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Electron impact excitation of 1^1S–2^1S transition in helium

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Abstract. The modified variable-charge Coulomb-projected Born approximation is applied to electron impact excitation of 1^1S–2^1S transition in helium. The results are compared with other theoretical and experimental results.

Keywords. Electron impact excitation; modified Coulomb-projected Born method; distorted wave; antisymmetrization; exchange potential.

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1. Introduction

In order to improve upon the original Coulomb-projected Born method (Geltman 1971), Schaub-Shaver and Stauffer (1980) suggested the variable-charge-Coulomb-projected Born (VCCPB) approximation and applied it to electron impact excitation of hydrogen atom. They obtained encouraging results. When the same method was applied to *e*-He (Singh *et al* 1983a) and *e*-He-like ion collisions (Singh *et al* 1983b) the expected improvements were not observed. This shortcoming was traced (Singh *et al* 1983b) to an inadequate treatment of the anti-symmetrization requirement when the distorted wave calculations for the radial wavefunction are made. A modification of the VCCPB approach in the form of modified variable-charge-Coulomb-projected Born (MVCCPB) method to correct for this inadequacy was made (Singh *et al* 1984) and was applied to the calculation of the total (Singh *et al* 1984) and differential (Singh and Rai 1987) cross-sections for the electron impact $1^1S \rightarrow 2^3S$ excitation of He. The results were encouraging and in the present study we extend the method to the calculation of the total and differential cross-sections for $1^1S \rightarrow 2^1S$ excitation of He due to the electron impact.

2. Modified variable-charge-Coulomb-projected Born method

Here we give a brief account of the MVCCPB method by describing the shortcoming of the VCCPB method and the attempt that was made to remove it in the MVCCPB

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method. The detailed description and formulae are contained in the review by Singh and Rai (1987).

A comparison of the original VCCPB method with distorted wave (DW) approximations (Scott and McDowell 1975; Bhatia and Temkin 1977; Baluja *et al* 1978) shows that the VCCPB method is a form of distorted wave approximation in which distortion of the continuum electron wavefunction is considered only in the final channel. The basic difference between the DW approximations and the VCCPB method is the following. In the VCCPB method distortion is included in the final channel and the total wavefunction there assumed to be a simple product (no antisymmetrization) of the atomic wavefunction and the distorted wavefunction for the incident electron while solving the Schrödinger equation for the system to get the radial function for the distorted wave. The initial channel total wavefunction is suitably antisymmetrized but the free electron is now represented as a plane wave (no distortion). On the contrary, in the distorted wave approach the free electron wavefunction includes the effect of distortion together with the proper antisymmetrization of the total wavefunction while solving the Schrödinger equation for the total system to get the radial function for the distorted wave. The effect of antisymmetrization introduces an 'exchange potential' in the radial equation to be solved for the distorted wave, in addition to the static potential which causes the distortion. This 'exchange potential' (also known as symmetrization potential), which is included in the radial equation for the distorted wave in DW methods, is missing in the VCCPB method.

In order to remove the shortcoming of the VCCPB method we have modified it and have taken the prior form of the T-matrix. While solving for the radial functions to the distorted wavefunctions for the continuum electron in the final and initial channels the final channel wavefunction (ψ_f^-) is properly antisymmetrized and the initial channel total wavefunction is taken as a simple product function without antisymmetrization. Since ψ_f^- is properly antisymmetrized, the distorted wavefunction for the free electron in that channel is forced to satisfy the symmetry constraint imposed by the antisymmetrization of the total wavefunction. Thus the radial part of the distorted wave of the continuum electron in the final channel satisfies an inhomogeneous differential equation and the distortion is due to the static potential plus the inhomogeneity term (exchange potential). The inhomogeneity term arises due to the antisymmetrization of the total wavefunction in that channel. In the VCCPB method this antisymmetrization potential is missing from the differential equation to the radial function of the distorted wave. The radial part, in the MVCCPB method, of the distorted wave of the continuum electron in the initial channel satisfies a homogeneous differential equation and the distortion is due to the static potential only.

For the ground state (1^1S) of the helium atom we have used the Hartree–Fock wavefunction due to Byron and Joachain (1966) and the excited state wavefunction is taken from Van den Bos (1969).

