Influence of laser radiation on charge transfer in proton–alkali-metal-atom collisions

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The atomic-eigenfunction-expansion method is used to investigate the influence of laser radiation on charge-transfer processes in proton–alkali-metal-atom collisions. The radiation is treated classically. The cross sections for charge transfer into the ground state of hydrogen in collisions between a proton and any of the atoms sodium, potassium, rubidium, and cesium in the presence of radiation of wavelengths varying between 3000 and 6000 Å are determined for incident-ion energy values of 1, 2, and 10 keV. Calculations are made for two different radiation intensities, 0.1 and 1 TW/cm^2. It is found that the effect of the radiation is to increase the charge-transfer cross section in some cases and decrease the cross section in others.

I. INTRODUCTION

Charge-transfer or electron-capture processes which occur during collisions between ions and atoms are known to play important roles under a wide variety of physical situations. Dalgarno[1] has explained how the consideration of such processes helped in the interpretation of a number of atmospheric and astrophysical data including the distribution of ions and neutral atoms in the upper atmosphere and the intensities of spectral lines emitted by planetary nebulas. Gilbody[2] has emphasized that the production and maintenance of a high-temperature plasma necessary for realization of controlled thermonuclear energy through fusion depend significantly on several charge-exchange processes occurring within the plasma. It has been suggested[3] that the charge-transfer mechanism may provide ways of getting laser radiations in the extreme-ultraviolet- or shorter-wavelength region. In view of the fact that the magnitude of the cross section of an electron-capture process is often crucial in determining its relative importance in a practical situation, there has arisen a need for the study of factors which may influence this magnitude. One such factor which has attracted considerable recent attention is the presence of an intense electromagnetic field due to radiation from a laser. Green *et al.*[4] has already observed how an intense laser beam induces charge transfer in collisions between ground-state calcium ions and strontium atoms with the production of calcium atoms and excited strontium ions.

Several theoretical works on radiation-assisted charge-transfer collisions have also been done by different groups of workers. We mention here some of the recent publications where references to earlier papers are given. Symmetrical resonance charge-transfer processes such as $H^+ + H(1s) \rightarrow H(1s) + H^+$ and $He^+(1s) + He(1s^2) \rightarrow He(1s^2) + He^+$ in presence of laser field have been dealt with by Mittleman[5] and Ganguly *et al.*,[6] respectively. Errea *et al.*[7] have investigated the cases of accidental resonance charge exchange in α-hydrogen and Li^{3+}-H collisions as modified by intense electromagnetic fields, employing a method developed earlier by Copeland and Tang.[8] The α-hydrogen problem has been considered also by Ho *et al.*[9] who used a semiclassical coupled dressed quasimolecular states approach. Very recently Hsu *et al.*[10] have studied the laser-assisted electron capture process $K^+ + Na(3s) + \gamma \rightarrow K(4s) + Na^+$.

The above works are all based on the method of expansion in terms of quasimolecular states. We have recently developed an alternative formalism[11] for investigating charge transfer processes in ion-atom collisions in the presence of intense radiation fields obtainable with lasers. In this method we expand the total state in terms of the products of the atomic eigenstates and the photon states. The relative advantages and disadvantages and the regions of validity of the atomic state and the molecular-state approach in ion-atom collisions are well known[12,13] and will not be discussed here. We only want to mention that the atomic state expansion method becomes more suitable as the collision velocity increases although, for very fast collisions, methods that take proper account of the continuum are needed. Further, one can conveniently use the available atomic wave functions. We applied[11] our formalism to calculate the ground-state electron-capture cross sections in proton-helium collisions in the presence of laser radiation of different wavelengths and intensities. The cross sections for electron capture with no photon exchange and one-photon absorption were determined for incident-ion energy values of several keV.

Although in the paper cited just now we described the radiation by resorting to quantum electrodynamics and using the creation and annihilation operators for photons, the alternative description of the radiation as a classical electromagnetic field is quite accurate for lasers.[14] In the present work, we use this alternative description and the atomic state expansion method to investigate the influence of laser radiation on charge transfer processes in collisions between a proton and any of the alkali-metal atoms, sodium, potassium, rubidium, and cesium. The model valence-electron ground-state wave functions and the core-electron potentials suggested by Hart and Goodfriend[15] have been employed in our calculations. These wave functions and potentials were earlier utilized by

Daniele *et al.*[16] and Basu Choudhury and Sural[17] in their works in high-energy proton–alkali-metal-atom charge exchange (in the absence of radiation field) in the eikonal and impulse approximations, respectively.

