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Excitation of Helium by Proton Impact

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The binary-encounter collision model for ionization of atoms by proton impact proposed by Gerjuoy and Vriens is extended to the problem of proton-impact excitation of a neutral atom from the ground state. We have calculated the proton-excitation cross sections from the ground state of a helium atom to the $n\,^1S$ $(n=2-5)$, $n\,^1P$ $(n=2-5)$, and n^1D $(n=3,\ 4)$ states using a δ function as well as a quantal-momentum distribution function for the target electrons. The calculated cross sections are compared with other theoretical calculations and the measured values.

INTRODUCTION

The direct collisional excitation of a helium target by proton impact has been the subject of intensive experimental and theoretical research. Experimental measurements for excitation to different states of helium from the ground state have been recently reported by Thomas and Bent,[1] Van den Bos *et al.*,[2] and Park and Schowengerdt.[3] These excitations have been considered theoretically by using the Born,[4-7] distortion,[8] and coupled-state[9] approximations.

No attempt has yet been made to calculate the excitation cross section of the helium atom by proton impact in the framework of the classical binary-encounter approximation. A number of methods (Gryzinski,[10] Gerjuoy,[11] and Vriens[12]) have been proposed to obtain the proton-impact ionization cross sections of the atoms in the binary-encounter approximation. The expressions for the differential cross section obtained by Gryzinski contain certain approximations. He used an approximate velocity distribution for atomic electrons to obtain the final expressions of cross sections. Gerjuoy has derived an exact expression for the differential cross section and his results have been used by Garcia[13] to calculate the ionization cross section of atoms. Vriens has derived expressions for the differential cross section in a different way by using the momentum transfer and the velocity of the incident particles as variables. However, Vriens's formula was derived under the assumption that the proton mass was very large compared to the electron mass. In this limit, Gerjuoy's formula also reduces to Vriens's formula. We therefore refer to this as the Gerjuoy-Vriens formula for proton-impact ionization.

Here we have extended the Gerjuoy-Vriens method to calculate the excitation cross section of atoms by proton impact. The classical binary-encounter theory is more valid for treating the case of ionization than excitation, since the energy transfers involved in the excitation process are small and it is difficult to correlate the classical energy continuum to the different possible quantized-angular-momentum final states. However, it is of some value to obtain the formulas in closed forms for computing the excitation by protons under the classical impulse approximation as advocated by Gryzinski. We have calculated cross sections for excitation to the n^1S $(n=2-5)$, n^1P $(n=2-5)$, and n^1D $(n=3,4)$ states of helium by protons of energy up to 5000 keV. Quantum-mechanical as well as δ-function-type velocity distribution functions have been used for the electron of the target (helium) atom.

THEORY

In the binary-encounter collision model, the excitation cross section from the ground state to a state n of an atom due to an incident charged particle of kinetic energy E_1, is given by[14]

$$\sigma_{\text{exc}}=\sum_i n_i\langle \int_{U_n}^{U_{n+1}} \sigma_E\,(v_1, v_{2i})\,dE\rangle \quad \text{if } E_1>U_{n+1}\ , \quad (1a)$$

$$\sigma_{\text{exc}}=\sum_i n_i\langle \int_{U_n}^{E_1} \sigma_E(v_1, v_{2i})\,dE\rangle \quad \text{if } U_n<E_1<U_{n+1}\ , \quad (1b)$$

where U_n and U_{n+1} are the relative energies of the states n and $n+1$, σ_E is the cross section for exchange of energy E, n_1 is the number of electrons in the shell whose energy is U_i, and $\langle\ \rangle$ denotes the average over the velocity distribution for the target electrons. v_1 and v_{2i} denote the velocities of the incident particle and the target electrons. The proton-atom collision cross section $\sigma_E\,dE$ for maximum energy transfer E is given by[12]

$$(\sigma_E)_A\,dE=\frac{2\pi e^4}{mv_1^2}\left(\frac{1}{E^2}+\frac{2mv_{2i}^2}{3E^3}\right)dE$$

$$\text{if } E\leq 2mv_1(v_1-v_{2i})\ , \quad (2a)$$

$$(\sigma_E)_B\,dE=\frac{\pi e^4}{3v_1^2 v_{2i}E^3}\ \{4v_1^3-\tfrac{1}{2}(v_2'-v_{2i})^3\}dE$$