3. Results and discussion

We have used the same computer program as used earlier (Singh *et al* 1984). In figure 1 the electron impact total excitation cross-section for 1^1S–2^1S transition in helium obtained in the present calculation is compared with other theoretical results (Hidalgo and Geltman 1972; Thomas *et al* 1974; Winters 1974; Scott and McDowell 1975;

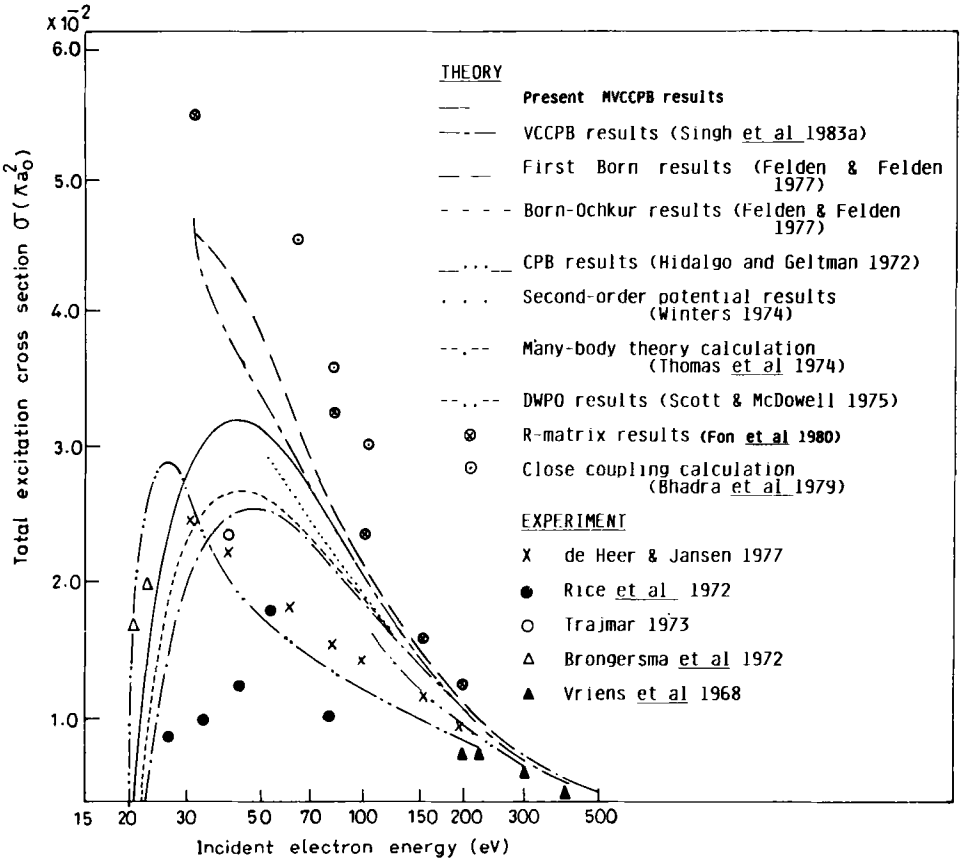

Figure 1. Total cross-section for 2^1S excitation.

Felden and Felden 1977; Bhadra *et al* 1979; Fon *et al* 1980) and experimental (Vriens *et al* 1960; Brongersma *et al* 1972; Rice *et al* 1972; Trajmar 1973; de Heer and Jansen 1977). We see that at low energies, where the VCCPB results are in very poor agreement with the experimental and other theoretical results (except for the *R*-matrix (Fon *et al* 1980) and close-coupling (Bhadra *et al* 1979) results), the MVCCPB results show better agreement. The experimental results of Rice *et al* (1972), below 50 eV, are not consistent with other experimental results. Their cross-sections are about a factor of two lower in this region. At higher energies (> 100 eV) all the results converge towards one another except the DWPO results due to Scott and McDowell (1975).

