Pramāṇa - J. Phys., Vol. 28, No. 2, February 1987, pp. 167–179. © Printed in India.

Electron impact excitation of hydrogen and helium in Coulomb-projected Born methods

C S SINGH and D K RAI
Department of Physics, Banaras Hindu University, Varanasi 221 005, India

MS received 21 July 1986; revised 4 December 1986

Abstract. Coulomb-projected Born methods for the theoretical study of electron impact excitation of hydrogen and helium are reviewed. The results obtained by using different forms of Coulomb-projected Born methods are compared with other theoretical and experimental results and analyzed. The inadequacy of the variable charge Coulomb-projected Born approximation (VCCPB)—the most recent form of the Coulomb-projected Born methods—in giving good results in processes where exchange is dominant is discussed in detail. The 'modified' VCCPB approximation obtained by modifying the VCCPB method to remove its shortcomings is also discussed and its application to electron impact excitation of 2^3s state of helium is studied.

Keywords. Electron impact excitation; hydrogen; helium; Coulomb projection; screening; distorted wave; exchange potential; antisymmetrized.

PACS No. 34·80

1. Introduction

The Coulomb-projected Born approximation consists basically of modifying the usual Born approximation by taking an explicit account of the Coulomb interaction between the projectile and the target nucleus. Different ways of taking this Coulomb interaction into account have led to different CPB methods—Geltman's Coulomb-projected Born approximation (CPB) (Geltman 1971, 1976), generalized Coulomb-projected Born approximation (GCPB) (Stauffer and Morgan 1975) and variable-charge Coulomb-projected Born approximation (VCCPB) (Schaub-Shaver and Stauffer 1980a). Geltman's CPB method has been applied by Geltman and Hidalgo (1971) and Hidalgo and Geltman (1972) to evaluate the direct scattering amplitude for electron impact with hydrogen and helium. No account of exchange was taken. A better CPB study of e^--H scattering was carried out by Stauffer and Morgan (1975) who also included exchange contributions. These authors extended the CPB approximation by introducing a screening parameter which takes partial account of the screening of the nuclear charge by the bound electrons. Calculations were carried out for several values of the screening parameter and results in (reasonable) agreement with experiment were obtained. More recently Schaub-Shaver and Stauffer (1980a) generalized this model by making the screening parameter a function of the distance between the incident particle and the target atom. This VCCPB approximation has been applied to electron impact excitation of hydrogen (Schaub-Shaver and Stauffer 1980a) and hydrogen-like ions (Schaub-Shaver and Stauffer 1980b) and it was found that the calculated total cross-

sections are in better (as compared to the results for a fixed screening parameter) agreement with experimental and other theoretical results. When applied to electron impact excitation of 1^1S-2^1S excitation in helium (Singh *et al* 1983a) and helium-like ions (Singh *et al* 1983b) it was seen that for low impact energy the VCCPB approximation gave results which were not as good as was expected. Comparing the VCCPB method with Bhatia and Temkin's (1977) distorted wave (DW) method it was concluded that the VCCPB approximation is inadequate for processes where exchange contribution is significant. This inadequacy of the VCCPB method was discussed by Singh *et al* (1984) who also modified the VCCPB approximation to remove this shortcoming. This 'modified' VCCPB method together with the original VCCPB method has been applied to electron impact excitation of 1^1S-2^3S transition in helium. The results obtained by the 'modified' VCCPB method are in much better agreement with the experimental and other accurate theoretical results.

2. General theory of the CPB approximation

It has long been accepted that the first Born approximation (FBA) gives a reasonably accurate account of total cross-sections for a large class of inelastic processes at some sufficiently high energy. It remains unclear how high this energy (of course, this limiting energy depends on the process under consideration) must be for FBA results to be reliable within some preassigned error. Comparison of experimental and theoretical results also shows that FBA does not describe well the inelastic differential cross-sections at large angles, but again, there is no way of specifying in advance the angular range over which one can expect FBA results to be accurate within a preassigned error at a specified energy. To improve upon the Born approximation modifications of this basic approximation e.g. distorted wave Born method, Vainshtein-Presnyakov and Sobelman (VPS) method, Eikonal Born series method, Coulomb-projected Born method etc have been suggested. These modified approximations take account of the incident particle-target nucleus and incident particle-bound electron interactions to different extents. We shall mainly discuss the CPB approximation in some details.

