ANL/PPRNT--89-107

DE89 008439

Removal of nonorthogonality in the Born theory used for study of electron capture in high energy ion-atom collisions*

M. Kimura

Argonne National Laboratory, Argonne, IL 60439

and

Rice University, Houston, TX 77251

We show the complete removal of the nonorthogonality of wave functions between initial and final states in the Born theory. Hence, this treatment offers more realistic electron capture cross sections in high energy ion-atom collisions. Representative results for resonant electron capture in $H^+ + H^*$ collision are discussed in conjunction with other perturbative results.

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*Work supported by U.S. Department of Energy, Office of Health and Environmental Research, under Contract W-31-109-Eng-38, and by Office of Basic Energy Sciences, Division of Chemical Science.

It is known that the deficiency of the Born approximation used for the study of electron capture in ion-atom collisions is due to the fact that initial and final wave functions are not orthogonal to each other.[1] Because of this defect, predictions of electron capture cross sections using the Born approximation or its variations differ substantially, particularly on the lower energy side.

Detailed analysis of the atomic orbital (AO) expansion method[2,3] clearly indicates that the AO expansion method properly accounts for the nonorthogonality of the initial and final wave functions in electron capture processes. In a two-state AO expansion method, a set of coupled equations can be written,[1]

$$i\,\dot{a}_A(t) = \left[\frac{h_{AB} - S_{AB}h_{BB}}{1 - S^2}\right] e^{i(\omega t+\alpha)t}\, a_B(t)$$

$$i\,\dot{a}_B(t) = \left[\frac{h_{BA} - S_{BA}h_{AA}}{1 - S^2}\right] e^{-i(\omega t+\alpha)}\, a_A(t) \qquad (1)$$

where

$$S_{ij} = \langle \phi_i^{AO} | e^{i\vec{v}\cdot\vec{r}} | \phi_j^{AO} \rangle$$

$$S^2 = S_{ij}\, S_{ji}$$

$$h_{ij} = \langle \phi_i^{AO} \left| -\frac{Z_i}{r_i} \right| \phi_j^{AO} \rangle$$

$$h_{ii} = \langle \phi_i^{AO} \left| -\frac{Z_j}{r_j} \right| \phi_i^{AO} \rangle \qquad (2)$$

$$\alpha = \int_{-\infty}^{t} [X(t') - Y(t')]\, dt'$$

and

$$X(t) = \frac{h_{AA} - S_{AB}h_{BA}}{1 - S^2}$$

$$Y(t) = \frac{h_{BB} - S_{BA}h_{AB}}{1 - S^2} \quad .$$

The α term is unique in the AO expansion method, which represents the electronic distortion effect due to two nuclei.

The coupled equations (1) can be solved in first order approximation provided the capture probability is small. Then, the scattering amplitude $a_B(+\infty)$ is given as,

$$a_B(+\infty) = i \int_{-\infty}^{\infty} \left[\frac{h_{BA} - S_{BA}h_{AA}}{1 - S^2}\right] e^{-(\omega t+\alpha)}\, dt \quad . \qquad (3)$$

Equation (3) serves as the starting point to simplify the scattering amplitude formula by further approximation. Also, the exactly identical result to Eq. (3) can be derived from the first Born approximation[1,3] as well as the distorted-wave approximation[3,4] by imposing the condition that the final wave function is orthogonal to the initial one.

The above analysis for electron capture processes in the two-state AO expansion method and the Born theory naturally leads one to the procedure for "forcing" the orthogonality between the initial and final states within the Born theory. One way to achieve this is to rewrite the electronic Hamiltonian in a sum of initial and final atomic states

$$H = \left(-\frac{1}{2}\nabla^2_{r_P} - \frac{Z_P}{r_P}\right) - \left(-\frac{1}{2}\nabla^2_{r_T} - \frac{Z_T}{r_T}\right) + V(r_P, r_T, R) \quad , \qquad (4)$$

where $\vec{r}_c$ represents a vector coordinate to an electron from projectile (c = P) and target (c = T). The interaction $V(r_P, r_T, R)$ can be written by the cross

term of the kinetic operators in Eq. (4), i.e., $-\nabla_{r_T} \cdot \nabla_{r_P}$ plus nuclear-nuclear interaction. Obviously, the present choice of electronic unperturbed Hamiltonian always guarantees the orthogonality of the initial and the final wavefunctions. Hence, this procedure removes the difficulty that arises from the nonorthogonality of wave functions within the Born theory.

We have applied the improved Born treatment explained above to study electron capture processes for $H^+ + H$ collisions in the energy range from 25 to 1000 keV. The calculated result is shown in Fig. 1 along with other theoretical results[4-8] and experimental data.[9,10] Also, the numerical results are tabulated in Table I. The OBK (Oppenheimer,[5] Brinkman and Kramers[6]) approximation in Fig. 1, which completely neglects the nuclear-nuclear interaction in evaluating the first Born term, apparently overestimates the cross section. However, as argued by Bates and Dalgarno,[7] the inclusion of the nuclear-nuclear interaction in the perturbation would compensate to some extent for the nonorthogonality of the initial and final wave functions. Consequently, calculated cross sections[7] in the figure are much smaller and in better accord with measurements.[9,10] The distorted-wave approximation by Bassel and Gerjuoy[4] (BG) has an identical form to Eq. (3) except for the neglect of the S^2-term in the denominator. This corresponds to the higher-velocity approximation where the overlap of the wave function between the initial and final states is small due to the short interaction period of particles. Evidently, the two-state AO expansion method by McCarroll[8] agrees quite well with the BG result above ~100 keV. The present result, which completely removes troublesome problems due to the non-orthogonality between wave functions of the initial and final states, lies about 36% below the Born result at 25 keV. However, this difference reverses itself to 10% at 1000 keV, as seen from Table I, making the present result

closer to the BG result[4] at higher collision energies. This characteristic can be easily understood from the fact that the two-state AO method, the BG method and the Born theory can give identical results for the scattering amplitude in Eq. (3) provided that wave functions between the initial and final states are orthogonal to each other.

