Singlet–singlet and triplet–triplet excitations of the helium atom by proton impact

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Abstract. Differential and integral cross sections for singlet-singlet (1S→nS, n = 2, 3, 4; 2S→1S, m = 3, 4) and triplet-triplet (2S→3S) excitations of the helium atom by proton impact are calculated in the framework of the distorted-wave approximation. A comparative study is made by taking the distorted-wave (Coulomb-wave) approximation in either the initial or final channel or both. The energy range studied is from 100–500 keV. The computed results are compared with the plane-wave results and other available theoretical results.

1. Introduction

For many years, the study of excitations in collisions between protons and helium atoms has remained a subject of considerable attention. The significance of this ion–atom collision in thermonuclear fusion, laser development, plasma diagnostics and other critical areas has led to a large number of theoretical calculations employing various approximations. With the exception of only a few calculations, all the reported measurements have dealt with the total cross sections for proton impact excitation of a target helium atom. It is well known that a knowledge of the differential cross sections can supply important information in this respect and can also provide a better test of the theoretical models against the experimental observations than can the total cross section data. The only measurement of the differential cross sections for the excitation of helium to the n = 2 level has been reported by Park et al (1978).

Extensive theoretical work has been carried out on the total cross sections for proton–helium inelastic scattering (Bell et al 1968, Flannery 1970, Tripathi et al 1971, Baye and Heenen 1973, Begum et al 1973, Roy and Mukherjee 1973, Issa 1977, Sur and Mukherjee 1979). Some calculations of the differential cross section for the excitations of the n = 2 level in He have been reported by Datta et al (1980), Flannery and McCann (1974), Sur et al (1981). No attempt (experimentally or theoretically) has yet been made to calculate the differential cross sections for the higher state excitations from ground and metastable states of the helium atom by proton impact.

In the present work, we have calculated the differential and total cross sections for singlet–singlet (1S→nS, n = 2, 3, 4; 2S→1S, m = 3, 4) and triplet–triplet (2S→3S) excitations of the helium atom by proton impact at energies 100–500 keV. A comparative study is made by taking the distorted-wave (Coulomb-wave) approximation in
either the initial or the final channel or both. The computed results are also compared with the plane-wave results and other available theoretical calculations. Atomic units are used throughout.

2. Theory

The Hamiltonian for the proton plus helium atom system, in the centre of mass reference frame, is given by (Datta et al 1980)

\[ H = \left( -\frac{1}{2\mu} \nabla^2 + \frac{1}{r_2} - \frac{1}{r_1} \right) + \left( \frac{2}{r_3} - \frac{1}{r_1} \right) \]

where \( r_1, r_2 \) and \( r_3 \) are the position vectors of the atomic electrons and incident proton respectively with respect to the nucleus of the atom. \( r'_1 \) is the position vector of the projectile with respect to the centre of mass of the atom. \( \nabla^2, \frac{1}{r_1}, \frac{1}{r_2}, \frac{1}{r_3} \) are the kinetic energy operators.

Rewriting equation (1) as

\[ H = \left( -\frac{1}{2\mu} \nabla^2 + \frac{2}{r_3} - \frac{1}{r_1} \right) + \left( \frac{2}{r_3} - \frac{1}{r_1} \right) \]

The contribution of the term \( 2/r_3 - 2/r'_1 \) to the \( T \) matrix would be negligible compared with the contribution from the \( 1/r_1^3 \) and \( 1/r_2^3 \) terms. Assuming the nucleus to be a fixed origin, terms of the order \( 1/M \) (where \( M \) is the mass of a proton) can be neglected. This implies the replacement of \( r'_1 \) by \( r_1 \).

The proton–helium Hamiltonian thus becomes

\[ H = \left( -\frac{1}{2\mu} \nabla^2 - \frac{1}{r_2} - \frac{1}{r_1^2} - \frac{2}{r_2} + \frac{1}{r_2^2} \right) + \left( \frac{2}{r_3} - \frac{1}{r_1} \right) \]

\[ = H_0 + V. \]

\( H_0 \) is the unperturbed Hamiltonian and \( V = 2/r_3 - 1/r_1^3 - 1/r_2^3 \) is the interaction potential of the incident proton with the target helium atom.