The Coulomb-projected Born (CPB) approximation was formulated by Geltman (1976) making use of the fact that one may split the total Hamiltonian H of a system in an arbitrary way between an unperturbed part H and a perturbation V. The most common choice is to assume that the unperturbed part consists of the (N-electron) target and a non-interacting incident particle (electron in our case). We thus write

$$H = H_A - \tfrac{1}{2}\nabla^2_{r_{N+1}} \tag{1}$$

and consequently

$$V = -\frac{Z}{r_{N+1}} + \sum_{i=1}^{N} \frac{1}{|\mathbf{r}_{N+1} - \mathbf{r}_i|}, \tag{2}$$

H_A is the Hamiltonian of the target atom with N electrons. $\mathbf{r}_{N+1}$ represents the co-ordinate of the projectile and $\mathbf{r}_i$'s, for $i = 1, \ldots N$ represent the co-ordinates of the N bound electrons. The target nucleus is assumed to be infinitely heavy and at rest and is also taken as the origin of the co-ordinate system.

The transition matrix element T_{if} for a transition in which the target atom goes from

an initial state i to a final state f can be written as

$$T_{if} = \langle \exp(i\mathbf{k}_f \cdot \mathbf{r}_{N+1})\, \varphi_f(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N) | V | \Psi_i(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_{N+1}) \rangle. \tag{3}$$

Geltman included the $-Z/r_{N+1}$ term in the unperturbed part of the full Hamiltonian and wrote

$$H_0 = H_A - \tfrac{1}{2}\nabla^2_{r_{N+1}} - \frac{Z}{r_{N+1}}, \tag{4}$$

and

$$V = \sum_{i=1}^{N} \frac{1}{|\mathbf{r}_{N+1} - \mathbf{r}_i|}. \tag{5}$$

With this choice of the interaction potential the T-matrix element takes the form

$$T_{if} = \left\langle \psi_f \left| \sum_{i=1}^{N} \frac{1}{|\mathbf{r}_{N+1} - \mathbf{r}_i|} \right| \Psi_i^{(+)} \right\rangle. \tag{6}$$

For this choice of H_0 the total wavefunction ψ_f for the final state can be written in the form

$$\psi_f = \chi_f(\mathbf{k}_f, \mathbf{r}_{N+1})\, \varphi_f(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N), \tag{7}$$

where χ_f is the Coulomb wavefunction of the projectile electron (with wave vector $\mathbf{k}_f$) in the Coulomb field of the nuclear charge Z of the target atom. In the earlier way of separating H (equations (1) and (2)) the corresponding ψ_f is similar to (7) but χ_f has to be replaced by a free wave $\exp(i\mathbf{k}_f \cdot \mathbf{r}_{N+1})$ (as in this case no net positive charge is acting). It is this replacement of a Coulomb wave in place of a plane wave in the expression for T_{if} due to which Geltman's procedure is referred to as the Coulomb-projected form of the transition matrix element.

The Coulomb-projected Born approximation is obtained in the usual manner by replacing the exact scattering solution $\Psi_i^{(+)}$ by an approximate solution of the form $\exp(i\mathbf{k}_i \cdot \mathbf{r}_{N+1})\, \varphi_i(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N)$ in equation (6). $\mathbf{k}_i$ is the initial wave vector of the projectile electron and φ_i is the wavefunction of the target atom in its initial state. If we make the same replacement for $\Psi_i^{(+)}$ in expression (3) we get the Born approximation. In the Born approximation the incident electron-nucleus interaction term $-Z/r_{N+1}$ makes no contribution to the direct excitation amplitude as it vanishes due to the orthogonality of the atomic wavefunction. However, in the Coulomb-projected Born approximation i.e. equation (6), the $-Z/r_{N+1}$ term does contribute significantly even in the direct amplitude and this approximation is a better representation of the electron-atom collision process.

When applied to electron impact excitation of hydrogen (Geltman and Hidalgo 1971) (1*s*-2*s*, 1*s*-2*p*, 1*s*-3*s* transitions) the evaluated CPB total cross-sections converge to Born results at high energies, but the differential cross-sections at large angles show marked disagreement with the Born approximation though the CPB values are in reasonable agreement with experimental results.

The reason for the qualitative success of the CPB is its inclusion of the interaction between the incident electron and the target nucleus, an effect which is neglected entirely in the first Born approximation but is included in higher Born approximations. The CPB is thus analogous to a complete summation of that part of the Born series which involves the interaction between the incident electron and the target nucleus.

However, the incident electron-atomic electron interaction is included only upto the first order.