$$\text{if } 2mv_1(v_1 - v_{2i}) \leq E \leq 2mv_1(v_1 + v_{2i}) \ , \quad (2b)$$

$$(\sigma_E)_C \, dE = 0 \qquad \text{if } E \geq 2mv_1(v_1 + v_{2i}) \ , \quad (2c)$$

where v_2' is the final velocity of atomic electron determined by

$$\tfrac{1}{2}m(v_2'^2 - v_{2i}^2) = E \ .$$

In calculation of the total cross section for the proton-impact excitation to a state n, Eqs. 2(a)–2(c) have to be integrated over the energy, and the range of the energy integral is determined by the conditions put forth in Eqs. 1(a)–1(b). This leads us to the following expressions for the excitation cross section:

When $E_1 > U_{n+1}$, we have

$$Q = \int_{U_n}^{2mv_1(v_1-v_{2i})} (\sigma_E)_A \, dE \quad \text{if } U_n \leq 2mv_1(v_1 - v_{2i}) \leq U_{n+1}, \quad (3a)$$

$$Q = \int_{U_n}^{U_{n+1}} (\sigma_E)_A \, dE \qquad \text{if } 2mv_1(v_1 - v_{2i}) \geq U_{n+1} \ , \quad (3b)$$

$$Q = \int_{U_n}^{U_{n+1}} (\sigma_E)_B \, dE$$

$$\text{if } 2mv_1(v_1 - v_{2i}) \leq U_n \leq 2mv_1(v_1 + v_{2i}) \ . \quad (3c)$$

When $U_n \leq E_1 \leq U_{n+1}$, we have

$$Q = \int_{U_n}^{2mv_1(v_1-v_{2i})} (\sigma_E)_A \, dE + \int_{2mv_1(v_1-v_{2i})}^{2mv_1(v_1+v_{2i})} (\sigma_E)_B \, dE$$

$$\text{if } U_n \leq 2mv_1(v_1 - v_{2i}) \ , \quad (4a)$$

$$Q = \int_{U_n}^{2mv_1(v_1+v_{2i})} (\sigma_E)_B \, dE$$

$$\text{if } 2mv_1(v_1 - v_{2i}) \leq U_n \leq 2mv_1(v_1 + v_{2i}) \ , \quad (4b)$$

$$Q = 0 \qquad \text{if } U_n \geq 2mv_1(v_1 + v_{2i}) \ . \quad (4c)$$

We can evaluate the integrals in the above equations and express the results in terms of dimensionless variables:

$$Q = \frac{4}{S^2U^2}\left(\frac{1}{M^2} + \frac{2t^2}{3M^4} - \frac{1}{4S(S-t)} - \frac{t^2}{24S^2(S-t)^2}\right)$$

$$\text{if } M^2 \leq 4S(S-t) \leq R^2 \ , \quad (5a)$$

$$Q = \frac{4}{S^2U^2}\left[\frac{1}{M^2} - \frac{1}{R^2} + \frac{2t^2}{3}\left(\frac{1}{M^4} - \frac{1}{R^4}\right)\right]$$

$$\text{if } 4S(S-t) \geq R^2 \ , \quad (5b)$$

$$Q = \frac{4}{S^2U^2}\left\{\frac{1}{3t}(2S^3 + t^3)\left(\frac{1}{M^4} - \frac{1}{R^4}\right) + \frac{1}{2}\left(\frac{1}{M^2} - \frac{1}{R^2}\right) + \frac{1}{3t}\left[\frac{(R^2+t^2)^{3/2}}{R^4} - \frac{(M^2+t^2)^{3/2}}{M^4}\right]\right\}$$

$$\text{if } 4S(S-t) \leq M^2 \leq 4S(S+t) \ , \quad (5c)$$

$$Q = \frac{4}{S^2U^2}\left(\frac{1}{M^2} + \frac{2t^2}{3M^4} - \frac{1}{4(S^2-t^2)}\right)$$

$$\text{if } M^2 \leq 4S(S-t), \quad (6a)$$

$$Q = \frac{4}{S^2U^2}\left(\frac{1}{8t(S+t)} + \frac{1}{2M^2} + \frac{1}{3M^4t}\left[2S^3 + t^3 - (M^2+t^2)^{3/2}\right]\right)$$