We write the total Hamiltonian \( H \) as

\[ H = H + W \]

with

\[ H = H + U \]

where \( U = \delta/r_3, \ W = (2 - \delta)/r_3 - 1/r_1 - 1/r_2 \) and \( \delta \) is the screening parameter. The functions \( \phi, \chi, \psi \) satisfy the following Schrödinger equation with Hamiltonians \( H_0, H_1 \) and \( H \) respectively:

\[ H_0\phi = E\phi \]
\[ H_1\chi = E\chi \]
\[ H\psi = E\psi \]

where \( E \) is the total energy of the system.
The integral and differential cross sections for the excitations of the helium atom from an initial state $i$ to a final state $f$ are respectively given by

$$\sigma_{i,f} = \frac{2}{k_i k_f} \int_{k_i-k_f}^{k_i+k_f} \left( \frac{d\sigma}{d\Omega} \right) q \, dq$$

and

$$\left( \frac{d\sigma}{d\Omega} \right)_{i,f} = \frac{\mu^2}{4\pi^2} \frac{k_f}{k_i} |T|^2$$

where $k_i$ and $k_f$ are the momenta of the incident and the scattered proton respectively and $q (=k_i-k_f)$ is the momentum transfer vector.

The $T$-matrix element appearing in equation (8), when the Coulomb distortion is taken in the initial channel, is given by (Saxena et al 1984, Junker 1975)

$$T = \langle \phi_f | V | \chi_i^{(+)} \rangle = \Gamma (1 + ia_i) \exp (-\pi a_i/2) I^{(I)}$$

with

$$I^{(I)} = \int dr_3 \exp (iq \cdot r_3) F_1 (-ia_i; 1; ik_f r_3 - ik_i \cdot r_3) \langle u_f (r_1, r_2) | V | u_i (r_1, r_2) \rangle.$$ (10)

The $T$-matrix element when the Coulomb distortion is taken in the final channel can be expressed as (Saxena et al 1984, Geltman and Hidalgo 1971)

$$T = \langle \chi_f | U | \chi_i^{(-)} \rangle = \Gamma (1 + ia_f) \exp (-\pi a_f/2) I^{(G)}$$

where $V' = -1/r_{i3} - 1/r_{f3}$ is the Coulomb interaction between the incident proton and the target electrons and

$$I^{(G)} = \int dr_3 \exp (iq \cdot r_3) F_1 (-ia_f; 1; ik_f r_3 + ik_i \cdot r_3) \langle u_f (r_1, r_2) | V' | u_i (r_1, r_2) \rangle.$$ (12)

When the Coulomb distortion is taken in both the initial and final channel, the $T$-matrix element, in the framework of a two-potential approach, is given by (Saxena et al 1984, Rodberg and Thaler 1970)

$$T = \langle \phi_f | U | \chi_i^{(+)} \rangle + \langle \chi_f | V | \chi_i^{(+)} \rangle$$

$$= \Gamma (1 + ia_i) \Gamma (1 + ia_f) \exp (-\pi (a_i + a_f)/2) I^{(M)}$$

with

$$I^{(M)} = \int dr_3 \exp (iq \cdot r_3) F_1 (-ia_i; 1; ik_f r_3 - ik_i \cdot r_3)$$

$$\times_1 F_1 (-ia_f; ik_f r_3 + ik_i \cdot r_3) \langle u_f (r_1, r_2) | W | u_i (r_1, r_2) \rangle.$$ (14)

where $a_i = \mu \delta_i / k_i$ and $a_f = \mu \delta_f / k_f$, $\delta_i$ and $\delta_f$ are the screening parameters corresponding to the initial and final states respectively, $_1 F_1$ is the confluent hypergeometric function, $u_i$ and $u_f$ are the spatial parts of the atomic wavefunctions for the initial and final states respectively.

Equations (9), (11) and (13) correspond to taking the projectile distortion in either the initial or the final channel or both, respectively.

The wavefunctions for the various discrete states of He are taken from (i) Byron and Joachain (1966, 1975) for the $1^1S$ and $2^1S$ states, (ii) Morse et al (1953) for the
2S and 3S states and (iii) Knox (1969) for the 3'1S and 4'1S states. With these wavefunctions, the integrals $I^{(N)}$ (equations (10), (12) and (14)) can be performed analytically (Saxena et al 1984) following the procedure of Nordsieck (1954).

3. Results and discussion

We have used equations (7) and (8) to compute the integral and differential cross sections for singlet-singlet and triplet-triplet excitations of helium by proton impact in the distorted-wave approximation. The range of energy studied is 100–500 keV. In all figures and tables, the results marked by IC, FC, BC and B are our calculations which include (i) distortion in the initial channel, (ii) distortion in the final channel, (iii) distortion in both channels and (iv) no distortion in either channel, i.e. the first Born approximation, respectively. In all our calculations (IC, FC, BC), we have taken $\delta_i$ and $\delta_f$ as equal to the full nuclear charge.