3. Generalization of the CPB method

Later Stauffer and Morgan (1975) argued that a more accurate description of electron-atom collisions must note that the incident (also the scattered) electron never 'sees' the bare nucleus, and hence does not experience its full charge but only 'sees' a partially screened charge. This screening is provided by the bound electrons in the target atom. Normally the most important contribution to the *e-A* inelastic processes involving the excitation or ionization of any particular electron from the atom A comes from impact parameters which are comparable to the appropriate shell radius. Since we are interested usually in excitation of outer valence electrons the incident electron spends most of its time outside the inner shells which effectively screen the nucleus, at least partially. At very low incident energies this argument may not hold and the incident particle may have to penetrate inside the shell in which case the screening gets changed drastically. Even the effective binding energy of the bound electrons may get changed. Such effects are well studied in the inner shell ionization of atoms by heavy charge particles (Brandt *et al* 1966a, 1966b). In this case the appropriate choices for the unperturbed Hamiltonian and the interaction are

$$H_0 = H_A - \tfrac{1}{2}\nabla^2_{r_{N+1}} - \frac{\xi}{r_{N+1}} \tag{8}$$

and

$$V = \frac{Z-\xi}{r_{N+1}} + \sum_{i=1}^{N} \frac{1}{|\mathbf{r}_{N+1} - \mathbf{r}_i|} \tag{9}$$

where $0 \leqslant \xi \leqslant Z$. The corresponding transition matrix element then becomes

$$T_{if} = \langle \varphi_f(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)\, \chi_f(\xi, \mathbf{r}_{N+1}) | V | \varphi_i(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N) \times \exp(i\mathbf{k}_i \cdot \mathbf{r}_{N+1}) \rangle. \tag{10}$$

In (10) χ_f is a Coulomb wavefunction describing the scattered free electron in the field of a charge situated at the position of the nucleus. This approximation (equation (10)) is referred to as the generalized Coulomb-projected Born (GCPB) approximation and reduces to the first Born approximation for $\xi = 0$ and to the Geltman's CPB approximation for $\xi = Z$. A further modification of the method was later suggested by Schaub-Shaver and Stauffer (1980a) in which one assumes that ξ, the screened nuclear charge, is a function of the position of the incident electron. This approximation is referred to as the variable-charge Coulomb-projected Born approximation (VCCPB) and is described in the following.

In the VCCPB approximation the perturbation potential V is taken as

$$V = -\frac{Z - \xi(\mathbf{r}_{N+1})}{\mathbf{r}_{N+1}} + \sum_{i=1}^{N} \frac{1}{\mathbf{r}_{N+1} - \mathbf{r}_i}. \tag{11}$$

Here $\xi(\mathbf{r}_{N+1})$ is the screened charge seen by the free scattered electron which depends on

the position of the scattered electron. The VCCPB choice for $\xi(r_{N+1})$ is based on the following arguments.

The charge density (in units of e) due to a single electron, say electron 1, in the N-electron system described by a wavefunction $\varphi(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N)$ can be written as

$$\rho_1(r_1) = \int d\mathbf{r}_2\, d\mathbf{r}_3 \ldots d\mathbf{r}_N |\varphi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2. \tag{12}$$

The charge density $\rho(r)$ at position $\mathbf{r}$ due to all the atomic electrons is therefore given by

$$\rho(r) = N\rho_1(r). \tag{13}$$

The potential experienced by the incident electron at position $\mathbf{r}_{N+1}$ due to this total electronic charge density $\rho(r)$ at the point $\mathbf{r}$ is given by

$$U(r_{N+1}) = \int \frac{\rho(r)}{|\mathbf{r} - \mathbf{r}_{N+1}|} d\mathbf{r}. \tag{14}$$

Hence from (12) and (13), we have

$$U(r_{N+1}) = N \int \frac{|\varphi(\mathbf{r}_1; \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2}{|\mathbf{r}_1 - \mathbf{r}_{N+1}|} d\mathbf{r}_1\, d\mathbf{r}_2 \ldots d\mathbf{r}_N. \tag{15}$$

The total potential of the incident electron is thus given by

$$-\frac{Z}{r_{N+1}} + U(r_{N+1}). \tag{16}$$

If we write $Q(r_{N+1})/r_{N+1} = U(r_{N+1})$, then the effective potential felt by the incident electron can be written as

$$-\frac{Z}{r_{N+1}} + \frac{Q(r_{N+1})}{r_{N+1}}$$

or by $$-[Z - Q(r_{N+1})]/r_{N+1}. \tag{17}$$

(This expression is just the static potential of the atom when it is in the state described by the wavefunction $\varphi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$). Based on this description the screened charge seen by the scattered particle can be taken as

$$\xi(r_{N+1}) = Z - Q(r_{N+1}). \tag{18}$$

It is clear that as long as the unperturbed part of the Hamiltonian i.e. H_0 can be written as the sum of two terms—one representing the target atom and another which is a function of the projectile electron co-ordinate $\mathbf{r}_{N+1}$, we can always write for ψ_f

$$\psi_f = \varphi_f(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \cdot F(\mathbf{r}_{N+1}). \tag{19}$$

$F(\mathbf{r}_{N+1})$ represents the wavefunction of the scattered particle. Since in the VCCPB approximation the above decomposition of H_0 holds, in this VCCPB method ψ_f is represented as in (19).