In figure 2 we have compared the differential cross-section results for the 1^1S–2^1S excitation at 29·6 eV impact energy with other experimental and theoretical results. We see that except the first Born results (Fon *et al* 1980), every calculation shows a minimum. The present results are close to the results of Scott and McDowell (1975) at both low and high angles; however, at intermediate angles the present results are closer to the *R*-matrix (Fon *et al* 1980) and close coupling calculations (Bhadra *et al* 1979)

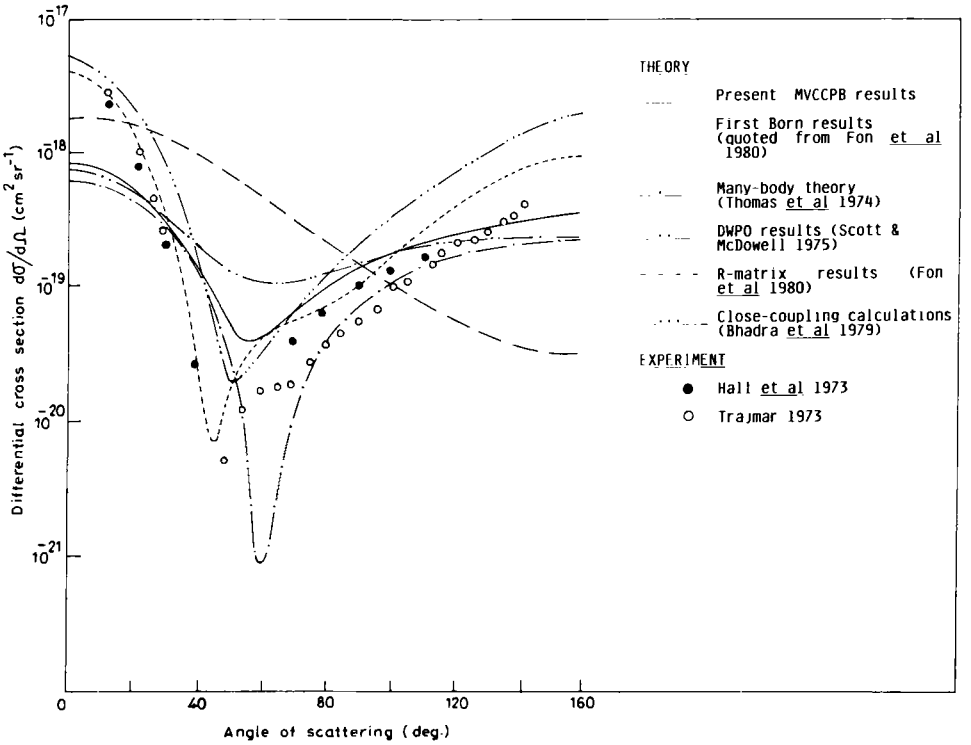

Figure 2. Differential cross-section for 2^1S excitation at 29·6 eV electron impact energy.

