and $2,3\,^3P$. The configuration-interaction calculation of these states is based on eight orbitals, namely $1,2,3,4s$; $2,3,4p$; $3d$; and the pseudo-orbitals $\bar{s},\bar{p},\bar{d}$ [9]. The CCO calculation includes polarization potentials in the couplings $1\,^1S-1\,^1S$, $1\,^1S-2\,^1P$, $2\,^1S-2\,^1S$, and $2\,^1P-2\,^1P$. Note that triplet states cannot be excited by positrons, since they require the exchange mechanism.

The comparison is shown in Table I. For both the total ionization σ_I and positronium-formation σ_{Ps} cross sections the estimate (8) is quite close to the more detailed calculation. For σ_{Ps} we calculate the formation of positronium in its $n=1$ and 2 states. According to the close-coupling calculations of Hewitt, Noble, and Bransden [10], this is about 90% of the total.

IV. CROSS SECTIONS FOR HELIUM

The CCO model has been quite successful [11] in calculating total cross sections for sodium and potassium, where the continuum is weakly excited. In the case of helium, continuum cross sections form a large fraction of

TABLE I. Comparison of the Q-space cross sections for the ten-channel positron-helium problem calculated by the CCO method and Eq. (8).

	σ_i (units of πa_0^2)		σ_{Ps} (units of πa_0^2)	
E (eV)	CCO	Eq. (8)	CCO	Eq. (8)
30	0.11	0.06	0.89	0.54
40	0.22	0.25	0.70	0.66
50	0.35	0.35	0.57	0.59
75	0.52	0.50	0.32	0.33
100	0.57	0.50	0.16	0.17
200	0.48	0.53	0.04	0.02

TABLE II. Comparison of theoretical estimates of the total scattering σ_{sc} and total ionization σ_I cross sections for electron-helium interaction with the semiempirical estimates of de Heer and Jansen [12]. Units are πa_0^2. Errors in the final significant figures are shown in parentheses.

E (eV)	σ_I (expt)	σ_I (CCO)	σ_{sc} (expt)	σ_{sc} (CCO)	σ_{sc} (CC)
30	0.074(3)	0.194	2.73(19)	2.83	2.54
40	0.192(7)	0.316	2.12(14)	2.22	
50	0.269(10)	0.412	1.79(13)	1.81	1.63
80	0.374(14)	0.529	1.12(7)	1.12	1.02
100	0.391(18)	0.556	0.90(5)	1.00	0.84
200	0.358(16)	0.419	0.48(3)	0.50	

the total cross section, which significantly tests the modeling of the continuum.

We test the description of the ionization continuum for electron scattering by comparing the total ionization cross section σ_I calculated by the CCO method, as described in Sec. III, with experiment. This comparison is shown in the second and third columns of Table II. σ_I is calculated by subtracting the total scattering cross section for the ten channels of P space σ_{sc} from the total cross section σ_T obtained from the optical theorem. It is significantly too large.

The last three columns of Table II test whether the overestimate of the Q-space cross section invalidates the description of the continuum for calculations of the P-space excitation. The calculation of σ_{sc} by the CCO method agrees closely with the semiempirical estimates of de Heer and Jansen [12], and is better than the ten-state coupled-channels (CC) method, which omits the continuum.

For positrons we test the description of the ionization and positronium-formation continuum by the CCO method. The total ionization cross section σ_I and the total positronium-formation cross section σ_{Ps} are compared with experiment in Tables III and IV, respectively. In both cases calculated and experimental values are quite close above about 50 eV. For σ_I the present model is better for positrons than electrons. The major difference is the presence of exchange amplitudes for electrons. The equivalent local approximation is quite rough for these amplitudes. For σ_{Ps} the present model is in semiquantitative agreement with the experiments, and with the close-coupling approximation of Hewitt, Noble, and Bransden [10].

TABLE III. Comparison of the CCO calculation of the total ionization cross section σ_I for positron-helium interaction with experiment. Units are πa_0^2. Expt. 1: data of Fromme *et al.* [13]. Expt. 2: data of Knudsen *et al.* [14]. Errors in the final significant figures are shown in parentheses.

Energy (eV)	Expt. 1	Expt. 2	CCO
30	0.058(6)	0.033(7)	0.11
40	0.222(26)	0.174(17)	0.25
60	0.415(49)		0.42
100	0.501(60)	0.596(56)	0.60
200	0.444(52)	0.444(50)	0.53

TABLE IV. Total positronium-formation cross section for helium. Column headings are as follows. Expt 1: experiment of Fromme *et al.* [13]. Expt. 2: experiment of Diana *et al.* [15] (energy interpolations of a few eV are made in the data). CCA: close-coupling approximation of Hewitt, Noble, and Bransden [10]. Units are πa_0^2.