Transition matrix element for the VCCPB approximation for electron-helium

scattering is obtained by putting $N = 2$ in (10), replacing $\chi_{\mathbf{k}_f}(\xi, \mathbf{r}_{N+1})$ by $F(\mathbf{r}_3)$ and antisymmetrizing the initial state wavefunction

$$T_{if}^{\text{VCCPB}} = \langle \varphi_f(1,2) F(\mathbf{r}_3) | V | \mathscr{A} \varphi_i(1,2) \exp(i\mathbf{k}_i \cdot \mathbf{r}_3) \rangle. \tag{20}$$

V is given by equation (11). $\mathscr{A}$ is the antisymmetrization operator.

Direct T^d and exchange T^{ex} transition matrices were obtained (Schaub-Shaver and Stauffer 1980b) separately by expanding $F(\mathbf{k}_f, \mathbf{r})$ as a sum over partial waves

$$F(\mathbf{k}_f, \mathbf{r}) = \frac{1}{\sqrt{k_f}} \sum_l \frac{(2l+1)\, i^l \exp(i\delta l)\, U_l(k_f, r)\, P_l(\cos\theta)}{r}, \tag{21}$$

where θ represents the angle between the final momentum vector $\mathbf{k}_f$ of the scattered electron and its radius vector $\mathbf{r}$ and $P_l(\cos\theta)$ is the Legendre polynomial of degree l. $U_l(k_f, r)$ satisfies the differential equation

$$\left(\frac{d^2}{dr^2} + k_f^2 - \frac{l(l+1)}{r^2} + \frac{2\xi(r)}{r}\right) U_l(k_f, r) = 0. \tag{22}$$

The boundary conditions to be satisfied by U_l are

$$U_l(k_f, r) = 0 \qquad r \to 0 \tag{23}$$

and

$$U_l(k_f, r) = k_f^{-1/2} \sin\left(k_f r - \frac{l\pi}{2} - \delta_l\right). \qquad r \to \infty$$

Equation (22) was solved by a non-iterative procedure due to Marriot (1958), the normalization being obtained by comparison with the JWKB solution (Burgess 1963).

The differential cross-section was obtained by using the expression

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2} |T^d - T^{ex}|^2. \tag{24}$$

The total cross-section σ is obtained after integrating this expression over the angular co-ordinates.

When applied to helium-like atoms (Singh *et al* 1983a, b) for 2^1S excitation by electron impact it is seen that the results obtained using VCCPB method at higher energies are in agreement with other theoretical and experimental results. Differential cross-section obtained by this method at 100 eV and 200 eV in the case of helium atom is in better agreement with the experimental results than CPB results (Singh *et al* 1983a). At low energies the results obtained by this method (VCCPB) diverge from other (similar) theoretical and experimental results (Singh *et al* 1983a, b).

This method (VCCPB) was further applied (Singh *et al* 1984) to electron impact excitation of 2^3S state in helium atom. The results obtained are in very poor agreement with other theoretical and experimental results (for all values of the impact energy) (figure 1). Looking at these results it was conjectured that the VCCPB approximation gives poor result in processes where exchange phenomenon is dominant. (The 2^3S excitation of helium atom by electron impact can occur only through exchange because

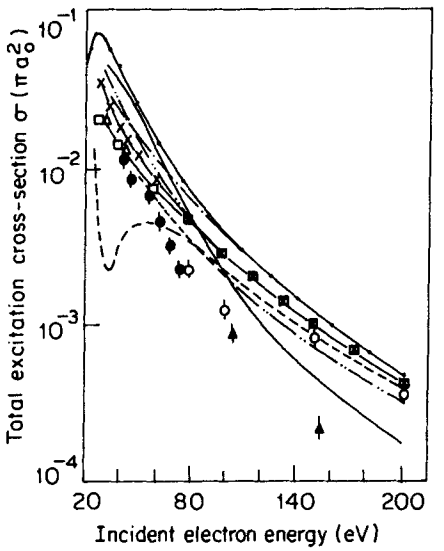

Figure 1. Total cross-section for 1^1S-2^3S transition in helium by electron impact. **Theory**: -□-□- 'modified' VCCPB results; —— VCCPB results; -..- R-matrix (Fon *et al* 1979); -.- Many body theory (Thomas *et al* 1974); — — DWPO results (Scott and McDowell 1975); - x - x - DW results (Baluja and McDowell 1979); ----- Second-order potential method (Winters 1974 cited in Scott and McDowell 1975); —·—·— Born calculation (Felden and Felden 1977). **Experiment**: ○ Yagishita (1978a); △ Trajmar (1973); ● Crooks *et al* (1972); ▲ Vriens *et al* (1968).

relativistic effects are being neglected and in electron impact excitation of 2^1S state of helium-like atoms exchange is considerable at low energies). To verify this conclusion we shall analyze the VCCPB method and compare it with Bhatia and Temkin's (1977) (BT) distorted wave approach as there is an apparent similarity between the two methods even though the results obtained by the VCCPB method in the case of electron impact excitation of helium-like ions (Singh *et al* 1983b) are not in reasonable agreement with those obtained by the BT method.