$$\text{if } 4S(S-t) \leq M^2 \leq 4S(S+t) \ , \quad (6b)$$

$$Q = 0 \qquad \text{if } M^2 \geq 4S(S+t) \ , \quad (6c)$$

where

$$S^2 = \frac{v_1^2}{U} \ , \quad t^2 = \frac{v_{2i}^2}{U} \ , \quad M^2 = \frac{U_n}{U} \ , \quad R^2 = \frac{U_{n+1}}{U} \ ,$$

and U is the ionization potential of the atom. Q is expressed in units of πa_0^2 where a_0 is the Bohr radius. The expressions (5a)–(5c) and (6a)–(6c) are then averaged over the velocity distribution of the bound electron of the target electron. If we take a δ-function velocity distribution, the expressions for σ_{exc} are given by

$$\sigma_{\text{exc}} = \sum_i n_i \frac{4}{S^2U^2}\left[\frac{1}{M^2} + \frac{2}{3M^4} - \frac{1}{4S(S-1)} - \frac{1}{24S^2(S-1)^2}\right]$$

$$\text{if } M^2 \leq 4S(S-1) \leq R^2 \ , \quad (7a)$$

$$\sigma_{\text{exc}} = \sum_i n_i \frac{4}{S^2U^2}\left[\frac{1}{M^2} - \frac{1}{R^2} + \frac{2}{3}\left(\frac{1}{M^4} - \frac{1}{R^4}\right)\right]$$

$$\text{if } 4S(S-1) \geq R^2 \ , \quad (7b)$$

$$\sigma_{\text{exc}} = \sum_i n_i \frac{4}{S^2U^2}\left[\frac{1}{3}(2S^3+1)\left(\frac{1}{M^4} - \frac{1}{R^4}\right) + \frac{1}{2}\left(\frac{1}{M^2} - \frac{1}{R^2}\right) + \frac{1}{3}\left(\frac{(R^2+1)^{3/2}}{R^4} - \frac{(M^2+1)^{3/2}}{M^4}\right)\right]$$

$$\text{if } 4S(S-1) \leq M^2 \leq 4S(S+1) \ , \quad (7c)$$

$$\sigma_{\text{exc}} = \sum_i n_i \frac{4}{S^2U^2}\left[\frac{1}{M^2} + \frac{2}{3M^4} - \frac{1}{4(S^2-1)}\right]$$

$$\text{if } M^2 \leq 4S(S-1) \ , \quad (8a)$$

$$\sigma_{\text{exc}} = \sum_i n_i \frac{4}{S^2U^2}\left(\frac{1}{8(S+1)} + \frac{1}{2M^2} + \frac{1}{3M^4} \times \left[2S^3 + 1 - (M^2+1)^{3/2}\right]\right)$$

$$\text{if } 4S(S-1) \leq M^2 \leq 4S(S+1) \ , \quad (8b)$$

$$\sigma_{exc} = 0 \qquad \text{if } M^2 \geq 4S(S+1) \ . \tag{8c}$$

We have also used the quantum-mechanical momentum distribution function given by

$$f(t) = 4\pi t^2 U \rho_{nl}(t U^{1/2}) \ , \tag{9}$$

where

$$\rho_{nl}(p) = \rho_{nl}(\vec{p}) = \frac{1}{2l+1} \sum_{m=-l}^{+l} \left| \psi_{nlm}(\vec{p}) \right|^2 \ ,$$

$$\psi_{nlm}(\vec{p}) = (2\pi)^{-3/2} \int \Phi_{nlm}(\vec{r})\, e^{i\vec{p}\cdot\vec{r}}\, d\vec{r} \ .$$

$\Phi_{nlm}(\vec{r})$ are the one-electron Hartree-Fock orbitals and are taken for this calculation from Clementi's tables.[15] When we use this distribution function σ_{exc} has to be obtained by evaluating the integrals in Eqs. (5) and (6) numerically.

