Proton-impact excitation of helium to the $n=2$ sublevels in the distorted-wave Born approximation

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Differential and total cross sections for proton-impact excitation of helium to the $n=2$ sublevels are calculated in the distorted-wave Born approximation. Many-parameter correlated wave functions are used to describe the helium atom. A comparison with recent theories and experimental measurements is made. The present calculations for differential cross sections for the $n=2$ substates yield good agreement with the measured values of Park *et al.* and Kvale *et al.* and the multistate eikonal calculations of Flannery and McCann.

I. INTRODUCTION

Considerable effort has gone into the study of discrete excitation of atomic helium by electron impact but relatively few studies are available for proton-impact excitation.[1,2] The proton-helium system provides one of the simplest types of heavy-particle collisions and is interesting both theoretically and experimentally because of the numerous applications of their cross-section data to the physics of the earth and planets of high atmospheres as well as to controlled thermonuclear fusion processes. Most of the theoretical or experimental studies done in the recent past concentrated only on the determination of the total cross section. Park *et al.*[3] and very recently Kvale *et al.*[4] have been successful in measuring angular differential cross sections (DCS's) for excitation of helium to the $n=2$ level and the individual $n=2$ sublevels, respectively, in the intermediate-energy region of proton impact. Obviously such angular measurements would provide a more reliable test in assessing the suitability of the theoretical approaches in understanding discrete excitations.

Looking at the theoretical literature for proton-helium excitation, we find that the various approaches developed for electron-helium excitation were logically extended to proton-helium studies as well. Among these studies, the work of Baye and Heenen[5] using a second-order diagonalization method, that of Joachain and Vanderpoorten[6] using an eikonal distorted-wave method, that of Flannery and McCann[7] employing a multistate impact-parameter method, and that of Sur and Mukherjee[8] and Sur *et al.*[9] using Glauber approximations are worth mentioning. The latter two approaches[7-9] also reported the differential-cross-section results for the $1\,^1S-2\,^1S,2\,^1P$ excitations of helium.

In recent years, the distorted-wave approximation and its variants[10] have proved to be quite successful in producing both differential and total cross sections for electron-helium excitation in the intermediate-energy region. We therefore feel that it would be desirable to perform similar calculations for proton-impact excitation of the helium atom for the above two transitions. In order to test such suitability, we present in this paper our results for both the DCS's and total cross sections for the $1\,^1S-2^1S,2\,^1P$ excitations using an earlier version[11] of the distorted-wave Born approximation (DWBA). In this approach, we incorporate the distortion in both incoming and outgoing channels of the projectile due to the Coulomb field of the target nucleus. The model we use is reasonably good and easily accessible as the expressions for the DCS can be obtained in closed form. The closed-form expressions have been given in an earlier paper (see Kumar *et al.*[11]) for both the trivial (s-s) and nontrivial (s-p) transitions. To avoid further uncertainties in the cross sections due to the input bound-state wave functions, we have used accurate target wave functions of the many-parameter correlated type (Weiss[12]). Instead of repeating the analysis, we shall outline in Sec. II briefly the present theoretical methodology. Results and discussion will be presented in Sec. III.

II. THEORY

The scattering amplitude for the excitation of the helium atom from an initial state (i) to a final state (f) by proton impact in the distorted-wave Born approximation is given as

$$T_{if}=-\frac{1}{4\pi}\frac{2\mu_r}{\hbar^2}\int d\mathbf{R}\,\chi_f^{(-)}(\mathbf{R})V_{if}(R)\chi_i^{(+)}(\mathbf{R}) \tag{1}$$

with

$$V_{if}(R)=\langle \phi_f^*(\mathbf{r}_2,\mathbf{r}_3)\,|\,V(\mathbf{r}_2,\mathbf{r}_3,\mathbf{R})\,|\,\phi_i(\mathbf{r}_2,\mathbf{r}_3)\rangle \ . \tag{2}$$