We present the theory of our method in Sec. II of the paper. Section III contains the results for the laser modified cross sections for electron capture into the ground state of hydrogen in proton–alkali-metal-atom collisions. Atomic units will be used throughout except for cross sections which are expressed in units of πa_0^2.

II. THEORY

We shall describe the motion of the active electron quantum mechanically and shall assume that the proton and the alkali-metal core move along classical straight-line trajectory with constant relative velocity. This last assumption is quite valid in the keV energy range under consideration.[12] We denote the position vectors of the active electron from the proton B, the alkali-metal core A, and from their center of mass by $\mathbf{r}_B$, $\mathbf{r}_A$, and $\mathbf{r}$, respectively. The Hamiltonian of the system interacting with a single-mode laser field may be written as

$$H = H_i + V_i + H' \tag{2.1a}$$

$$= H_f + V_f + H' , \tag{2.1b}$$

where H' represents the interaction between the electron and the radiation. Treating the laser radiation classically and making the usual dipole approximation, we have $H' = \mathbf{r}\cdot\mathbf{E}_0 \sin(\omega t)$, where $\mathbf{E}_0$ is the amplitude of the electric field and ω is the angular frequency of radiation. V_i and V_f are the respective interaction potentials in the initial and final channels.

We now approximate the wave function of the total system by

$$\Psi(\mathbf{r},t) = a(t)\phi_A(\mathbf{r}_A)\exp(-i\varepsilon_A t - \tfrac{1}{2}iv_A^2 t + i\mathbf{v}_A\cdot\mathbf{r}) + b(t)\phi_H(\mathbf{r}_B)\exp(-i\varepsilon_H t - \tfrac{1}{2}iv_B^2 t + i\mathbf{v}_B\cdot\mathbf{r}) , \tag{2.2}$$

where ϕ_A and ϕ_H are the wave functions of the ground states of the alkali-metal and hydrogen atoms with ε_A and ε_H being the corresponding eigenenergies, and $\mathbf{v}_A$ and $\mathbf{v}_B$ are the velocities of the alkali-metal core and the proton in the center of mass system. The coupled equations satisfied by $a(t)$ and $b(t)$ may be derived by using a variational principle,[18] and are obtained as

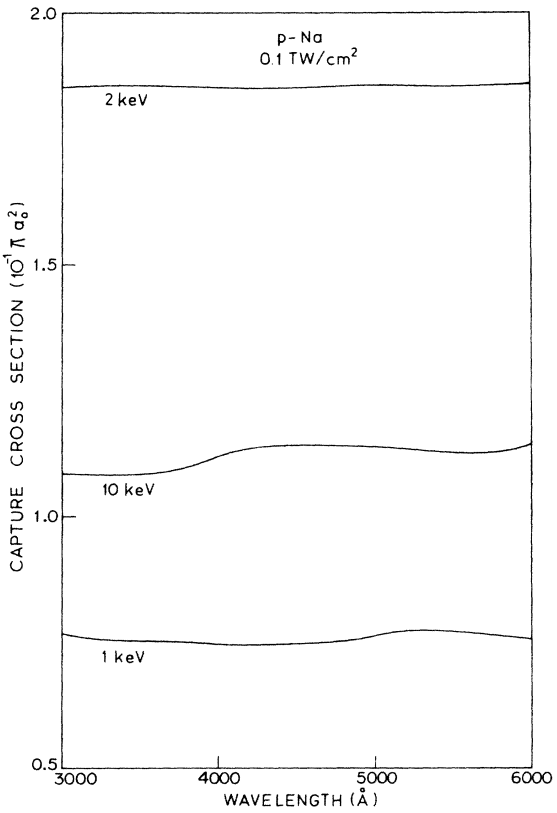

FIG. 1. Cross sections for electron capture into the ground state of hydrogen in proton-sodium collisions in presence of radiation of intensity 0.1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

