Cross sections for the excitation of the projectile He^+ ions in collision with hydrogen atoms

Shyamal Datta, Kanika Roy, and S. C. Mukherjee
Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700032, India
(Received 16 January 1980)

The two-state distortion approximation and a corresponding second Born approximation are employed to calculate the 2*s* excitation cross section of the projectile $He^+(1s)$ in $He^+(1s) + H(1s)$ collision process, keeping the target atom unexcited for the incident energy ranging from 30 to 4000 keV. The distortion effect in the second Born calculation is taken into consideration in the present work by retaining the couplings between the initial and the final states in the infinite summation. The present results are compared with the existing theoretical and experimental cross sections. Our calculations give results in reasonably good agreement with the many-state close-coupling calculations of Bell and Kingston, but like the existing calculation, the present results are not in good agreement with the observed results.

INTRODUCTION

The collision between helium ions (He^+) and hydrogen atoms (H) is one of the simplest and most basic collision problems involving two composite atomic systems. The wave functions for these systems are known exactly. Consequently the theoretical predictions of cross sections involving these systems are more reliable and the experimental measurements of such cross sections thus become stringent tests of the theory.

Shah and Gilbody[1] have recently measured in the energy region 22.5–346 keV the cross sections σ_{11}^* for the direct excitation process

$$He^+(1s)+H(1s) \to He^+(2s)+H(\Sigma)\,, \qquad (1)$$

where(Σ) denotes all discrete and continuum final states of the target atom. The only theoretical study for the process (1) has been made by Bell and Kingston.[2] The measurements[1] and the theoretical calculations[2] of the excitation cross sections for the projectile in the above collision process were made simultaneously. Because of the remarkable difference between the total cross-section measurements[1] and the existing theoretical calculations[2] we became interested in performing a fresh theoretical investigation on this problem. Bell and Kingston[2] applied the first Born approximation to compute the cross sections for the formation of He^+ (2*s* or 2*p*) ion up to an incident He^+-ion energy of 4000 keV. They also employed a coupled-state calculation in the impact parameter treatment to calculate these cross sections. In the present work we propose to employ the distortion approximation and the corresponding second Born approximation in the impact-parameter treatment to calculate the excitation cross sections.

The two-state distortion approximation was first introduced by Bates[3] in the impact-parameter formulation for the calculation of the inelastic cross sections in ion-atom collision processes and, in the intermediate energy region, he obtained much better results in comparison with the first Born approximation. Several other investigations on the heavy-particle collision have thereafter been carried out using this approximation. The application of distortion approximation by Bell[4] and Davison[5] for ^1P and ^1D excitation of helium atom by protons and alpha-particle impact have shown good agreement with experiments at intermediate energies. Skinner[6] has studied the excitation process of a hydrogen atom by the impact of alpha particle or proton using a modified distortion approximation so as to include the coupling between $2p_0$ and $2p_{\pm1}$ states. Bell and Skinner[7] have reconsidered the same problem to study the effect of back coupling to the 1*s* state. The effect of distortion in the asymmetric charge transfer $He^{2+}+H \to He^+ + H^+$ has been found to be quite significant.[8,9] The distortion approximation has also been applied to calculate the $2\,^1S$, $3\,^1S$, and $4\,^1S$ excitation cross sections of helium atoms by proton and alpha-particle impact.[10,11] It is confirmed by all the above-mentioned investigations that the inclusion of the distortion greatly influences the results of the cross sections, and it is further observed that the effect of distortion is more important for the case of *s*-*s* transition than for *s*-*p* transition. For proton impact $3\,^1S$ excitation of a helium atom, the distortion calculation of Roy and Mukherjee[10] gives nearly the same results as observed experimentally at lower energies. In the second Born approximation the distortion effect can be taken into consideration by retaining couplings only to the initial and the final states in the infinite summation. Assuming that the major contribution to the scattering amplitude is provided by the 1*s*, 2*s*, $2p_{0,\pm1}$ intermediate states, Kingston *et al.*[12] have carried out calculations for the $1s \to 2s$ excitation of atomic hydrogen by electron, positron, and proton impact. The same approach has been used by Kingston and Skinner[13] on the problem of elastic scattering of electrons and positrons by hydrogen atoms and by Moiseiwitsch and Perrin[14] on the problem of $1s \to 2p$ excitation of atomic hydrogen by electron, positron, and proton impact. Chaudhuri and Bhattacharya[15] have calculated the $1s \to 2s$ and $1s \to 3s$ excitation cross sections of the hydrogen atom by alpha-particle impact in the second Born approximation using the impact-parameter formulation and, taking only the couplings corresponding to the initial and the final states in the infinite summation, obtained good agreement with their calculated results of the distortion approximation. The above methods are employed here to calculate the $2s$ excitation cross sections of the projectile $He^+(1s)$ for the single-transition process (target atom in ground state)

