Calculations of the energy distribution of electrons ejected in ion-atom collisions using pseudostates

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Calculations of the energy distribution of electrons ejected in ion-atom collisions have been performed by representing continuum wave functions in terms of pseudostates. It is illustrated that for proton-hydrogen collisions the electron spectrum in the low-energy region is in good agreement with that calculated by the use of exact continuum wave functions. In the case of ionization of helium by proton impact, the present results are compared with experimental data as well as with Born Hartree-Fock calculations.

I. INTRODUCTION

The inner-shell ionization process in ion-atom collisions has been a subject of great theoretical interest for many years, and various theoretical models have been developed. A common approach for the calculation of ionization cross sections is to use a continuum wave function for the final state. However, continuum wave functions are complicated even for a simple Coulomb field, and it is very tedious to evaluate matrix elements involving continuum wave functions for the ionization processes. For this reason there have been several attempts to approximate the wave function in a limited region of configuration space by expansion into atomic and pseudostate basis sets.

Another great advantage of this latter approach lies in its simplicity for extension beyond the first-order Born approximation, such as the distortion approximation, and the coupled-state calculations. Furthermore, this method can be readily adapted to atomic potentials other than hydrogenic. The pseudostate method has achieved great success for the calculation of the K-shell hole production cross section by light ions[1] and for the two-center expansion model of proton-hydrogen collisions.[2,3]

Until now, the pseudostate method has been used only for calculations of total ionization cross sections and no application has been made for the energy distribution of ejected electrons. It is the aim of the present paper to show the validity of the pseudostate method for estimating the energy spectrum of electrons ejected from atoms in ion-atom collisions.

II. ENERGY SPECTRUM

In the present work, the continuum states of the target atom are represented in terms of Slater-type orbitals (STO's). In order to obtain the pseudostates, we diagonalize the atomic Hamiltonian with a set of STO's. As pointed out previously,[3] the precise form of STO is not important. These pseudostates are used for the calculations of ionization cross sections within the framework of the semiclassical approximation[4] (SCA). We assume that the projectile moves along a straight-line trajectory.

The energy spectrum of ejected electrons, or, more precisely, the ionization probability density at energy $E=(E_i+E_{i+1})/2$, df/dE, is calculated from

$$\frac{df}{dE}\left[E=\frac{E_i+E_{i+1}}{2}\right]=\frac{f(E_i)+f(E_{i+1})}{2(E_{i+1}-E_i)}\ , \tag{1}$$

where E_i is the energy of the pseudostate and $f(E_i)$ is the transition probability of the target electron from the initial bound state to the pseudostate with positive energy E_i. This procedure was widely used in the calculation of photoionization cross sections.[5]

III. RESULTS AND DISCUSSION

To test the present method, the energy spectra of electrons calculated from Eq. (1) for proton-hydrogen collisions are compared with those obtained from the SCA with exact continuum wave functions. For the case of orbital angular momentum $l=0$, the basis set used consists of ten STO's from $1s$ to $4s$. In Table I, a typical example of the parameters used in the calculations and the energy eigenvalues obtained by diagonalizing the hydrogenic Hamiltonian are listed for the cases of $l=0$ and 1. The parameters of other basis sets are similar to those in Table I with different values of n and ζ. A different choice of the basis set gives a different set of energy points in the spectrum.

In Fig. 1(a), the energy spectra for electrons, corresponding to $l=0$, ejected from hydrogen atom by 25-keV proton impact are shown for various impact parameters. The results from different basis sets are indicated with different symbols. Figure 1(b) shows the corresponding spectra for $l=1$. These pseudostate results are to be compared with the SCA results shown in solid lines. In the SCA calculation, exact continuum wave functions were used. We note from Fig. 1 that the energy spectra calculated from different sets of pseudostates all lie on the SCA curves in the low-energy region, while at higher energies the pseudostate approach gives higher values. Notice that the discrepancy at higher energies does not give much error to the total ionization cross sections, because of the small probabilities in-

TABLE I. Principal quantum number n and orbital exponent ζ for the Slater-type basis functions, and the energy eigenvalues E_i obtained by diagonalizing the hydrogenic Hamiltonian.