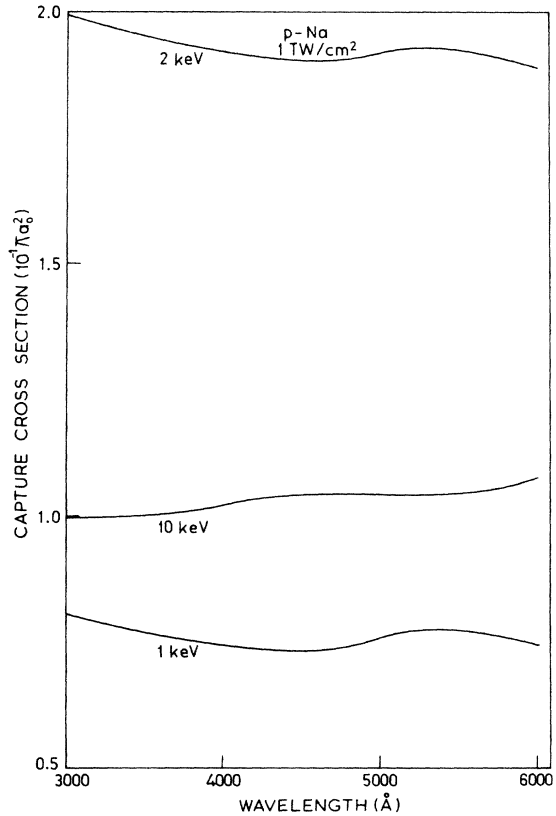

FIG. 2. Cross sections for electron capture into the ground state of hydrogen in proton-sodium collisions in presence of radiation of intensity 1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

$$i(1-|f_{01}|^2)\frac{da}{dt}=\left[F_{00}+D_{00}-\tfrac{1}{2}f_{01}\left[F_{10}+F_{01}^*-i\frac{df_{01}^*}{dt}\right]-f_{01}D_{01}^*\right]a(t)$$
$$+\left[\frac{1}{2}\left[F_{01}+F_{10}^*-i\frac{df_{01}}{dt}\right]+D_{01}-f_{01}(F_{11}+D_{11})\right]b(t)\,, \tag{2.3}$$

$$i(1-|f_{01}|^2)\frac{db}{dt}=\left[\frac{1}{2}\left[F_{10}+F_{01}^*-i\frac{df_{01}^*}{dt}\right]+D_{01}^*-f_{01}^*(F_{00}+D_{00})\right]a(t)$$
$$+\left[F_{11}+D_{11}-\frac{1}{2}f_{01}^*\left[F_{01}+F_{10}^*-i\frac{df_{01}}{dt}\right]-f_{01}^*D_{01}\right]b(t)\,. \tag{2.4}$$

In Eqs. (2.3) and (2.4), the overlap integrals and the interaction integrals occurring from collision dynamics are given by

$$f_{01}=\int\phi_A^*(\mathbf{r}_A)\phi_H(\mathbf{r}_B)\exp(-i\varepsilon t+i\mathbf{v}\cdot\mathbf{r})d\mathbf{r}\,, \tag{2.5a}$$

$$F_{00}=\int\phi_A^*(\mathbf{r}_A)V_i\phi_A(\mathbf{r}_A)d\mathbf{r}\,, \tag{2.5b}$$

$$F_{01}=\int\phi_A^*(\mathbf{r}_A)V_f\phi_H(\mathbf{r}_B)\exp(-i\varepsilon t+i\mathbf{v}\cdot\mathbf{r})d\mathbf{r}\,, \tag{2.5c}$$

$$F_{10}=\int\phi_H^*(\mathbf{r}_B)V_i\phi_A(\mathbf{r}_A)\exp(i\varepsilon t-i\mathbf{v}\cdot\mathbf{r})d\mathbf{r}\,, \tag{2.5d}$$

$$F_{11}=\int\phi_H^*(\mathbf{r}_B)V_f\phi_H(\mathbf{r}_B)d\mathbf{r}\,, \tag{2.5e}$$

with $\varepsilon=\varepsilon_H-\varepsilon_A+\frac{1}{2}(v_B^2-v_A^2)$ and the relative velocity of collision $\mathbf{v}=\mathbf{v}_B-\mathbf{v}_A$.