4. Excitation of 2^3S state of helium

It is easy to show that the VCCPB model, in which the effective nuclear charge as seen by the projectile varies with the latter's position, is essentially a distorted wave Born (DWB) approximation wherein the distortion is included in the final channel only. The screening parameter determines the static potential of the target system in its initial state and the distortion of the scattered particle wavefunction by this potential is considered.

The VCCPB method when applied to electron impact excitation of 1^1S-2^1S transition in helium-like ions yields cross-section results, at low incident energies (where exchange contributions are significant), which are in very poor agreement with results obtained by Bhatia and Temkin (1977). This particular form (BT model) of the DW model is very similar to the VCCPB model differing only in the choice of channel in which distortion is included. The BT model includes distortion in the initial channel

while the VCCPB model includes it in the final channel. Both models do not take any account of polarization. To explain the large discrepancy between the VCCPB results and the other DW results in the case of electron impact 1^1S-2^1S excitation in helium and helium-like ions and in the case of 1^1S-2^3S transition in helium atom we examine (Singh *et al* 1984) the DW methods and the VCCPB method.

We see that in the DW methods distortion is taken into account in both the channels or, if in only one channel, in the initial channel for which the wavefunction is properly antisymmetrized. On the other hand in the VCCPB method, distortion is considered in the final channel where the wavefunction ψ_f is unsymmetrized. In the DW methods the distorted radial wavefunction $U_l(r)$ satisfies the differential equation

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-2V_{1s,1s}(r)+k_f^2\right)U_l(r)=W(r)U_l(r), \tag{25}$$

whereas in the VCCPB method the distorted radial function satisfies the equation

$$\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-V_{1s,1s}(r)+k_f^2\right)U_l(r)=0. \tag{26}$$

These two equations differ from one another in an important manner, namely the presence of an additional antisymmetrization (also sometimes referred to as exchange potential, Baluja *et al* 1978) potential $W(r)$ in the former equation. $V_{1s,1s}(r)$ and $V_{1s,2s}(r)$ are the static potentials of helium in the ground and excited configurations respectively. Thus in the DW methods the additional Hartree-Fock exchange potential $W(r)$ is included while solving the radial part of the distorted wavefunction whereas in the VCCPB method this is not so. The distortion introduced in the VCCPB method is, therefore, inadequate.

Recently we used a VCCPB type DW model utilizing the prior form of T-matrix to remove this discrepancy and obtained very good results for 1^1S-2^3S excitation of helium by electron impact. The mathematical details are as follows:

In the case of electron helium scattering

$$H=-\sum_{i=1}^{3}\frac{1}{2}\nabla_i^2-\sum_{i=1}^{3}\frac{Z}{r_i}+\sum_{\substack{i=1\\j>i}}^{3}\frac{1}{r_{ij}}. \tag{27}$$

Z is the nuclear charge and is equal to 2 in the case of helium, but can take other values for other helium-like systems. In the decomposition

$$H=H_i+V_i \tag{28}$$

we take

$$H_i=\sum_{i=1}^{3}\frac{1}{2}\nabla_i^2-\sum_{i=1}^{2}\frac{Z}{r_i}+\frac{1}{r_{12}} \tag{29}$$

and

$$V_i=-\frac{Z}{r_3}+\sum_{i=1}^{2}\frac{1}{r_{13}}. \tag{30}$$

Let us write V_i as a sum of two terms

$$V_i=U_i+W_i \tag{31}$$

and take

$$U_i = \langle \varphi_f(1,2) | V_i | \varphi_f(1,2) \rangle. \tag{32}$$

In other words U_i is the static potential of the target in the final state. The prior form of the T-matrix element then takes the form

$$\langle \mathscr{A}\varphi_f(1,2)\, F_f(3) | V_i - U_i | \varphi_i(1,2)\, F_i(3) \rangle. \tag{33}$$

In the above equation we have replaced the exact total wavefunction of the final channel i.e. $\Psi_f^{(-)}$ by an approximate but properly antisymmetrized function $\mathscr{A}\varphi_f(1,2)F_f(3)$.