$$He^+(1s) + H(1s) \to He^+(2s) + H(1s). \tag{2}$$

The distortion effect in second Born calculation is taken into consideration in the present work by retaining the couplings between the initial and the final states in the infinite summation. The first Born-approximation results for the double-transition process as calculated by Bell and Kingston[2] are then added with the present results to obtain the $He^+(2s)$ cross sections for the reaction (1).

The present theoretical approach though very simple and based on only two-state calculations give results in reasonably close agreement with the many-state close-coupling calculations of Bell and Kingston.[2] In the high-energy region, the present two-state distortion calculation almost coincides with the close-coupling calculations. It may, however, be noted that like the close-coupling calculations of Bell and Kingston the present theoretical results also are not in satisfactory agreement with the observed results. Atomic units have been used throughout.

THEORY

The incident ion A having a nuclear charge Z_i is assumed to follow a classical straight-line trajectory with velocity $\vec{v}$ relative to the target nucleus B. The Hamiltonian H describing the system may be written as

$$H = -\tfrac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{Z_i}{r_{A2}} - \frac{Z_i}{r_{A1}} - \frac{1}{r_{B1}} - \frac{1}{r_{B2}} + \frac{1}{r_{12}},$$

where $\vec{r}_{A1}$, $\vec{r}_{A2}$, $\vec{r}_{B1}$, and $\vec{r}_{B2}$ are the radius vectors of electrons 1 and 2 for the nuclei A and B, respectively, and r_{12} is the distance between the two electrons. The internuclear interaction term has been neglected since it has no effect in the total cross sections.

The electronic wave function $\Psi(\vec{r}_{A1}, \vec{r}_{B2}, t)$ may be expanded in terms of the bound eigenfunctions as[16]

$$\Psi(\vec{r}_{A1}, \vec{r}_{B2}, t) = \sum_n A_n(t)\Phi_n(\vec{r}_{A1}, \vec{r}_{B2}, t),$$

where[17]

$$\Phi_n(\vec{r}_{A1}, \vec{r}_{B2}, t) = \Phi_n^{He^+}(\vec{r}_{A1}, t)\Phi^{H}(\vec{r}_{B2}, t), \tag{3}$$

neglecting electron exchange and noting that the nuclei are distinguishable. Here $\Phi_n^{He^+}$ represents the ground and excited states of the helium ion and Φ^H represents the ground state of the hydrogen atom. The collision is then described by the time-dependent Schrödinger equation

$$H\Psi(\vec{r}_{A1}, \vec{r}_{B2}, t) = i\frac{\partial}{\partial t}\Psi(\vec{r}_{A1}, \vec{r}_{B2}, t). \tag{4}$$

The total Hamiltonian H can be split up into two parts,

$$H = H_i + V_i,$$

H_i being the unperturbed Hamiltonain and V_i the interaction potenital given by

$$V_i = -\frac{2}{r_{A2}} - \frac{1}{r_{B1}} + \frac{1}{r_{12}}. \tag{5}$$

Following a procedure similar to Bates,[3] we obtain the following set of coupled differential equations:

$$\frac{dA_m(s)}{ds} = \frac{i}{v}\sum_n A_n(s)F_{mn}(s), \tag{6}$$

where $s = vt$,

$$F_{mn} = -\langle\Phi_m | V_i | \Phi_n\rangle = V_{mn}\exp(i\epsilon_{mn}s/v),$$

$$\epsilon_{mn} = \epsilon_m - \epsilon_n, \tag{7}$$

ϵ_m and ϵ_n being the eigenenergies corresponding to Φ_m and Φ_n. The set of equations (6) is solved for $A_m(s)$ with the initial conditions $A_m(-\infty) = \delta_{m1}$, when the probability of excitation from the ground state 1 to a state m is given by

$$P_m = |A_m(\infty)|^2.$$

Formal integration of (6) yields

$$A_m(s) = \delta_{m1} + \frac{i}{v}\sum_n \int_{-\infty}^{s} A_n(s')F_{mn}(s')ds' \tag{8}$$