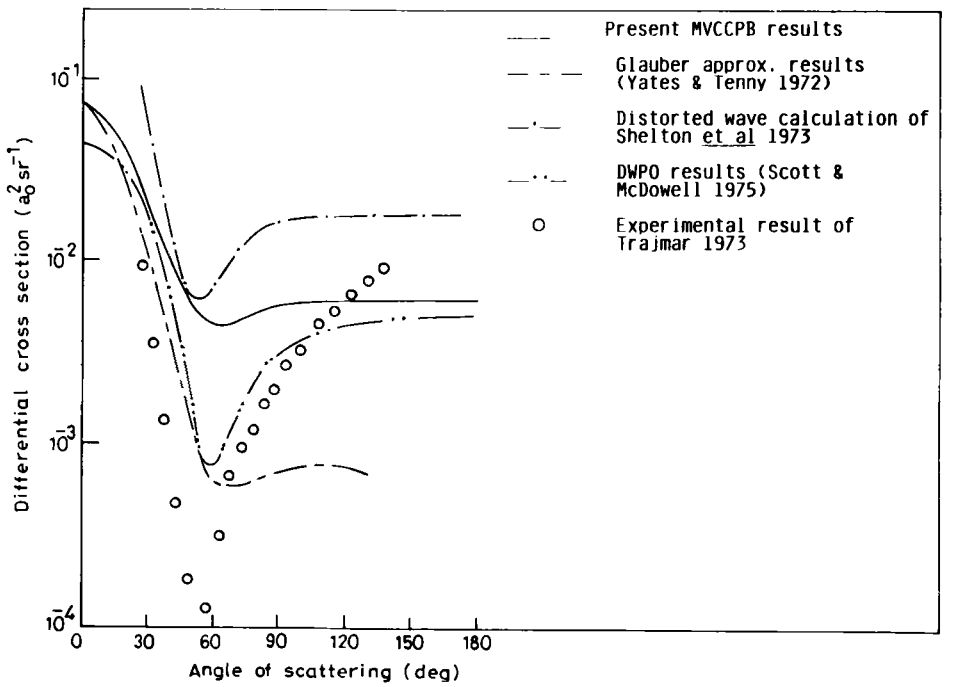

Figure 3. Same as figure 2 but for 40·1 eV impact energy.

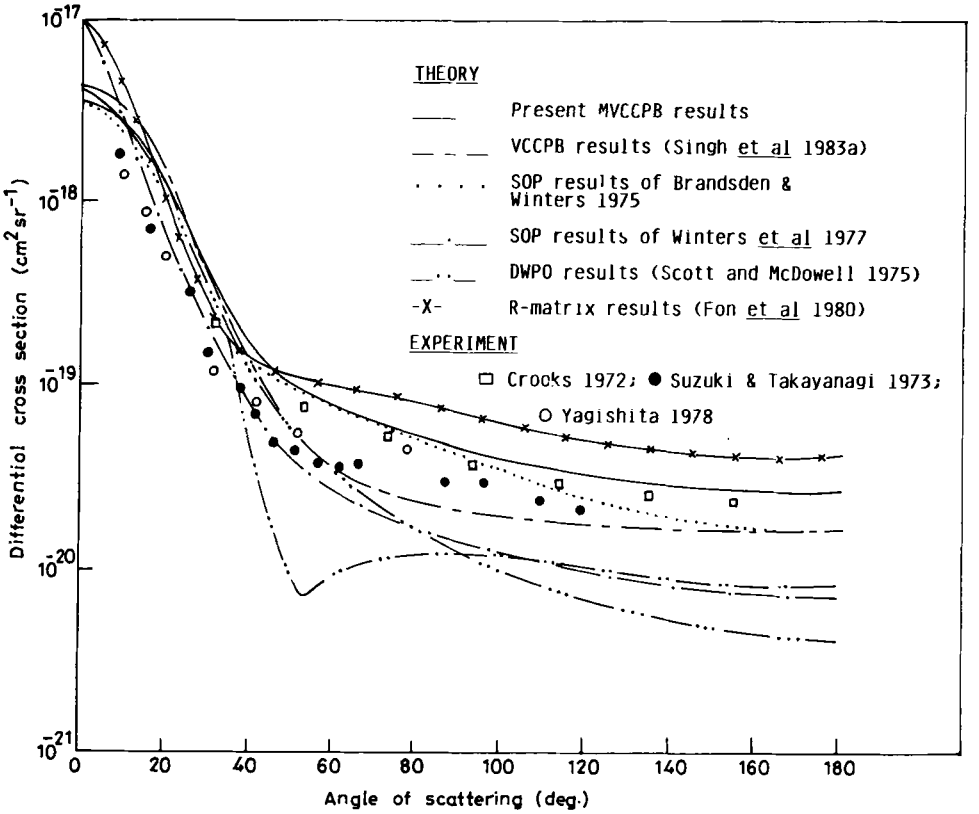

Figure 4. Same as figure 2 but for 100 eV impact energy.

than to those of Scott and McDowell (1975). All the theoretical results, except perhaps the *R*-matrix results, give poor agreement with the experimental results (Hall *et al* 1973; Trajmar 1973).

The differential cross-section results for impact energy 40·1 eV are shown in figure 3. None of the available theoretical results is in good agreement with the experimental results of Trajmar (1973). As in figure 2, our results here too are close to the results of Scott and McDowell at low and high angles but at intermediate angles the agreement is poor. At 100 eV (figure 4) our results show good agreement with experimental results due to Crooks (1972) as well as the second order potential calculations due to Bransden and Winters (1975).

The numerical results for total and differential cross-sections are also presented in table 1 for the 1^1S–2^1S transition.