The radiation-dependent coupling matrix elements are

$$D_{00}=E_0\sin(\omega t)\int\phi_A^*(\mathbf{r}_A)\mathbf{r}\cdot\hat{\boldsymbol{\epsilon}}\phi_A(\mathbf{r}_A)d\mathbf{r}\,, \tag{2.6a}$$

$$D_{01}=E_0\sin(\omega t)\int\phi_A^*(\mathbf{r}_A)\mathbf{r}\cdot\hat{\boldsymbol{\epsilon}}\phi_H(\mathbf{r}_B)\exp(-i\varepsilon t+i\mathbf{v}\cdot\mathbf{r})d\mathbf{r}\,, \tag{2.6b}$$

$$D_{11}=E_0\sin(\omega t)\int\phi_H^*(\mathbf{r}_B)\mathbf{r}\cdot\hat{\boldsymbol{\epsilon}}\phi_H(\mathbf{r}_B)d\mathbf{r}\,, \tag{2.6c}$$

where $\hat{\boldsymbol{\epsilon}}$ is the unit polarization vector. In our present work we have taken the radiation to be linearly polarized with $\hat{\boldsymbol{\epsilon}}$ parallel to the direction of the relative velocity $\mathbf{v}$. As already mentioned in the Introduction, the wave function ϕ_A and the potential between the alkali-metal core and the electron are taken to be the same as the model valence-electron wave function and the corresponding potential given by Hart and Goodfriend.[15] The required parameters for the alkali-metal elements—sodium, potassium, rubidium, and cesium—can be found in their paper. In view of the fact that our calculations are generally restricted to the laboratory energy region of 1–10 keV, the effect of the electron translational factors is not expected to be high and is neglected. The coupled differential equations (2.3) and (2.4) are then numerically integrated with proper initial conditions and the capture probabilities determined using a method similar to that used in our previous work.[11] In this method the Runge-Kutta integration technique is used with step size sufficiently small to take care of the rapidly oscillating time-dependent coefficients. It may be emphasized that the probability conservation condition

$$a^*a+a^*bf_{01}+b^*af_{01}^*+b^*b=\text{const}\,, \tag{2.7}$$

follows as a consequence of the coupled differential Eqs. (2.3) and (2.4), and is a valuable check on the accuracy of the solution. This constant has initially been taken to be unity and whenever, in the course of the integration of the differential equation, the left side of Eq. (2.7) has tended to differ from unity by a preassigned small number, the step size is reduced so that the condition of probability conservation is satisfied to sufficient accuracy. We have worked out the charge transfer probabilities at different impact parameters (ρ) for each set of laser parameters and

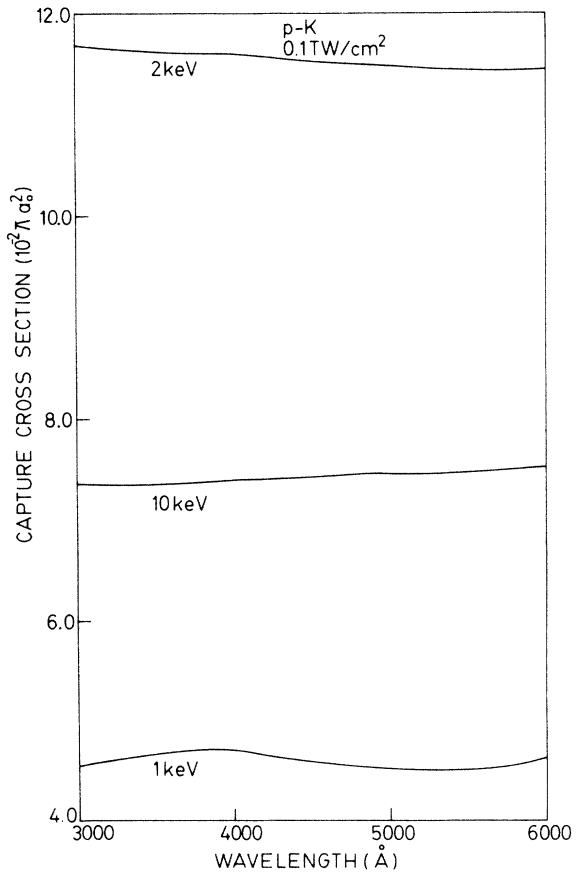

FIG. 3. Cross sections for electron capture into the ground state of hydrogen in proton-potassium collisions in presence of radiation of intensity 0.1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

collision energy. The cross sections are finally evaluated by the standard method of multiplying by $2\pi\rho$ and integration over ρ.