The first Born approximation corresponds to the substitution $A_m(s) = A_m(-\infty) = \delta_{m1}$ on the right-hand side of Eq. (8), yielding the first Born amplitude as

$$A_m^B(\infty) = \delta_{m1} + \frac{i}{v} \int_{-\infty}^{\infty} F_{m1}(s) ds . \tag{9}$$

This expression is substituted on the right-hand side of (9) and all couplings, except those involving the initial and the final state ($n=1$ and m) in the infinite summation, are neglected. The resulting second Born amplitude is given by

$$A_m^{B2}(\infty) = \frac{i}{v} \int_{-\infty}^{\infty} F_{m1}(s) ds - \frac{1}{v^2} \int_{-\infty}^{s} \left(F_{m1}(s) \int_{-\infty}^{s} F_{11} ds' + F_{mm}(s) \int_{-\infty}^{S} F_{m1} ds' \right) ds . \tag{10}$$

Alternatively, retaining coupling only to initial and final states in the original set of coupled equations (6), one obtains

$$\frac{dA_1}{ds} = \frac{i}{v} \left(A_1 F_{11} + A_m F_{1m} \right) \tag{11a}$$

and

$$\frac{dA_m}{ds} = \frac{i}{v} \left(A_1 F_{m1} + A_m F_{mm} \right). \tag{11b}$$

Neglecting the back-coupling term involving F_{1m} on the right-hand side of (11a) and solving, we obtain the two-state distortion amplitude

$$A_m^D(\infty) = \exp\left(\frac{i}{v} \int_{-\infty}^{\infty} F_{mm}(s) ds \right) \times \frac{i}{v} \int_{-\infty}^{\infty} A_1 F_{m1}(s) \exp\left(-\frac{i}{v} \int_{-\infty}^{s} F_{mm} ds' \right) ds . \tag{12}$$

For s-state excitations, all the $V_{mn}(s)$ involved are even in s, and on simplification one obtains the first Born probability as

$$P_m^B = (A_m^B)^2 ,$$

where

$$A_m^B = \frac{2}{v} \int_0^{\infty} V_{m1} \cos(\epsilon_{m1} s / v) ds , \tag{13}$$

and the second Born probability is

$$P_m^{B2} = P_m^B - \frac{2}{v} A_m^B A_m'^{B2} ,$$

where

$$A_m'^{B2} = \frac{2}{v} \int_0^{\infty} V_{m1}(s) \sin(\epsilon_{m1} s / v) \times \left(\int_0^{s} (F_{11} - F_{mm}) ds' \right) ds \tag{14}$$

(neglecting terms of the fourth order in interaction energy). One also obtains the distortion probability as

$$p_m^D = (A_m^D)^2 ,$$

where

$$A_m^D = \frac{2}{v} \int_0^{\infty} V_{m1}(s) \cos\left[\frac{1}{v} \left(\int_0^{s} (F_{11} - F_{mm}) ds' + \epsilon_{m1} s \right) \right] ds . \tag{15}$$

The double integrals are evaluated numerically: hence the total cross section for excitation from the ground state to the mth state is given by

$$\sigma_m = 2\pi \int_0^{\infty} P_m p \, dp , \tag{16}$$

p being the impact parameter.

Analytical expressions for the required matrix elements can be obtained from Eq. (7). The evaluation of matrix elements is tedious and requires much attention due to the occurrence of the term $1/r_{12}$ in Eq. (6). This term is present in the interaction potential due to structure of the projectile.

The integrals occurring in the expressions for the amplitudes have been evaluated numerically. In these computations sufficient care has been taken to ensure the desired accuracy. The Gauss-Legendre quadrature method has been used for the integration over p in the calculation of the cross sections. The value of p has been increased stepwise until the desired accuracy of 1% in the total cross sections is obtained. For the amplitude expression the outer integral has been evaluated in the same manner by increasing stepwise the value of "s" and the inner integral has been performed by repeated application of Simpson's rule.

RESULTS AND DISCUSSIONS

In Table I we present our calculated values for the total cross sections of the single-transition process (2) for the incident energy ranging from 30 to 4000 keV obtained by applying the distortion approximation (σ_m^D) and the corresponding second Born approximation (σ_m^{B2}).