ϕ_i and ϕ_f are the initial and final bound states of the helium atom. μ_r is the reduced mass of the system. V is the interaction potential expressed as

$$V(\mathbf{r}_2,\mathbf{r}_3,\mathbf{R})=\frac{Ze^2}{\mathbf{R}}-\frac{e^2}{|\mathbf{R}-\mathbf{r}_2|}-\frac{e^2}{|\mathbf{R}-\mathbf{r}_3|}\ , \tag{3}$$

here $\mathbf{R}$ and $\mathbf{r}_2,\mathbf{r}_3$ are the coordinates of the projectile and the bound electrons, respectively. Z is the nuclear charge of the helium atom. χ_i^+ and χ_f^- are, respectively, the incident and scattered waves with $\mathbf{k}_{i\,(f)}$ as the associated wave vectors, given by

$$\chi_{i\,(f)}^{(\pm)}=\exp\left[\frac{\pi Z^{*}\mu_r}{2k_{i\,(f)}}\right]\Gamma(1\mp a_{i\,(f)})e^{i\mathbf{k}_{i\,(f)}\cdot\mathbf{R}}$$

$$\times {}_1F_1(\pm a_{i\,(f)},1;i(\pm k_{i\,(f)}R-\mathbf{k}_{i\,(f)}\cdot\mathbf{R})) \tag{4}$$

with $a_{i\,(f)}=i\mu_r Z^{*}/k_{i\,(f)}$. Z^{*} is the screened nuclear charge[13] and is always taken as -1.4. Now, after taking the Fourier transform of the interaction potential given in Eq. (3), Eq. (2) becomes

$$V_{if}(R)=\frac{e^2}{2\pi^2}\int d\mathbf{q}\,q^{-2}e^{-i\mathbf{q}\cdot\mathbf{R}}f_{if}(\mathbf{q})\ , \tag{5}$$

here $f_{if}(\mathbf{q})$ is the transition integral defined as

$$f_{if}(\mathbf{q})=\int d\mathbf{r}_2 d\mathbf{r}_3\phi_f^{*}(\mathbf{r}_2,\mathbf{r}_3)\left[\sum_{j=2}^{3}e^{i\mathbf{q}\cdot\mathbf{r}_j}\right]\phi_i(\mathbf{r}_2,\mathbf{r}_3)\ . \tag{6}$$

We have used properly orthonormalized many-parameter correlated wave functions[12] for both initial and final states of the target for calculating $f_{if}(\mathbf{q})$. Using Eqs. (6) and (5) along with Eq. (3), Eq. (1) for the scattering amplitude can be evaluated in closed form. The closed-form expressions for both transitions $1\,^1S-2\,^1S$ and $1\,^1S-2\,^1P$ are given in the recent paper by Kumar, Srivastava, and Tripathi.[11]

III. RESULTS AND DISCUSSION

A. Differential cross section

Figures 1 and 2 show our results for the DCS's at 100 keV (where our model is expected to work well) for the $1\,^1S-2\,^1S$ and $1\,^1S-2^1P$ excitations, respectively. We have also included in these figures our first-Born-approximation (FBA) calculation along with the calculations of Flannery and McCann[7] using the multistate (two- and four-state) eikonal approximation and the calculation of Sur *et al.*[9] using the Glauber approximation (GA).

Figure 1 shows the DCS results at 100 keV for the $1\,^1S-2\,^1S$ transition. In the small-angle region ($\theta_{\text{c.m.}}\le 0.02°$), the present calculation underestimates the DCS by an order of magnitude compared to the four-state calculations of Flannery and McCann[7] as well as with the experiment.[4] For scattering angles $\theta_{\text{c.m.}}\ge 0.02°$, the present results are higher within a factor of 2 than those of the four-state calculations.[7] In this angular region our results are overall in better agreement with experiment.[4] It should be noted that the two eikonal calculations, i.e., the two- and four-state calculations differ over the entire angular region. The Glauber calculations of Sur *et al.*[9] also show a large difference when compared to the present calculations. In particular the GA calculations show a broad minima around 0.04°. This feature is absent in our calculations as well as in the multistate eikonal calculations of Flannery and McCann.[7]