	$l=0$			$l=1$	
n	ζ	E_i (a.u.)	n	ζ	E_i (a.u.)
1	1.0	−0.5	2	0.5	−0.125
1	0.5	−0.125	2	0.3333	−0.0555
2	0.5	−0.0555	3	0.3333	−0.0304
3	0.5	−0.0203	2	0.8	−0.0030
4	0.5	0.0483	3	0.5	0.0615
1	0.8	0.2054	2	1.25	0.2049
1	1.25	0.5684	3	0.8	0.5198
1	1.4531	1.4866	3	1.0	1.2575
1	1.5625	4.4092	2	1.5625	3.3138
1	2.4414	21.6011	2	2.4414	12.0957

volved. Similar results were obtained for proton energies of 100 and 400 keV.

These agreements at low energies come from the fact that the wave function for the pseudostate, if appropriately normalized, can approximate the exact continuum wave function at the corresponding energy in the important inner region, where it overlaps with the initial bound state. At higher energies, the continuum wave function oscillates rapidly within the inner region. This oscillatory behavior cannot be represented as a superposition of a few STO functions unless the STO basis set is enlarged. In the case of hydrogen, we found poor agreement between the pseudostate and the continuum wave functions for $E \gtrsim 1.5$ a.u. using the small basis size displayed above.

For target atoms other than hydrogen, we need to use more realistic wave functions and realistic atomic potentials. Here we used the Hartree-Fock-Slater (HFS) potential[6] for He in the atomic Hamiltonian and diagonalized it in the basis set of STO's. By this procedure, we can reproduce the energy eigenvalue of the HFS calculation for the He atom to within an accuracy of 0.1%. The calculations of electron spectra ejected from He by proton impact were performed in the manner similar to the case for protons on hydrogen. In order to compare with experimental data and other theoretical calculations, the obtained results were integrated over impact parameters and single differential cross sections as a