RESULTS AND DISCUSSION

The results of our calculations for the excitation of single discrete states $n\,^1S$ ($n = 2-5$), $n\,^1P$ ($n = 2-5$), and $n\,^1D$ ($n = 3, 4$) of atomic helium from the ground state by proton impact are shown in Figs. (1)–(5). We have also shown in these figures the results of other calculations and measurements. The Born cross sections were calculated by Bell and coworkers and the experimental data are from measurements of Thomas and Bent, and of Van den Bos.

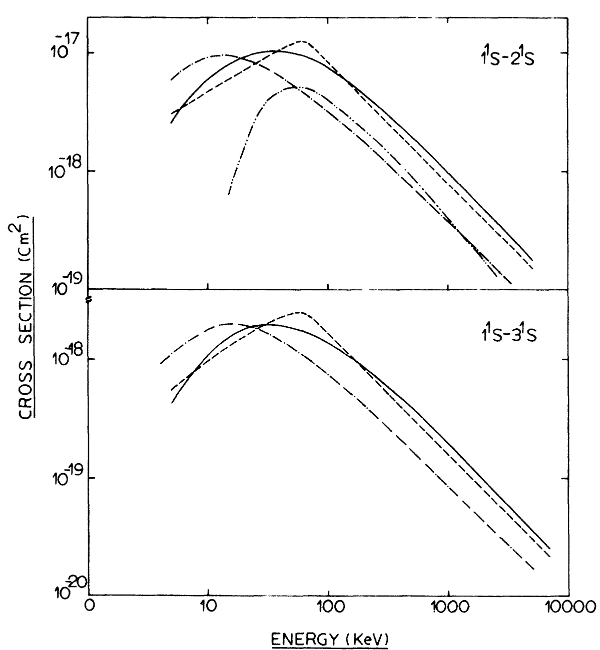

FIG. 1. Cross section for proton excitation of helium atom from the ground state to the $2\,^1S$ and $3\,^1S$ states. Present calculations: (——) quantal distribution; (----) δ-function distribution; (-•-•-) Born approximation (Ref. 4); (-••-••-) coupled-state approximation (Ref. 9).

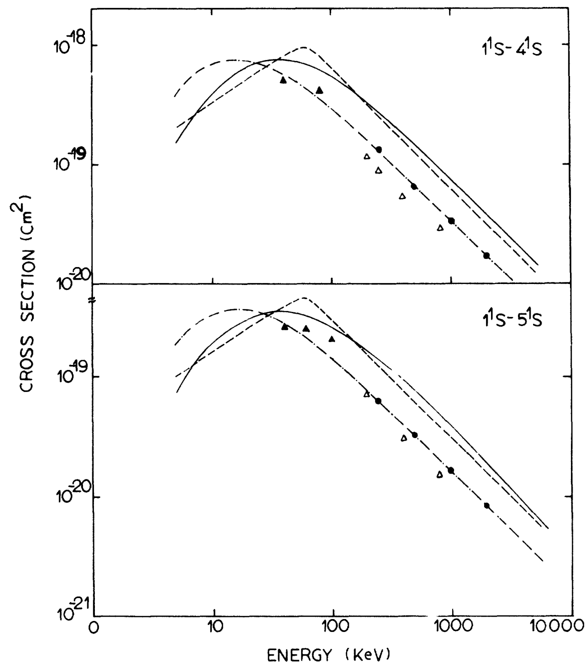

FIG. 2. Cross section for proton excitation of helium atom from the ground state to the $4\,^1S$ and $5\,^1S$ states. Present calculations: (——) quantal distribution; (---) δ-function distribution;(-•-•-) Born approximation (Ref. 4); ● (Ref. 5). Experimental data: ▲ Van den Bos *et al.* (Ref. 2); △ Thomas and Bent (Ref. 1).