It may be noted that in the approximate wave function given by Eq. (2.2) we have not made explicit allowance for any shifts and widths of the atomic levels induced by the electromagnetic field. Mittleman[19] has estimated that a laser intensity of about 10^4 TW/cm^2 is required to produce an electric field of the same order as the average field experienced by the electron in a hydrogen atom. For the case of the alkali-metal atoms the required intensity will be about one hundredth of the above-mentioned value. For our problem of ground state charge transfer in proton—alkali-metal-atom collisions in the keV region, the field-induced shifts and widths of the atomic energy levels are expected to become important when the laser intensity values become greater than several TW/cm^2. An approximate wave function based upon the expansion in terms of field-free atomic states is thus adequate below these intensities. For more intense laser beams, an expansion using field-dressed states will be preferable.

III. RESULTS AND DISCUSSION

We have determined the cross sections for electron capture into the ground state of hydrogen in proton—alkali-metal-atom collisions in the presence of laser radiation with wavelength varying between 3000 and 6000 Å. All the calculations are done for two different values of laser intensity, 0.1 and 1 TW/cm^2. We present in Figs. 1 and 2 our results at these two intensities for a sodium target and incident-proton energy of 1, 2, and 10 keV. Figures 3—8 show the corresponding results for potassium, rubidium, and cesium atoms as target. It is seen that all the cross-section—wavelength curves at 1 keV exhibit characteristic undulations of small amplitude, the amplitude being greater for the higher-intensity value. At the higher energies of 2 and 10 keV for the incident proton, the charge transfer cross sections, particularly for 1-TW/cm^2 radiation intensity, change with wavelength, though not in the same typical manner as at 1 keV. These curves demonstrate the nature of the effect of the laser radiation on the charge exchange process. The collision dynamics is of course the more important mechanism affecting the charge transfer at these energies but the influence of the radiation is quite perceptible. The frequency dependence of the cross section comes through the dependence on ω of the matrix elements D_{00}, D_{01}, and D_{11} occurring in the coupled differential equations (2.3) and (2.4), its nature and magnitude being determined by the relative magnitudes of these matrix elements as compared to the other

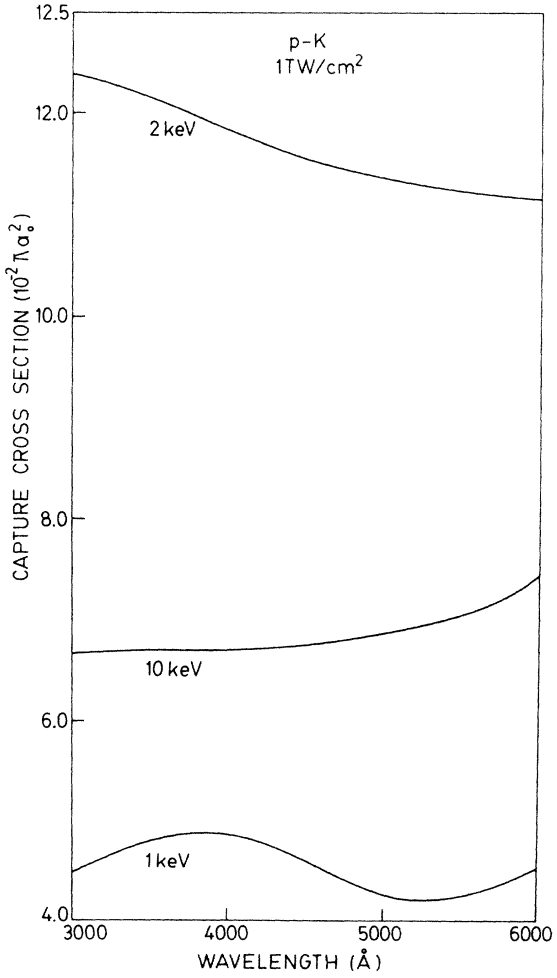

FIG. 4. Cross sections for electron capture into the ground state of hydrogen in proton-potassium collisions in presence of radiation of intensity 1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