It is evident from the table that at high energies (from 1000 to 4000 keV) the two sets of cross sections calculated by the two different approximations almost converge. It may, however, be noted that in the lower-energy side, although the values obtained by the second Born approximation are somewhat lower than those obtained by the distortion approximation, with the increase of incident energy these two cross sections gradually become almost identical.

We present our results for the excitation cross sections of the single-transition process (2) in

TABLE I. Distortion and second Born-approximation cross sections (10^{-18} cm^2/atom) for $He^+(2s)$ excitation in the reaction $He^+(1s) + H(1s) \rightarrow He^+(2s) + H(1s)$. The numbers in parentheses denote the powers of ten by which the numbers are to be multiplied.

Energy of incident He^+ ion (keV)	$\sigma_m^D(2s$ excitation)	$\sigma_m^{B2}(2s$ excitation)
30	5.23(−2)	
50	4.33(−1)	
64	6.48(−1)	3.04(−1)
90	8.48(−1)	7.66(−1)
100	8.80(−1)	8.41(−1)
144	8.95(−1)	9.19(−1)
196	8.18(−1)	8.50(−1)
256	7.17(−1)	7.43(−1)
324	6.20(−1)	6.39(−1)
400	5.35(−1)	5.49(−1)
600	3.90(−1)	3.97(−1)
800	3.06(−1)	3.10(−1)
1000	2.51(−1)	2.54(−1)
2000	1.33(−1)	1.33(−1)
3000	9.02(−2)	9.06(−2)
4000	6.83(−2)	6.85(−2)

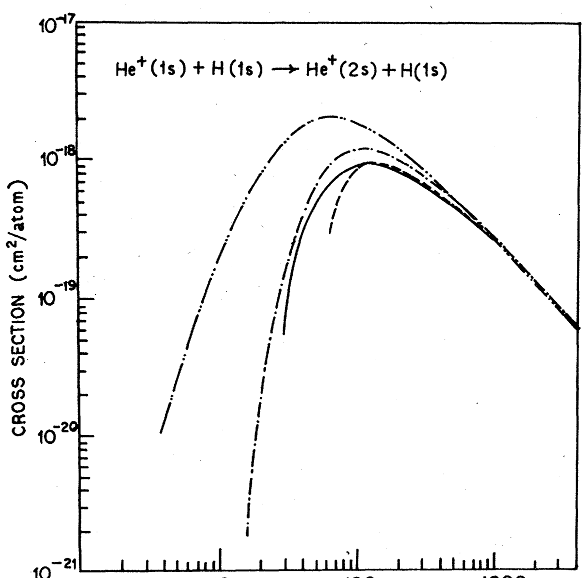

FIG. 1. Total cross section σ_{11}^* for $1s$-$2s$ excitation of He^+ in the reaction $He^+(1s) + H(1s) \rightarrow He^+(2s) + H(1s)$. Theory: —··— Bell and Kingston (Ref. 2), first Born approximation. —·— Bell and Kingston (Ref. 2), close-coupling cross section for single-transition processes. —— Present calculation, distortion approximation. --- Present calculation, second Born approximation.

Fig. 1 and compare them with the theoretical results of Bell and Kingston,[2] calculated by the coupled-state method as well as by the first Born approximation.

The cross sections of Bell and Kingston[2] calculated by close-coupling method shown in Fig. 1 agree reasonably well with the present distortion approximation calculation both in shape and magnitude. The calculated values obtained by the first Born-approximation method, however, differ considerably from other theoretical results. From the figure it appears that over a limited low-energy region (30 to 80 keV), the present two-state distortion results are in much better agreement with the results obtained by the many-state close-coupling calculation of Bell and Kingston,[2] as compared to the results obtained by using the first Born approximation. The Born-approximation results, however, grossly overestimate other predicted calculated results on the low-energy side. At high-impact energies of the projectile, the cross sections obtained by the present two-state calculations and the coulped-state calculations of Bell and Kingston[2] agree well with each other. The cross sections obtained by the present two-state distortion calculation and the corresponding second Born-approximation exhibit the maximum nearly on the same incident energy as obtained by the many-state close-coupling calculation, whereas the first Born approximation