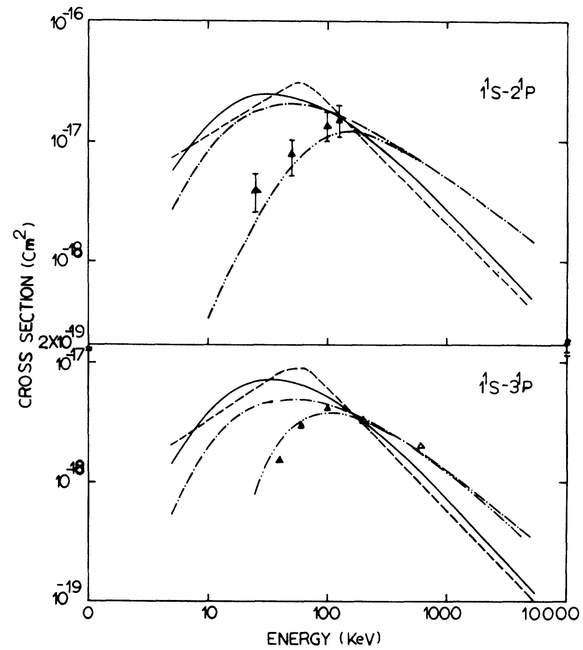

FIG. 3. Cross section for proton excitation of helium atom from the ground state to the $2\,^1P$ and $3\,^1P$ states Present calculations: (——) quantal distribution; (----) δ-function distribution; (-•-•-) Born approximation (Ref. 4); (-••-••-) coupled-state approximation (Ref. 9). Experimental data: ▲ Park and Schowengerdt (Ref. 3); ▲ Van den Bos *et al.* (Ref. 2); △ Thomas and Bent (Ref. 1).

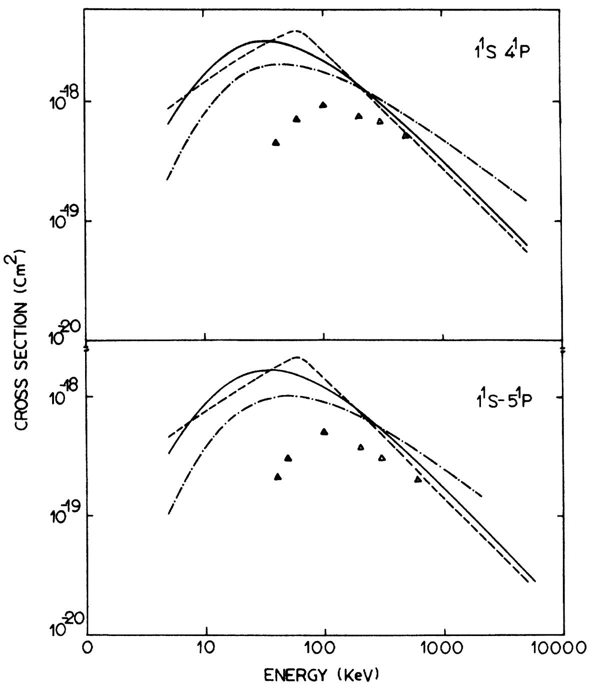

FIG. 4. Cross section for proton excitation of helium from the ground state to the $4\,^1P$ and $5\,^1P$ states. Present calculations: (——) quantal distribution; (----) δ-function distribution; (-•-•-) Born approximation (Ref. 4). Experimental data: ▲ Van den Bos *et al.* (Ref. 2); △ Thomas and Bent (Ref. 1).

$1\,^1S$-n^1S

The results for excitation to the various S states have many common features. In the lower-energy range up to 15 keV the Born cross sections are larger than our results based on the δ function and quantal-velocity distribution function. The values of σ_{exc} calculated by Van den Bos using the coupled-state approximation are much lower in this energy region than our results. Within 20–40-keV energy there is good agreement between our calculations and the Born cross sections, but the results of Van den Bos are comparatively lower. At higher energy, i.e., beyond 60 keV, the shape of the present curve agrees well with results of the Born-approximation calculation and the calculation of Van den Bos; the cross section decreases linearly with energy. For the $2\,^1S$ excitation our results at higher energy agree slightly better with the calculation of Van den Bos than with the Born approximation. For excitation to the $4\,^1S$ and $5\,^1S$ levels, our results with the quantal-momentum distribution are in good agreement with the data of Van den Bos in the energy range 40–100 keV. In the higher-energy region the agreement with the data of Thomas and Bent is not good. In general, for all other S excitations our results at higher energy are higher within a factor of 2 compared to the Born-approximation results.