Figure 2 shows the DCS results at 100 keV for the $1\,^1S-2\,^1P$ transition. The general trend of variation and the relative agreement with other theoretical calculations are similar to those noted in the $1\,^1S-2\,^1S$ excitation case. The present calculation shows a better agreement with the

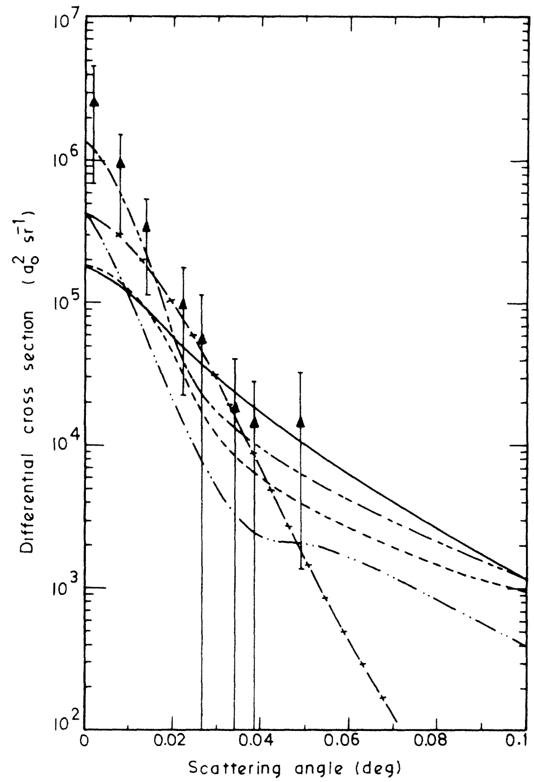

FIG. 1. Differential cross section for $H^{+}+He(1\,^1S)\rightarrow H^{+}+He(2\,^1S)$ at 100-keV proton-impact energy. Theoretical calculations: ——, DWBA results; —×—, first Born results; —··—, Glauber results (Ref. 9); — — —, two-state eikonal results (Ref. 7); — — — —, four-state eikonal results (Ref. 7); ▲, experiment (Ref. 4).

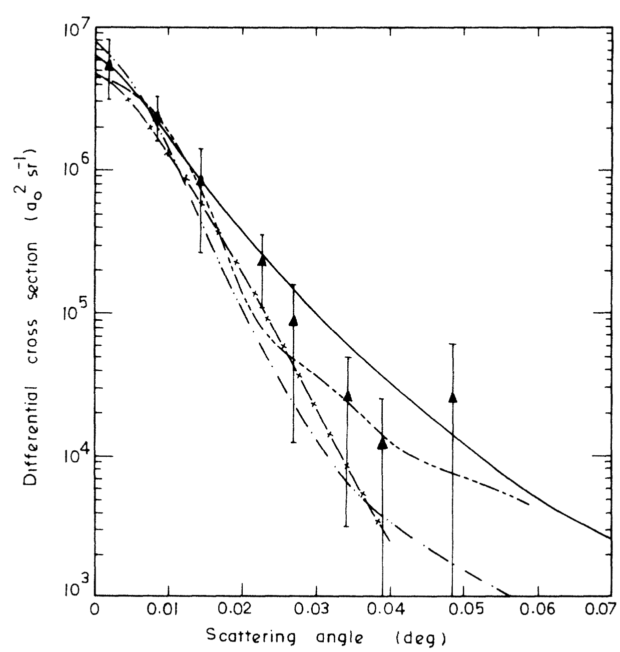

FIG. 2. Differential cross section for $H^{+}+He(1\,^1S)\rightarrow H^{+}+He(2\,^1P)$ at 100-keV proton-impact energy. Same as Fig. 1.