Energy (eV)	Expt. 1	Expt. 2	CCA	Eq. (8)
30	0.43(5)		0.45	0.542
40	0.49(5)		0.463	0.658
50	0.49(5)	0.53(7)	0.340	0.586
80	0.36(4)	0.27(12)	0.237	0.287
100	0.31(4)	0.20(4)	0.200	0.173
200	0.10(4)	0.04(4)	0.014	0.022

V. TOTAL IONIZATION CROSS SECTION FOR INERT GASES

The total ionization cross section for both electron and positron impact has been calculated for He, Ne, Ar, Kr, and Xe. In the case of inert-gas atoms larger than helium it is difficult to model the excited states accurately. We therefore estimate continuum cross sections by Eq. (8). This is justified for helium in Sec. III. Hartree-Fock or-

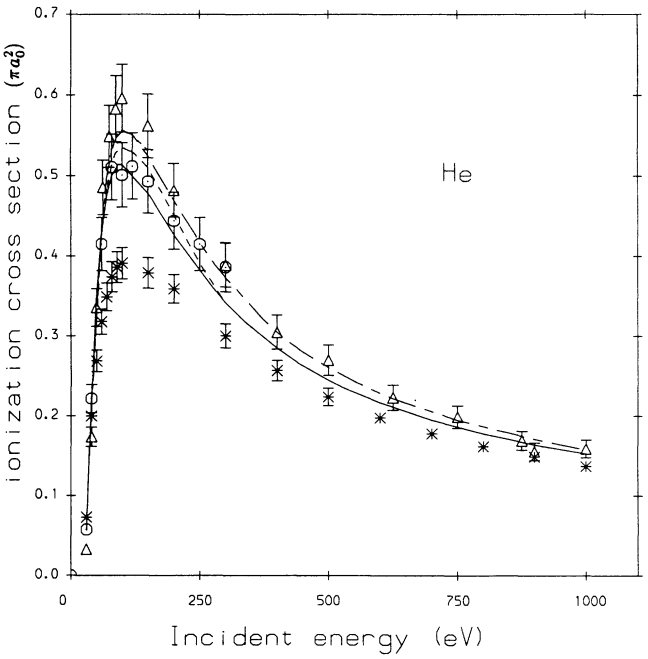

FIG. 1. Total ionization cross section (units of πa_0^2) for electron and positron impact on helium. Experimental data for positrons are due to Fromme *et al.* [13] (circles) and Knudsen *et al.* [14] (triangles). For electrons the data (asterisks) are due to de Heer and Jansen [12]. Solid curve: present calculation for positrons; short-dashed curve: positron calculation of Campeanu, McEachran, and Stauffer [16]; and chain curve: present calculation for electrons.