Figure 1 shows our results (IC, FC, BC and B) for the 1'1S $\rightarrow$ 2'1S excitation of helium by proton impact at 100 keV. For comparison, we have also shown (i) the Glauber approximation calculation of Sur et al (1981, curve $G$), (ii) the single-scattering Glauber calculations of Sur et al (1981, curve $SSG$), (iii) the two-state eikonal calculation of Flannery and McCann (1974, curve $\tau$) and (iv) the four-state eikonal calculation of Flannery and McCann (1974, curve $F$). From the figure, it can be seen that for scattering angles greater than 0.6 mrad the BC calculation gives the highest value for the cross section. For scattering angles above 1 mrad, we find that the IC calculation is in good agreement with the SSG calculation. The FC calculation underestimates the cross section.

![Figure 1](http://example.com/figure1.png)

**Figure 1.** Differential cross sections for the 1'1S $\rightarrow$ 2'1S excitation of helium at an incident proton energy of 100 keV. B, the first Born calculation; IC, the calculation with distortion in the initial channel only; FC, the calculation with distortion in the final channel only; BC, the calculation with distortion in both channels; G, full Glauber calculation of Sur et al (1981); SSG, the single-scattering Glauber calculation of Sur et al (1981); $\tau$, two-state eikonal calculation of Flannery and McCann (1974); F, four-state eikonal calculation of Flannery and McCann (1974).
Excitations of the helium atom by proton impact

over almost the entire angular range. The first Born calculation shows a rapid fall in the large-angle region. This is because in the FBA the scattering of the incident particle is considered from the target electrons only and not from the target nucleus. The contribution of the Coulomb interaction with the target nucleus, which would lead to large angle deflections, vanishes in the FBA because of the orthogonality of the bound-state wavefunctions. The effect of this Coulomb interaction is, however, included in the IC, FC and BC calculations by replacing the plane waves (associated with the particle in the FBA) with Coulomb waves. This leads to significant changes in the large-angle deflection probabilities.

In the large-angle region the largest deflection is obtained in the BC calculation because the effect of Coulomb distortion is considered in both the initial and final channels. The increase is less in the IC and FC calculations where the Coulomb distortion is included only in one (initial or final) channel.

From the figure it is noted that all other calculations (G, SSG, F and T) also differ considerably from the first Born calculation in the large-angle region. This is due to the fact that in the Glauber and eikonal approximations the projectile-nucleus interaction is considered in the form of phase-modulated plane waves, which in effect corresponds to the use of a variable nuclear charge.

Figure 2. Differential cross sections for the $1S \rightarrow 2S$ excitation of helium at an incident proton energy of 500 keV. The description of the curves is the same as in figure 1.

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Table 2. Differential cross section $d\sigma/d\Omega(a_0^2 \text{sr}^{-1})$ and total cross sections $\sigma(\pi a_0^2)$ for the excitations of helium by proton impact at 500 keV.

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Figure 2 shows our results (IC, FC, BC and B) for the $1^1S \rightarrow 2^1S$ excitation at 500 keV. At this energy, no other theoretical calculations are available at present to compare with our results. Here we find that as the incident energy increases from 100 to 500 keV the difference between IC, FC and BC decreases. This is to be expected from physical considerations also, as with the increase of energy the effect of distortion will become less. Also the first Born calculation (B) shows a more rapid fall towards the large-angle region at this energy. This is because for higher energies the amount of momentum transfer $q$ at large scattering angles becomes quite large. The first Born cross section (which for $e^{-}$-H inelastic (1s $\rightarrow$ 2s) scattering falls as $f_{B} \sim q^{-6}$ for large $q$) would thus decrease rapidly.

In table 1, we compare the various available results for the total cross sections for the $1^1S \rightarrow 2^1S$ excitation at energies in the range 100-500 keV.

Table 2 gives our results for DCS and TCS for the $1^1S \rightarrow n^1S$ ($n = 3, 4$), $2^1S \rightarrow n^1S$ ($n = 3, 4$) and $2^3S \rightarrow 3^3S$ excitations at 500 keV energy†. To our knowledge, no other calculations are available at present to compare with the above results.

In our calculations, we have taken the value of the screening parameter (either in the initial channel ($\delta_{i}$) or in the final channel ($\delta_{f}$)) as equal to two, i.e. the full nuclear charge of the helium atom. This is reasonable since at the energies studied here the major contribution to the cross sections comes only from the static term which is of short range. Through this short-range force the incident particle (proton) will be nearer to the target atom and will therefore see nearly the full charge.

We expect that, amongst the various calculations (B, IC, FC, BC) reported by us here, the BC calculation would provide the best results, particularly at large angles, since in this calculation distortion effects are included in both the channels. Large-angle results are significantly influenced by these distortion effects as, through the use of Coulomb waves, the incident particle can penetrate deeply into the atom.

To the best of our knowledge at present no experimental data exist for the differential or the total cross sections to compare with our results. We hope that these will be available in the near future and will provide a test for the various calculations.

Acknowledgments

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† The results at other energies, say 100 or 200 keV, can be obtained on request.
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