recent experimental measurements[4] for this transition in the entire angular region except in the angular region $0.025° \leq \theta_{\mathrm{c.m.}} \leq 0.045°$. However, in this angular region, the four-state results of Flannery and McCann[7] compare better with experimental measurements.[4] The Glauber results of Sur *et al.*[9] differ vastly from the present calculations. The Glauber calculations improve the situation only over the FBA results at large angles ($\theta_{\mathrm{c.m.}} \geq 0.05°$) where the predictions of the FBA are well known to be unreliable.[14]

Figure 3 shows the total DCS for the $n=2$ transition of helium at 100 keV. The results of the present calculations are compared with the angular differential cross-section measurements of Park *et al.*[3] and with the recent experimental measurement of the Kvale *et al.*[4] for the $n=2$ state. The present as well as other theoretical calculations are only the sum of the contributions from the $2\,^1S$ and $2\,^1P$ states. It is well known that the contributions due to transitions from the ground state to any of the triplet states are negligible because of spin conservation.[15] In the small-angle region, all the calculations show almost similar behavior and also agree with the experimental measurements.[3,4] With an increase in scattering angle, the Born and Glauber results decrease rapidly and show a large discrepancy from the measurements whereas the present DWBA results remain mostly within the error bars of the experimental measurements.[3,4] Among all the calculations, the four-state results show overall good agreement with the measurements in the entire angular region. The reason that our DWBA method does not reproduce well the experimental data as compared to the four-state eikonal method could be the simplicity of our DWBA method. For example, we have not included the effect of polarization of the target by the proton projectile in the distorted waves. It seems that one has to go to higher-order terms in the distorted-wave Born series to be able to account for this feature.

In Figs. 4 and 5, we have displayed all our other results for the differential cross sections of both transitions at energies where our model should provide good results; these may be useful for comparison purposes in the future.

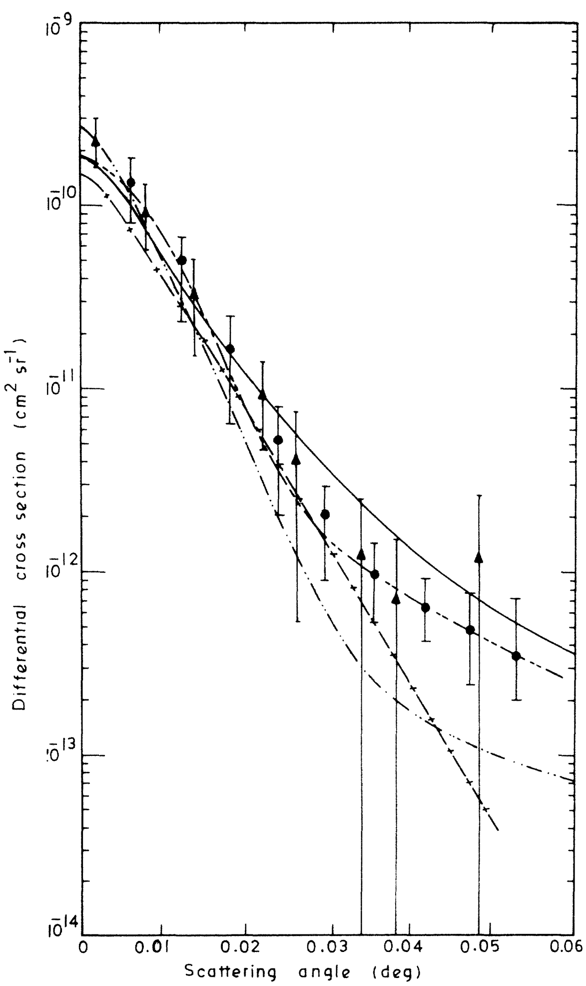

FIG. 3. Differential cross section for $H^+ + He(1\,^1S) \rightarrow H^+ + He(2\,^1S + 2\,^1P)$ at 100-keV proton-impact energy. Same as Fig. 1. ●, experiment (Ref. 3).