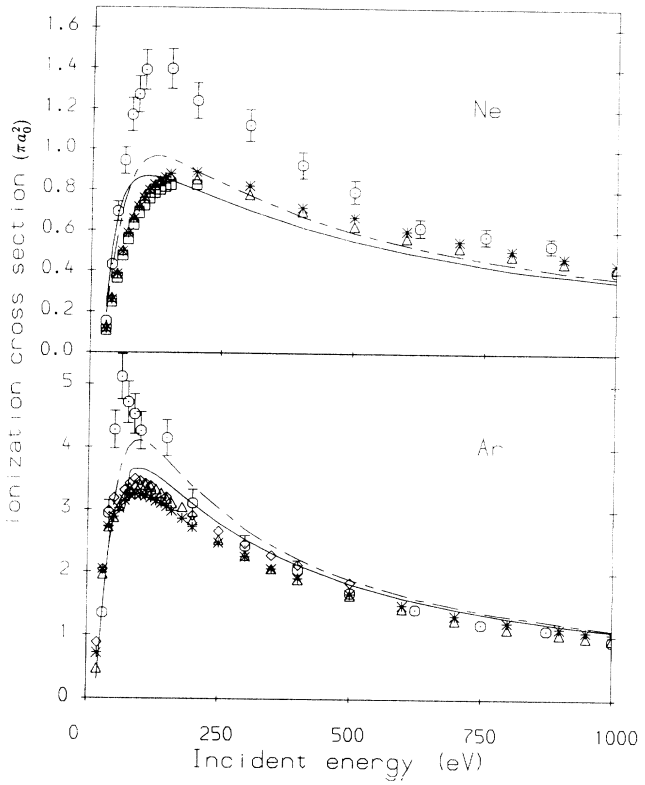

FIG. 2. Total ionization cross section (πa_0^2) for electron and positron impact on neon and argon. Circles represent the positron data of Knudsen *et al.* [14]. For electrons the data are represented by asterisks: Rapp and Englander-Golden [17]; triangles: Krishnakumar and Srivastava [18]; and diamonds: Fletcher and Cowling [19]. The present calculation is represented by a chain curve: positrons; and a solid curve: electrons.

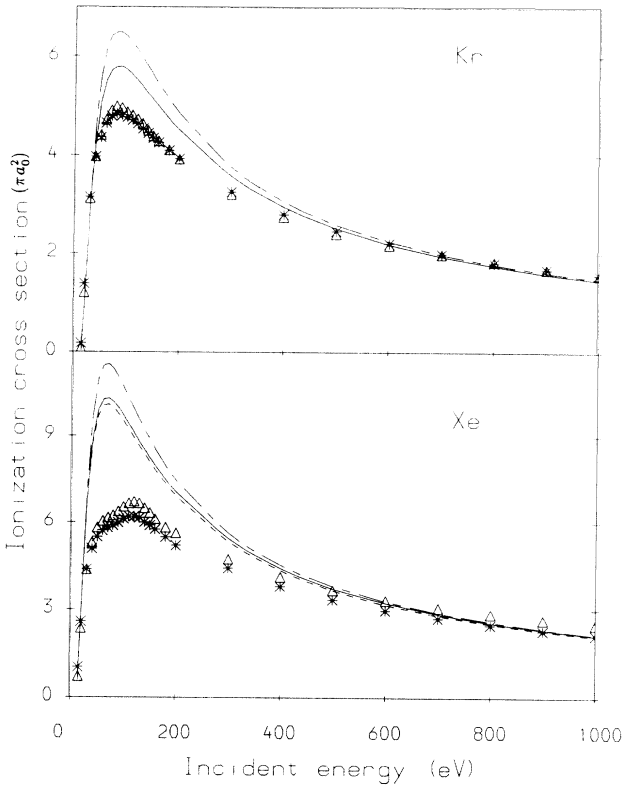

FIG. 3. Total ionization cross section (πa_0^2) for electron and positron impact on krypton and xenon. The notation is the same as for Fig. 2. The short-dashed and solid curves for xenon show the electron calculations for the relativistic and nonrelativistic Hartree-Fock approximations, respectively.

bitals are used to model the states of the target (relativistic in the case of Xe).

The comparison of theory and experiment for He is summarized by Fig. 1. In addition to the present calculation we have included the distorted-wave calculation of Campeanu, McEachran, and Stauffer [16] for positrons, which agrees closely with the present one.

The comparison for Ne and Ar is shown in Fig. 2. The present method describes both electron and positron reactions for argon rather well, but for electrons on Ne there is a shift of the peak, which does not occur for other cases here or in Ref. [7]. We suspect that the Hartree-Fock calculation gives an unexpectedly poor description of the ground state in this case.

The discrepancy between theory and experiment for electrons on Kr and Xe (Fig. 3) is similar to that for helium.

VI. CONCLUSIONS

The equivalent-local description of continuum cross sections is reasonably good at energies above about 50 eV in the case of helium, where the excitation of discrete target states may be described accurately. It is better for positrons than electrons, the difference being the rather rough equivalent-local approximation to the exchange amplitudes for electrons.

For electron-helium scattering the total cross section σ_{sc} for the excitation of P space is well described by the CCO calculation, including the equivalent-local polarization potential. This indicates that the errors in the polarization potential are not large enough to cause difficulties with calculations of P-space excitations in which the continuum effects are included. Omission of the Q space has a significant effect.

For larger inert gases the quality of the calculations of the total ionization cross section varies. It is good for argon, but inexplicably bad for neon. For all gases except neon, theory and experiment tend to agreement above 500 eV. The bad description of neon reactions is probably due to a comparative failure of the Hartree-Fock description for the target. The model predicts electron and positron cross sections for krypton and xenon that are too high at intermediate energies when loss of flux from the entrance channel to discrete excitations is ignored. It is not yet possible to calculate discrete excitations accurately enough in these cases to test whether this is the reason for the discrepancy.

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