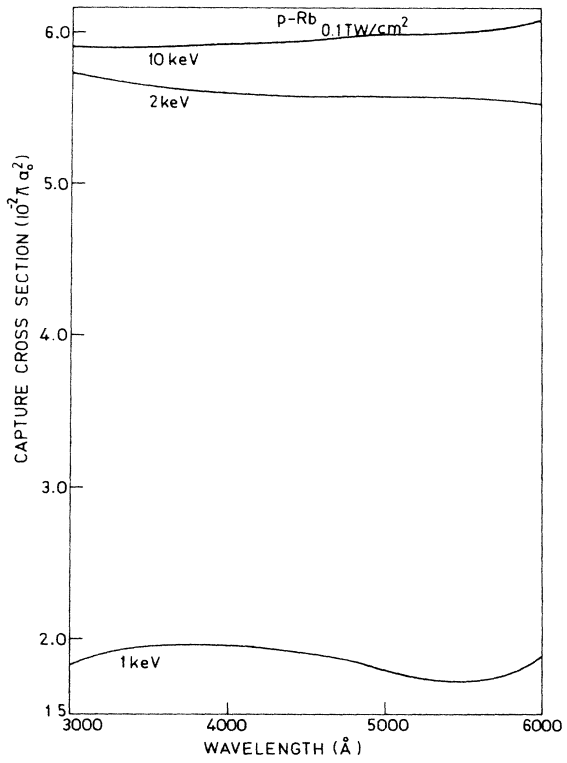

FIG. 5. Cross sections for electron capture into the ground state of hydrogen in proton-rubidium collisions in presence of radiation of intensity 0.1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

terms such as F_{00}, F_{01}, etc. arising from the collisional interaction. Since the radiation-dependent matrix elements are proportional to the square root of the laser intensity, the nature of the variation with intensity is simpler—any effect obtained with laser is generally magnified with higher intensity.

For a particular target element, the differences obtained in the values of the cross sections for different incident energies are by and large accountable to collision-induced process. The Massey criterion[20] tells us that the cross section for a nonsymmetric charge transfer in the absence of radiation field will show a maximum at an incident energy determined by the energy defect for the reaction and an "adiabatic parameter." For energy values both lower and higher than that corresponding to this maximum, the cross section decreases. The energy variations of the cross sections obtained by us have this general pattern. However, an interesting result has been obtained for a rubidium target and a laser intensity of 1 TW/cm^2. As can be seen from Fig. 6, the capture cross sections at 2 keV, while remaining lower than those at 10 keV in presence of radiation of longer wavelength ($\lambda > 5000$ Å), have become larger than the 10-keV results for $\lambda < 5000$ Å. In fact, in the lower-wavelength region of the laser field considered, the charge transfer at the two energies have been affected by radiation in opposite ways, the cross section increasing in one case and decreasing in the other. It may be pointed

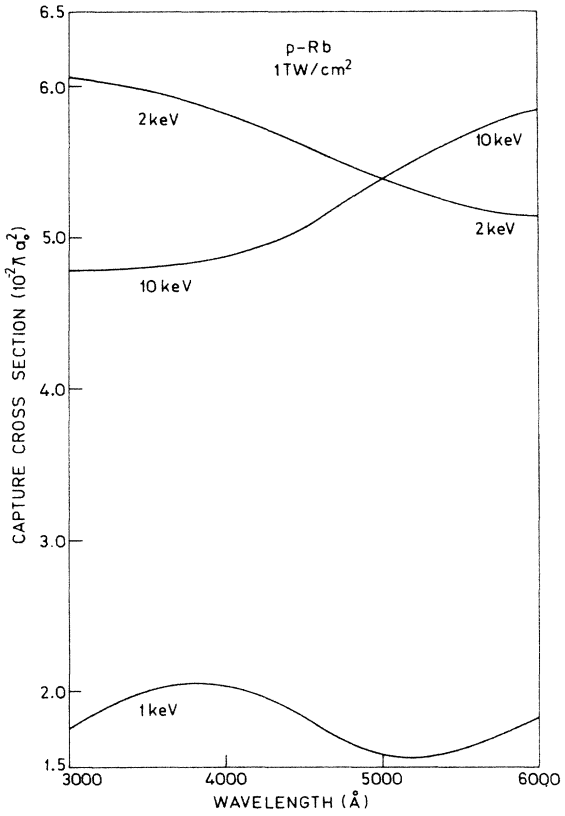

FIG. 6. Cross sections for electron capture into the ground state of hydrogen in proton-rubidium collisions in presence of radiation of intensity 1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