B. Total cross section

The total cross section for the $n=2$ state is obtained by summing the contributions from the $2\,^1S$ and $2\,^1P$ states and is displayed in Fig. 6. We have shown the curves for the $n=2$ cross section obtained from the various theoretical models along with the experimental results.[3,4,16] On comparison, we find that the first Born calculation overestimates the cross section near the maximum value of the cross section. It can also be seen that the different models predict total cross sections which differ by an order of magnitude before the peak value of the cross section. In general, the total cross section peaks between 70–100 keV. Beyond 100 keV, the differences among the

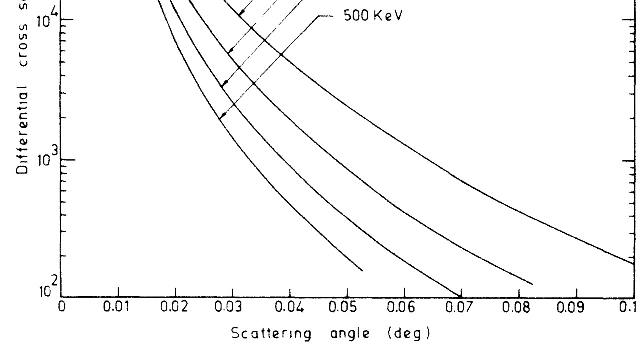

FIG. 4. Differential cross section for $H^+ + He(1\,^1S) \rightarrow H^+ + He(2\,^1S)$ at 200-, 300-, 400-, and 500-keV proton-impact energies. Same as Fig. 1.

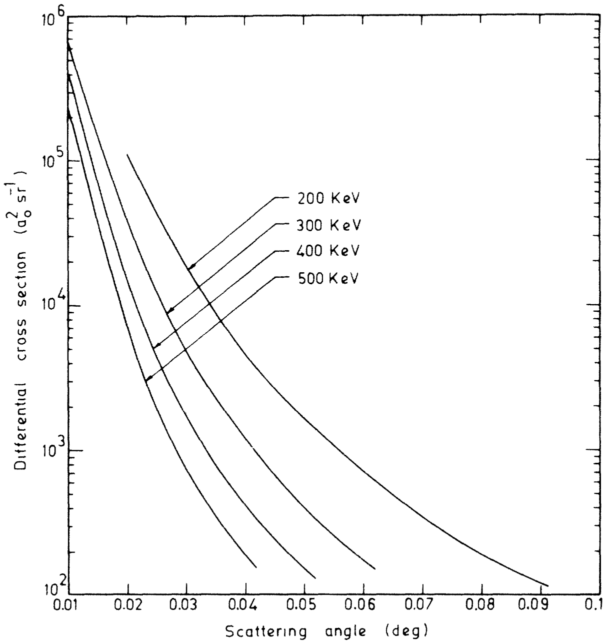

FIG. 5. Differential cross section for $H^+ + He(1\,^1S) \rightarrow H^+ + He(2\,^1P)$ at 200-, 300-, 400-, and 500-keV proton-impact energies.