For the ground state 1^1S of helium atom we have used a wavefunction due to Byron and Joachain (1966) of the form

$$\varphi_i(\mathbf{r}_1, \mathbf{r}_2) = (4\pi)^{-1} R_i(r_1, r_2) \tag{34}$$

with
$$R_i(r_1, r_2) = R_{1s}(r_1) R_{1s}(r_2) \tag{35}$$

The one-electron radial functions were represented by a sum of two exponentials:

$$R_{1s}(r) = (Ae^{-pr} + Be^{-qr}). \tag{36}$$

The parameters have the values

$$A = 2{\cdot}60505, \quad B = 2{\cdot}081144, \quad p = 1{\cdot}41, \quad q = 2{\cdot}61$$

The excited state wavefunction $\varphi_f(\mathbf{r}_1, \mathbf{r}_2)$ for the 2^3S state is represented in the form (Van den Bos 1969)

$$\varphi_f(\mathbf{r}_1, \mathbf{r}_2) = (4\pi)^{-1} R_f(r_1, r_2) \tag{37}$$

with
$$R_f(r_1, r_2) = \phi_1(r_1)\, \phi_2(r_2) - \phi_1(r_2)\, \phi_2(r_1). \tag{38}$$

The one-electron functions ϕ_1 and ϕ_2 are again represented in terms of exponentials:

$$\phi_1(r) = \exp(-a_n r) \quad \text{and} \quad \phi_2(r) = N[\exp(-c_n r) - br\exp(-b_n r)]. \tag{39}$$

The parameters have the values

$$a_n = 2{\cdot}0, \quad c_n = 1{\cdot}57, \quad b_n = 0{\cdot}61, \quad N = 4{\cdot}1956, \quad b = 0{\cdot}340.$$

If we expand $F_n(\mathbf{r}_3)$ $[n = i, f]$ in terms of partial waves in the form

$$F_n(\mathbf{r}_3) = k_n^{-1/2} r_3^{-1} \sum_{l=0}^{\infty} (2l+1)\, i^l \exp[\pm i\{\delta_l + \eta_l(k_n)\}] \times U_l^n(k_n, r_3)\, P_l(\cos \hat{k}_n \cdot \hat{r}_3) \tag{40}$$

($\pm$ sign is used in the exponential according to whether it is an outgoing or an incoming distorted wave), we see that U_l^n satisfies the differential equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - 2U_i(r) + k_n^2\right) U_l^n(r) = \delta_{nf}\left[\frac{4}{2l+1}(F_1 Y_l^{(1)}(r) + F_2 Y_l^{(2)}(r)) + 2\delta_{l0}\, r\, S(r)\right]. \tag{41}$$

We have used the following definitions of $Y_l^{(1)}$ and $Y_l^{(2)}$

$$Y_l^{(1)}(r_3) = r_3 \int_0^\infty \phi_1(r_1)\, U_l^n(r_1) r_1 \frac{(r_{13})_<^l}{(r_{13})_>^{l+1}}\, dr_1 \tag{42}$$

and

$$Y_l^{(2)}(r_3) = r_3 \int_0^\infty \phi_2(r_1)\, U_l^n(r_1) r_1 \frac{(r_{13})_<^l}{(r_{13})_>^{l+1}}\, dr_1. \tag{43}$$

These quantities $Y_l^{(1)}$ and $Y_l^{(2)}$ satisfy the following Hartree type exchange equations:

$$\frac{d^2}{dr^2} Y_l^{(j)}(r) = \frac{l(l+1)}{r^2} Y_l^{(j)}(r) - (2l+1)\, \phi_j(r)\, U_l^n(r) \tag{44}$$

$$j = 1, 2.$$

F_1, F_2 and S are functions of r and depend on the final state atomic wavefunction parameters.

From equation (41) the following points emerge:

(i) The radial part $U_l^i(r)$ of the wavefunction $F_i(\mathbf{r})$ satisfies a homogeneous differential equation as in this case the right hand side vanishes as $\delta_{nf} = \delta_{if} = 0$. The resulting homogeneous differential equation is

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_i^2 - U_i(r)\right) U_l^i(r) = 0$$

and differs from a free partial wave of momentum $\mathbf{k}_i$ only in the presence of the potential $U_i(r)$. This potential as already mentioned above is the static potential of the helium atom in the final state. So the radial wave $U_l^i(r)$ contains distortion effects only due to this potential.