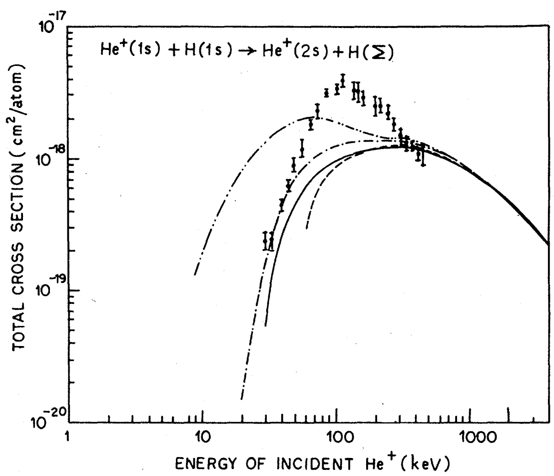

FIG. 2. Total cross section σ_{11}^* for $1s$-$2s$ excitation of He^+ in the reaction $He^+(1s) + H(1s) \rightarrow He^+(2s) + H(\Sigma)$. Theory: —··— Bell and Kingston (Ref. 2), first Born approximation. —·— Bell and Kingston (Ref. 2), close-coupling cross section for single-transition process plus first Born approximation for double-transition process. —— Present calculation, distortion approximation. --- Present calculation, second Born approximation. Experiment: ● Shah and Gilbody (Ref. 1).

indicates the maximum at somewhat lower energy.

Figure 2 represents our results for the distortion calculation, as well as those obtained by the corresponding second Born calculation for the total cross sections of $He^{+}(2s)$ excitation compared with the corresponding theoretical results of Born and close-coupling calculations, as well as the experimental findings of Shah and Gilbody.[1] The theoretical values of the total cross sections are calculated by combining the values of the cross sections obtained by the present method keeping the target at ground state (single-transition process) together with the results[2] of the cross sections obtained in the Born method by considering the target in excited states as well as in the continuum state (double-transition process). The results of the cross sections are found to have very little dependence on the inclusion of the excited states of the target in the low-energy domain. However, its inclusion above 300 keV shows some change in the theoretical results of the cross sections where the calculated results exhibit somewhat better agreement with the experimental findings. The present two-state distortion results show a trend similar to the close-coupling calculations of Bell and Kingston throughout the energy region considered; beyond about 500 keV these two methods give almost identical results for the cross sections. Although the present two-state distortion results for the total cross sections are in qualitative agreement with the many-state close-coupling calculations of Bell and Kingston, both these theoretical curves show a quantitative disagreement with the experimentally observed curve. The large difference between the theoretical results and the experimental findings definitely suggest further study in this line.

ACKNOWLEDGMENTS

The authors would like to express their sincere gratitude to Professor N. C. Sil of the Indian Association for the Cultivation of Science, Calcutta, for his interest in the problem. Thanks are also due to the authorities of the Regional Computer Centre, Calcutta, for making available their Burroughs 6700 computer in course of this work.

[1]M. B. Shah and H. B. Gilbody, J. Phys. B 11, 121 (1978).
[2]K. L. Bell and A. E. Kingston, J. Phys. B 11, 1259 (1978).
[3]D. R. Bates, Proc. Phys. Soc. London 73, 227 (1959).
[4]R. J. Bell, Proc. Phys. Soc. London 78, 903 (1961).
[5]W. D. Davison, Phys. Lett. A 27, 570 (1968).
[6]B. G. Skinner, Proc. Phys. Soc. London 79, 717 (1962).
[7]R. J. Bell and B. G. Skinner, Proc. Phys. Soc. London 80, 404 (1962).
[8]R. McCarroll and M. B. McElroy, Proc. R. Soc. London Ser. A 266, 422 (1962).
[9]M. McElroy, Proc. R. Soc. London Ser. A 272, 542 (1963).
[10]K. Roy and S. C. Mukherjee, Phys. Lett. A 44, 147 (1973).
[11]S. K. Sur, K. Roy, S. Roy, and S. C. Mukherjee, Phys. Rev. A 16, 1986 (1977).
[12]A. E. Kingston, B. L. Moiseiwitsch, and B. G. Skinner, Proc. Phys. Soc. London 258, 237 (1960).
[13]A. E. Kingston and B. G. Skinner, Proc. Phys. Soc. London 77, 724 (1961).
[14]B. L. Moiseiwitsch and R. Perrin, Proc. Phys. Soc. London 85, 51 (1965).
[15]J. Chaudhuri and D. M. Bhattacharya, Ind. J. Phys. 44, 63 (1970).
[16]D. R. Bates, in *Quantum Theory. I. Elements*, edited by D. R. Bates (Academic, New York and London, 1961), p. 252.
[17]M. R. Flannery, J. Phys. B 2, 1044 (1969).