The comparison of our MVCCPB results with other theoretical calculations as well as the experimental results indicates that when solving the distorted wave of the continuum electron the wavefunction of the total system should be properly antisymmetrized so that the exchange potential is included in the radial equation for the distorted wave.

Table 1. Differential and total cross-sections for 2^1S excitation of helium.

	1^1S–2^1S excitation				
$E^\dagger$(eV)	29·6	40·1	60	80	100
θ(deg)	$\frac{d\sigma}{d\Omega}(a_0^2\mathrm{Sr}^{-1})$				
0	$3{\cdot}03^{-2*}$	$6{\cdot}66^{-2}$	$1{\cdot}05^{-1}$	$1{\cdot}31^{-1}$	$1{\cdot}49^{-1}$
10	$2{\cdot}70^{-2}$	$5{\cdot}65^{-2}$	$8{\cdot}38^{-2}$	$9{\cdot}70^{-2}$	$1{\cdot}01^{-1}$
20	$1{\cdot}90^{-2}$	$3{\cdot}54^{-2}$	$4{\cdot}49^{-2}$	$4{\cdot}37^{-2}$	$3{\cdot}84^{-2}$
30	$1{\cdot}06^{-2}$	$1{\cdot}77^{-2}$	$1{\cdot}95^{-2}$	$1{\cdot}68^{-2}$	$1{\cdot}31^{-2}$
40	$4{\cdot}64^{-3}$	$8{\cdot}42^{-3}$	$9{\cdot}45^{-3}$	$7{\cdot}81^{-3}$	$5{\cdot}84^{-3}$
50	$1{\cdot}90^{-3}$	$5{\cdot}14^{-3}$	$6{\cdot}10^{-3}$	$5{\cdot}05^{-3}$	$3{\cdot}82^{-3}$
60	$1{\cdot}46^{-3}$	$4{\cdot}67^{-3}$	$4{\cdot}97^{-3}$	$3{\cdot}89^{-3}$	$2{\cdot}71^{-3}$
70	$2{\cdot}21^{-3}$	$5{\cdot}07^{-3}$	$4{\cdot}41^{-3}$	$3{\cdot}04^{-3}$	$2{\cdot}20^{-3}$
80	$3{\cdot}43^{-3}$	$5{\cdot}47^{-3}$	$3{\cdot}91^{-3}$	$2{\cdot}57^{-3}$	$1{\cdot}80^{-3}$
90	$4{\cdot}79^{-3}$	$5{\cdot}74^{-3}$	$3{\cdot}56^{-3}$	$2{\cdot}23^{-3}$	$1{\cdot}50^{-3}$
100	$6{\cdot}14^{-3}$	$5{\cdot}93^{-3}$	$3{\cdot}33^{-3}$	$1{\cdot}93^{-3}$	$1{\cdot}34^{-3}$
110	$7{\cdot}44^{-3}$	$6{\cdot}02^{-3}$	$3{\cdot}13^{-3}$	$1{\cdot}77^{-3}$	$1{\cdot}17^{-3}$
120	$8{\cdot}69^{-3}$	$6{\cdot}05^{-3}$	$2{\cdot}99^{-3}$	$1{\cdot}64^{-3}$	$1{\cdot}09^{-3}$
140	$1{\cdot}09^{-2}$	$6{\cdot}05^{-3}$	$2{\cdot}83^{-3}$	$1{\cdot}48^{-3}$	$9{\cdot}57^{-4}$
160	$1{\cdot}23^{-2}$	$5{\cdot}96^{-3}$	$2{\cdot}76^{-3}$	$1{\cdot}41^{-3}$	$8{\cdot}99^{-4}$
180	$1{\cdot}28^{-2}$	$5{\cdot}99^{-3}$	$2{\cdot}73^{-3}$	$1{\cdot}40^{-3}$	$9{\cdot}07^{-4}$
$\sigma(\pi a_0^2)$	$2{\cdot}81^{-2}$	$3{\cdot}23^{-3}$	$2{\cdot}91^{-2}$	$2{\cdot}46^{-2}$	$2{\cdot}08^{-2}$

†Incident electron energy. *Superscripts denote the power of ten by which the number is to be multiplied.

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