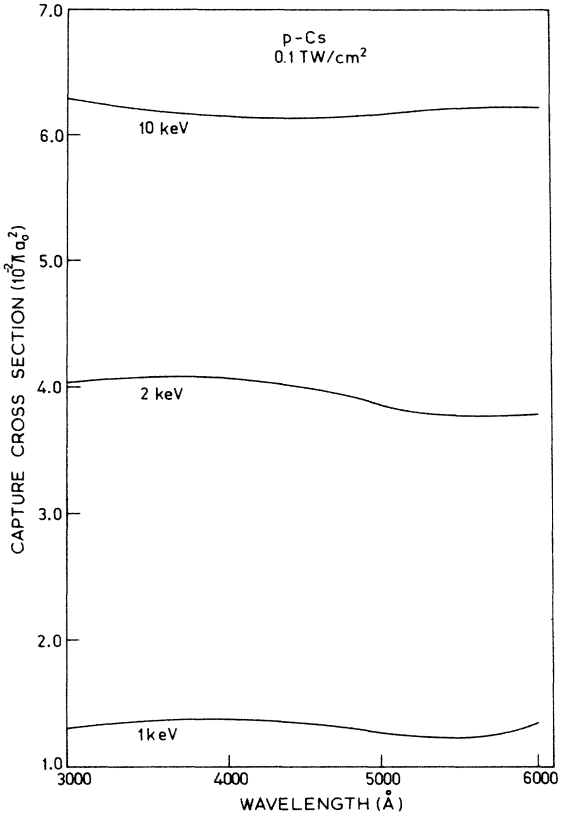

FIG. 7. Cross sections for electron capture into the ground state of hydrogen in proton-cesium collisions in presence of radiation of intensity 0.1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

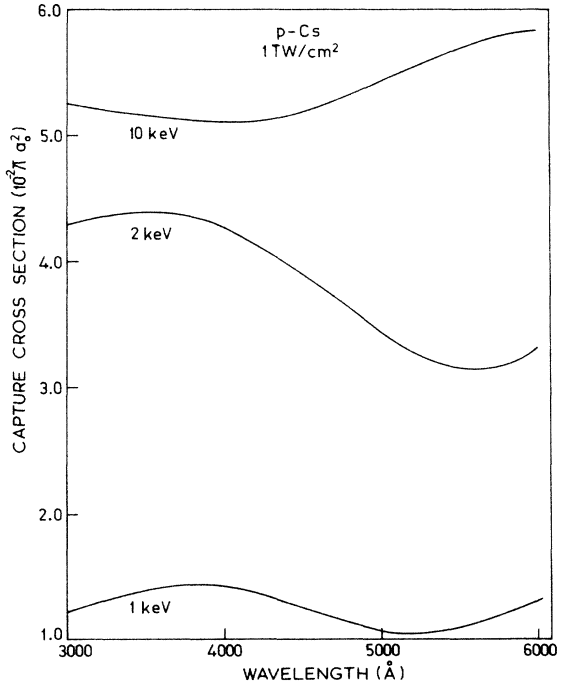

FIG. 8. Cross sections for electron capture into the ground state of hydrogen in proton-cesium collisions in presence of radiation of intensity 1 TW/cm^2 as functions of radiation wavelength for incident-ion energies of 1, 2, and 10 keV.

out that in the present work we have found that for all the alkali-metal elements concerned, depending upon the incident proton energy and the radiation wavelength used, the presence of laser increases the charge transfer cross section in some situations and diminishes it in others. This can be compared to what was found by Copeland and Tang[8] for H^+-Na and H^+-Cs collisions at considerably lower values of impact energy, where the electromagnetic field enhanced the electron capture cross sections. It would have been instructive to compare the cross sections for laser-assisted charge transfer for the proton—alkali-metal-atom case with those for other systems in the same energy region. A direct comparison with the findings of our earlier work[11] for proton-helium collisions is not possible as in that work we treated the radiation as an assembly of photons and determined only the cross sections for ground-state charge transfer with no photon exchange and one photon absorption. However, assuming that the cross sections for other types of photon exchanges are small, we notice that significant effect of the laser radiation is obtained in the proton-helium case at intensity values larger than those required for the proton—alkali-metal-atom collisions.

Our present results clearly show the type of the influence of a strong laser field on an asymmetric charge transfer phenomenon like that occurring in a collision between a proton and an alkali-metal atom. The effect of the variation of the wavelength and the intensity of the radiation can, by our method, be conveniently studied for different collision energies in the keV range. The method can be easily applied to other ion-atom collisions in presence of radiation. The accuracies of the results can be systematically improved by the inclusion of more states and the use of better wave functions.

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