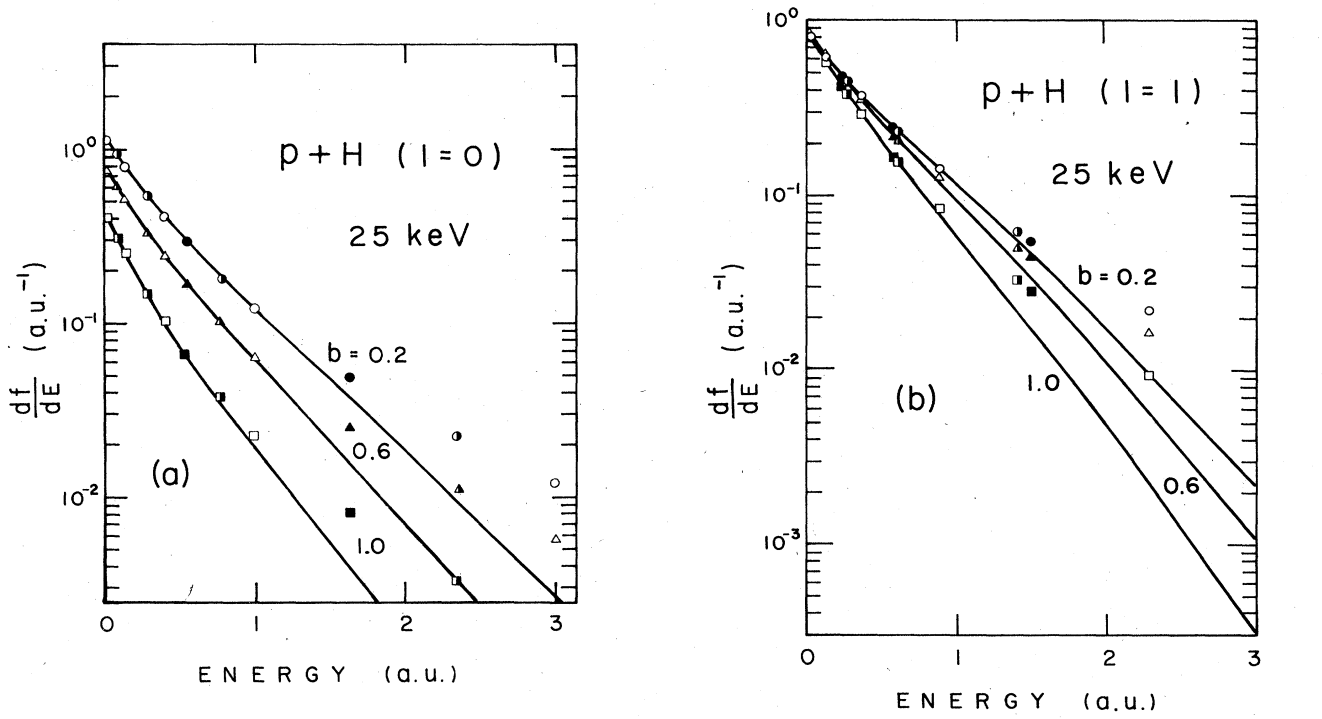

FIG. 1. Ionization probability density df/dE vs electron energy for 25-keV protons on a hydrogen atom at impact parameters $b = 0.2$, 0.6, and 1.0 a.u. for (a) $l = 0$ and (b) $l = 1$. The solid curves represent the SCA calculations with exact continuum wave functions. The present results are shown in circles ($b = 0.2$), triangles ($b = 0.6$), and squares ($b = 1.0$). Results from the same basis set are indicated by similar full, half-full, and open symbols.