(ii) (a) The radial function Uf for the $l = 0$ partial wave in the final channel satisfies an inhomogeneous equation. The inhomogeneous term in this case consists of two parts namely

$$\frac{4}{2l+1}(F_1(r) Y_l^{(1)}(r) + F_2(r) Y_l^{(2)}(r)) \quad \text{and} \quad 2rS(r).$$

Both these terms contain contributions from both initial and final atomic states. In addition, the first term, i.e. the term involving $Y_l^{(1)}(r)$ and $Y_l^{(2)}(r)$, incorporates exchange terms of the type one sees in atomic calculations using the Hartree-Fock method.

Thus we find that $U_0^f(r)$ satisfies an equation which differs from a free wave equation and includes distortion effects not only due to the static potential U_i but also due to the Hartree exchange potential.

(b) For waves with $l \neq 0$ the term $2\delta_{l0} rS(r)$ on the right-hand side of equation (41) vanishes and hence the inhomogeneity consists of one term i.e.

$$\frac{4}{2l+1}(F_1(r) Y_l^{(1)}(r) + F_2(r) Y_l^{(2)}(r)).$$

However, in view of the remarks in (iia) even this partial wave includes distortion due to Hartree exchange potential in addition to that due to the static potential U_i.

We compared the present results (total cross-section) (figure 1) obtained for the 1^1S-2^3S excitation of helium atom by electron impact using the VCCPB method as well as the 'modified' VCCPB method with other calculations. The results obtained in the VCCPB model are in very poor agreement with the results of other distorted wave models (Scott and McDowell 1975; Baluja and McDowell 1979, Winters 1974) and also with other calculations (Thomas *et al* 1974; Fon *et al* 1979; Felden and Felden 1977). The results obtained by using the 'modified' VCCPB method on the other hand are in close agreement with the experimental results (Yagishita 1978; Trajmar 1973; Crooks 1972; Vriens *et al* 1968) even for low incident energies. For incident energies $\geqslant 80$ eV the 'modified' VCCPB results nearly coincide with the results obtained in the very sophisticated DW calculation due to Baluja and McDowell (1979). Differential cross-sections obtained at 40·1 eV and 100 eV also show a qualitative agreement with the experimental results (figures 2–3).

We take the prior form of the T matrix in the modified VCCPB method and write

$$T = \langle \Psi_f^{(-)} | V_i - U_i | \psi_i \rangle$$

and include the effect of distortion in $\Psi_f^{(-)}$. Since $\Psi_f^{(-)}$ is now a properly symmetrized wavefunction the distorted wavefunction is forced to satisfy the symmetry constraint (see equation (41) and comments on it) referred to above. This results in a proper inclusion of the Hartree-Fock exchange (symmetrization) potential in the radial part of the distorted wave equation thereby removing the shortcoming of the original VCCPB method. The wave-function ψ_i in the initial channel also includes distortion but only due to the potential U_i which we took as the static potential in the final state of the target helium atom. Since we retain the concept of the variable screening in our calculations with this scheme and retain distortion in the final channel as in the VCCPB

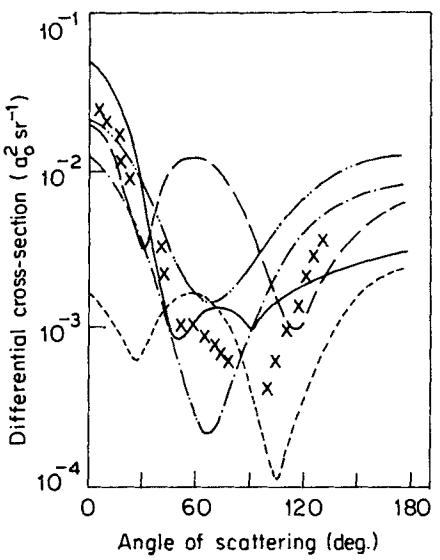

Figure 2. 1^1S-2^3S differential cross-section at 40·1 eV electron impact energy. — — 'modified' VCCPB results; —— VCCPB results; – – – – DWPO results (Scott and McDowell 1975); –.– DW results (Shelton *et al* 1973); –..– Many-body theory (Thomas *et al* 1974); × Experimental results of Trajmar (1973).