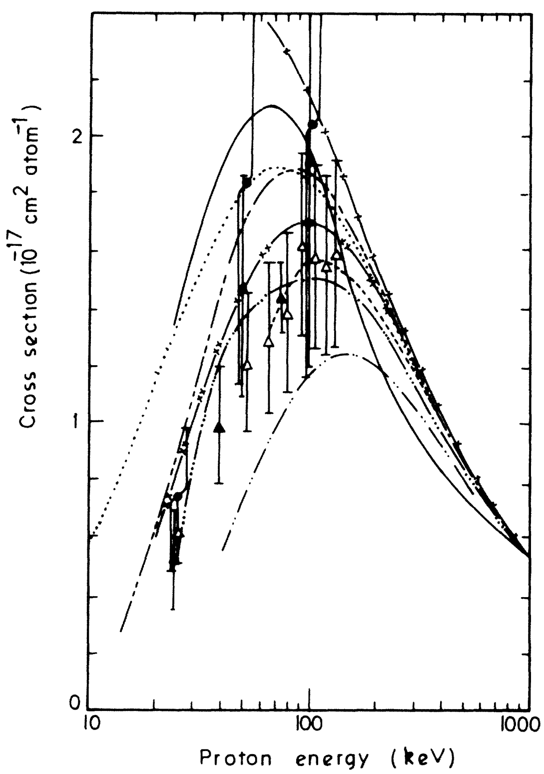

FIG. 6. Total cross section for $H^+ + He(1\,^1S) \rightarrow H^+ + He(2\,^1S + 2\,^1P)$. Theoretical calculations: ——, DWBA results; —×—, first Born results; — — — —, four-state eikonal results (Ref. 3); · · · ·, second-order diagonalization (Ref. 5); —××—, first-order potential (Ref. 6); —· · ·—, second-order potential (Ref. 18); — — —, second Born (Ref. 17); —··—, Glauber results (Ref. 6); ●, experiment (Ref. 3); △, experiment (Ref. 16); ▲, experiment (Ref. 4).

different theoretical results become smaller. They all seem to merge to the first Born results in the region beyond 400 keV. In the region between 100–400 keV, the present calculation underestimates the cross section by 40% compared to other calculations. It merges with all the results around 1000 keV. The second Born results of Holt *et al.*[17] and the second-order potential results of Begum *et al.*[18] agree better with the experimental data of Park and Schowengerdt[16] in the entire energy region where data are available. The large experimental uncertainties in the measurements preclude choosing the most reliable approach from among the different theoretical results obtained using different models.

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[1]J. T. Park, Adv. At. Mol. Phys. **19**, 67 (1983).

[2]R. Hippler, Comments At. Mol. Phys. 9, 219 (1980).

[3]J. T. Park, J. M. George, J. L. Peacher, and L. E. Aldag, Phys. Rev. A **18**, 48 (1978).

[4]T. J. Kvale, D. G. Seely, D. M. Blankenship, E. Redd, T. J. Gay, M. Kimura, E. Rille, J. L. Peacher, and J. T. Park, Phys. Rev. A **32**, 1369 (1985).

[5]D. Baye and P. H. Heenen, J. Phys. B **6**, 1255 (1973).

[6]C. J. Joachain and R. Vanderpoorten, J. Phys. B **7**, 817 (1974).

[7]M. R. Flannery and K. J. McCann, J. Phys. B **7**, 1558 (1974).

[8]S. K. Sur and S. C. Mukherjee, Phys. Rev. A **19**, 1048 (1979).

[9]S. K. Sur, Shyamal Datta, and S. C. Mukherjee, Phys. Rev. A **24**, 2465 (1981).

[10]K. H. Winters, J. Phys. B **11**, 149 (1978).

[11]M. Kumar, R. Srivastava, and A. N. Tripathi, Phys. Rev. A **31**, 652 (1985).

[12]A. W. Weiss, J. Res. Natl. Bur. Stand. **71A**, 163 (1967).

[13]B. R. Junker, Phys. Rev. A **11**, 1552 (1975).

[14]E. Gerjuoy and B. K. Thomas, Rep. Prog. Phys. **37**, 1345 (1974).

[15]*Quantum Collision Theory*, edited by C. J. Joachain (North-Holland, Amsterdam, 1974), Vol. II, Chap. 4.

[16]J. T. Park and F. D. Schowengerdt, Phys. Rev. **185**, 152 (1969).

[17]A. R. Holt, J. Hunt, and B. L. Moiseiwitsch, J. Phys. B **4**, 1318 (1971).

[18]S. Begum, B. H. Brandsden, and J. Coleman, J. Phys. B **6**, 837 (1973).