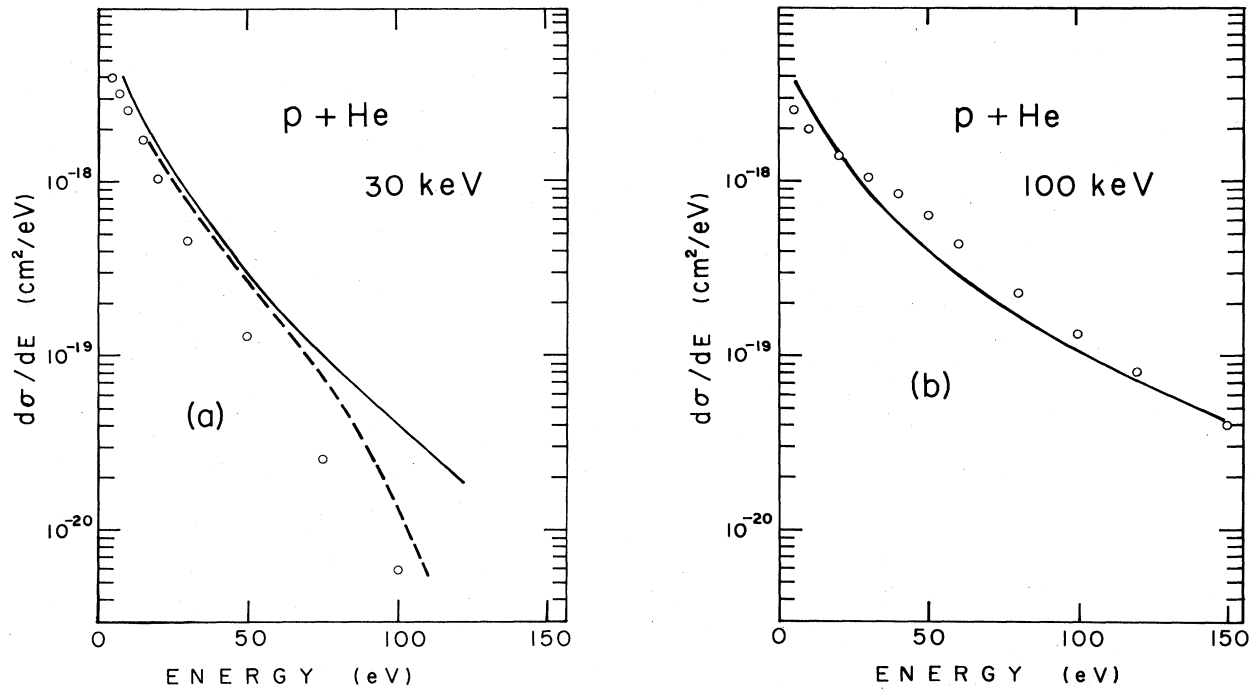

FIG. 2. (a) Energy distribution of electrons ejected from a helium atom by 30-keV protons. The solid curve represents the present results and the dashed curve indicates the Born Hartree-Fock calculations (Ref. 7). The circles are the experimental data taken from Ref. 7. (b) As in (a), for 100-keV protons.

function of ejected electron energy were evaluated.

In Fig. 2(a), we show the energy distribution of electrons integrated over all impact parameters for 30-keV protons on He. Calculations were made with four different basis sets for each orbital angular momentum $l=0$, 1, and 2. The number of STO's for all the basis sets is chosen to be ten and the STO's from $1s$ to $4s$ are used for $l=0$, from $2p$ to $4p$ for $l=1$, and from $3d$ to $5d$ for $l=2$. The results for these partial waves are summed up after numerical integration over b.

The experimental and theoretical results of Rudd and Madison[7] are also plotted in Fig. 2. Their theoretical values are based on the Born approximation with simplified Hartree-Fock wave functions.[8] It can be seen from Fig. 2 that the present results agree well (for low-energy electrons) with the Born Hartree-Fock calculations, and are close to the experimental data. The discrepancy between the Born Hartree-Fock and the present pseudostate results at low energy is due to the different potentials used. However, at high energies the pseudostate method gives larger values than both experimental and Born Hartree-Fock results. For projectile energies of 15 and 50 keV, we have obtained similar conclusions. Comparison of the present results with the experimental data of Rudd and Madison[7] for 100-keV protons on He is shown in Fig. 2(b). In this case the calculated values are in good agreement with the experimental ones.

In conclusion, we have demonstrated that the energy spectrum of low-energy electrons ejected during the ion-atom collisions can be well represented by pseudostates if an averaging procedure is employed. The spectrum shape is found to be insensitive to the details of the choice of pseudostates. Within the first-order approximation, the pseudostate results are in good agreement with the SCA calculation where exact continuum wave functions were used. In the case of protons on helium, the pseudostate approach also agrees with Born Hartree-Fock calculations and with experiments in the predicted electron energy distribution. The discrepancy of this approach at high energies is due to the fact that the STO-based pseudostates cannot reproduce the rapid oscillation of continuum wave functions for high-energy electrons. This discrepancy would be removed by the use of the basis set which contains rapidly oscillating functions. For practical applications, however, the present pseudostate approach is quite adequate, since the ionization cross sections are dominated by the low-energy electrons. The present calculation is demonstrated with the first Born approximation. Progress is being made in employing these pseudostates in coupled-channel calculations.

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[1]A. L. Ford, E. Fitchard, and J. F. Reading, Phys. Rev. A **16**, 133 (1977).

[2]R. Shakeshaft, Phys. Rev. A **18**, 1930 (1978).

[3]W. Fritsch and C. D. Lin, Phys. Rev. A **27**, 3361 (1983).

[4]J. Bang and J. M. Hansteen, K. Dan. Vidensk. Selsk. Mat.-Fys. Medd. **31**, No. 13 (1959).

[5]R. F. Steward, C. Laughlin, and G. A. Victor, Chem. Phys. Lett. **29**, 353 (1974).
[6]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, NJ, 1963).
[7]M. E. Rudd and D. H. Madison, Phys. Rev. A **14**, 128 (1976); M. E. Rudd, L. H. Toburen, and N. Stolterfoht, At. Data Nucl. Data Tables **18**, 413 (1976).
[8]Rudd and Madison used the exact Hartree-Fock wave functions for the initial bound state. However, the final continuum wave function was obtained by the use of the Hartree-Fock potential modified to give the asymptotically Coulombic behavior. This means that the orthogonality condition is fulfilled approximately.