$1\,^1S$-n^1P

For excitation to different P states, the present calculations yield a higher value of cross section compared to the Born approximation in the low-energy range. For energies beyond 200 keV the Born-approximation calculation gives higher cross-section values than the present calculations. For the $2\,^1P$ excitation in the energy region 20–200 keV there is good agreement between our results and the Born-approximation calculations as well as the experimental data of Park and Schowengerdt. For $3\,^1P$ excitation the present calculation agrees well with the experimental data of Van den Bos and of Thomas and Bent in the 100–200-keV region. The Born approximation and coupled-state approximation lie close to each other in the high-energy region beyond 200 keV and the present calculation gives a lower cross-section value compared to

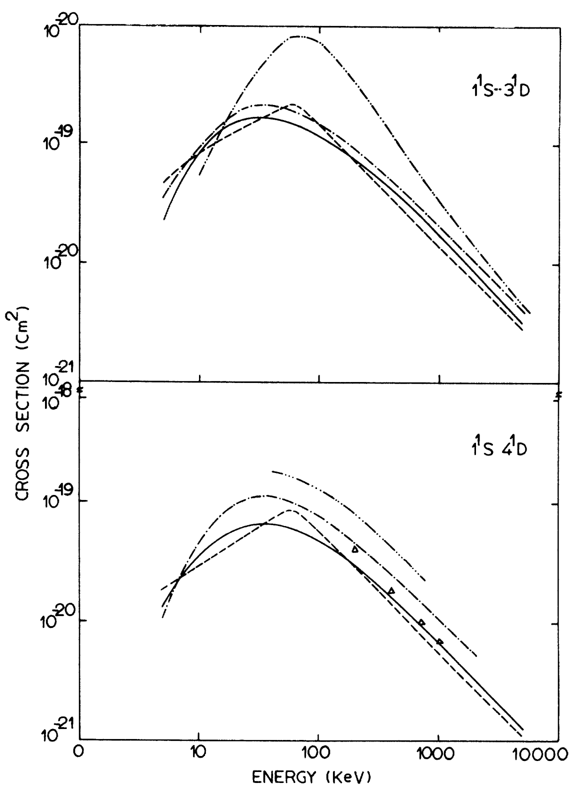

FIG. 5. Cross section for proton excitation of helium atom from the ground state to the $3\,^1D$ and $4\,^1D$ states. Present calculations: (——) quantal distribution; (---) δ-function distribution; (-•-•-) Born approximation (Ref. 4); (-••-••-) coupled-state approximation (Ref. 9); (-•••-•••-) calculation of McDowell and Pluta (Ref. 13); △ data of Thomas and Bent (Ref. 1).

these. The maximum deviation from the quantum-mechanical calculation is about 30%. For excitation to the $4\,^1P$ and $5\,^1P$ states the present calculation agrees well with the experimental data of Thomas and Bent in the energy region beyond 200 keV. The Born approximation in this region yields a higher cross-section value. For $4\,^1P$ and $5\,^1P$ excitations the agreement with the experimental data of Van den Bos is not good in the energy range up to 100 keV.

$1\,^1S$-$n\,^1D$

For the excitation to the $3\,^1D$ state we observe that the present calculation agrees closely with the Born-approximation results in the entire energy range, whereas the calculation of Van den Bos yields a high cross-section value, especially in the energy region from 40–1000 keV. For excitation to the $4\,^1D$ state the present calculation with quantal-momentum distribution agrees very well with the experimental data of Thomas and Bent in the energy region from 200 to 1000 keV. In this region the Born-approximation results and the calculations of McDowell and Pluta[16] yield a higher cross-section value.

The above calculations for the proton–helium-atom inelastic collisions based on the classical binary-encounter model have a $1/E$ dependence of cross section at higher energies. This is similar to the case of electron-atom collisions treated classically. Calculations based on the quantal approximation have a $\ln(E/E)$ dependence for optically allowed transition. However, for optically forbidden transition the Born approximation has an asymptotic $1/E$ dependence as seen from Figs. 1, 2, and 5. It is also noted that the present classical calculation using the δ-function velocity distribution and the quantal-momentum distribution function approaches to the same cross-section value at high incident energies. This feature is in agreement with our earlier observations.[17] Thus we observe that, at best, the present calculation illustrates broadly the features of the excitation function and gives a qualitative agreement with other theoretical calculations and experimental data. This is simply due to the inherent limitations of the classical approach for studying the excitation problem.

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