This short note reports the complete removal of the nonorthogonality of wave functions between the initial and final states in the Born theory and hence can provide more realistic electron capture cross sections. This treatment has been applied to the study of resonant electron capture in H^+ + H(1s) collisions. The present method can also be applied easily to the study of ionization processes. Work along this line is now under way.

This work is supported in part by the U.S. Department of Energy, Office of Health and Environmental Research, under Contract W-31-109-Eng-38 and by Office of Basic Energy Sciences, Division of Chemical Science.

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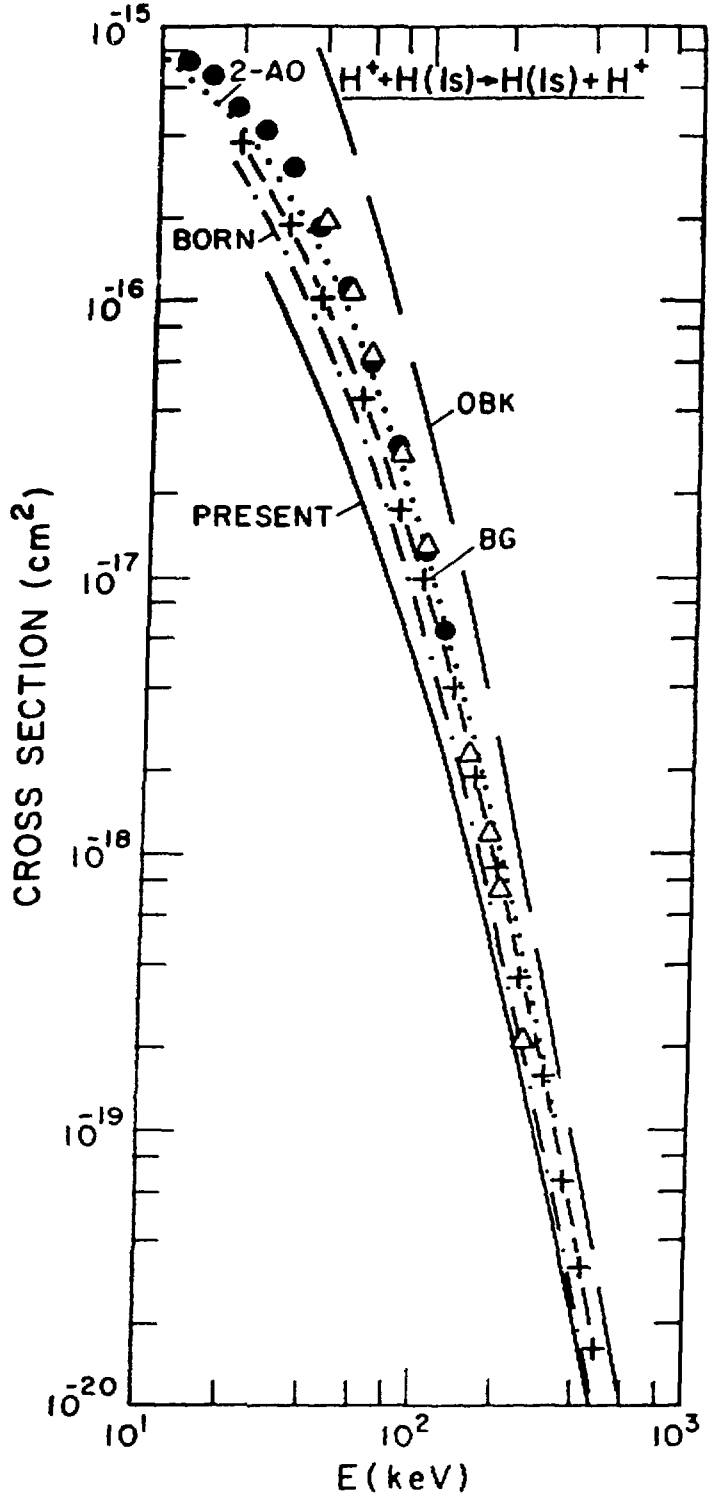
TABLE I. $H^+ + H(1s) \rightarrow H(1s) + H^+$ resonant electron capture cross section (10^{-16} cm^2).

E (keV)	Present	Born (Ref. 7)	BG (Ref. 4)	Two-state AO (Ref. 8)
25	1.27	2.01	2.58	2.75
50	2.65^{-1}	4.58^{-1}	6.05^{-1}	8.85^{-1}
100	3.97^{-2}	6.46^{-2}	9.79^{-2}	1.01^{-1}
200	3.83^{-3}	5.27^{-3}	8.88^{-3}	9.72^{-3}
500	8.78^{-5}	8.79^{-5}	1.68^{-4}	1.72^{-4}
1000	2.86^{-6}	2.56^{-6}	4.85^{-6}	5.12^{-6}

Figure Caption

Fig. 1. $H^+ + H(1s) \rightarrow H(1s) + H^+$ cross sections. Theory: solid line, present; Born, Ref. 7; BG, Ref. 4; OBK, Refs. 5 and 6; two-AO, Ref. 8. Experiment: Δ, Ref. 9; ●, Ref. 10.


$H^+ + H(1s) \rightarrow H(1s) + H^+$
2-AO
BORN
OBK
PRESENT
BG
CROSS SECTION (cm^2)
10^{-15}
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^{-20}
10^1
10^2
10^3
E (keV)