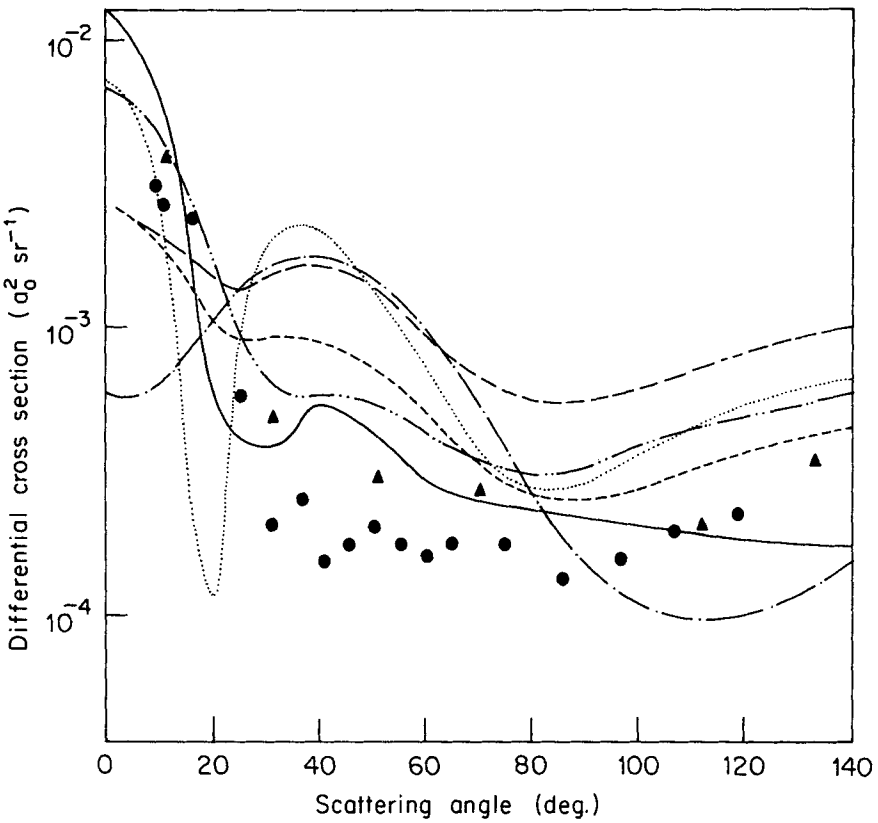

Figure 3. Same as figure 2 but for 100 eV electron impact energy. **Theory**: ..... 'modified' VCCPB results; —— VCCPB results; -.- DWPO results (Scott and McDowell 1975); —— Many body theory (Thomas *et al* 1974); ----- Second order potential method (Bransden and Winters 1975); -..- R-matrix (Fon *et al* 1979). **Experiment**: ▲ Crooks (1972); ● Yagishita *et al* (1976).

method (in contrast to BT model where the distortion is in the initial channel only) we refer to this model as the 'modified' VCCPB prior form model.

In order to convince ourselves that a simple inclusion of distortion (in the sense of the VCCPB method) in both the channels is not capable of allaying the deficiency of the VCCPB method as exemplified by its failure to reproduce 1^1S-2^3S excitation cross-sections we made separate calculations in the VCCPB method itself after including distortion in the initial channel also. In these calculations, however, we did not include symmetrization potential while solving the radial equation for the distorted wave in the initial channel. The right-hand side (exchange potential) of equation (41) was put equal to zero in both the cases. The cross-sections obtained in this set of calculations are almost indistinguishable from the earlier unmodified VCCPB results.

References

Baluja K L and McDowell M R C 1979 *J. Phys.* **B12** 835
Baluja K L, McDowell M R C, Morgan L A and Myerscough V P 1978 *J. Phys.* **B11** 715

Bhatia A K and Temkin A 1977 *J. Phys.* **B10** 981
Brandt W, Laubert R and Sellin I 1966a *Phys. Lett.* **21** 518
Brandt W, Laubert R and Sellin I 1966b *Phys. Rev.* **151** 51
Bransden B H and Winters K H 1975 *J. Phys.* **B8** 1459
Burgess A 1963 *Proc. Phys. Soc.* **81** 442
Byron F W and Joachain C J 1966 *Phys. Rev.* **146** 1
Crooks G B 1972 Ph.D. Thesis, University of Nebraska (unpublished)
Crooks G B, Dubois R D, Golden D E and Rudd M E 1972 *Phys. Rev. Lett.* **29** 329
Felden M M and Felden M A 1977 *Can. J. Phys.* **55** 396
Fon W C, Berrington K A, Burke P G and Kingston A E 1979 *J. Phys.* **B12** 1861
Geltman S 1971 *J. Phys.* **B4** 1288
Geltman S 1976 *Electron and photon interactions with atoms* (ed.) H Kleinpoppen and M R C McDowell (New York: Plenum Press) p. 387
Geltman S and Hidalgo M B 1971 *J. Phys.* **B4** 299
Hidalgo M B and Geltman S 1972 *J. Phys.* **B5** 617
Marriot R 1958 *Proc. Phys. Soc.* **72** 121
Schaub-Shaver J A and Stauffer A D 1980a *J. Phys.* **B13** 1457
Schaub-Shaver J A and Stauffer A D 1980b (Private communication)
Scott T and McDowell M R C 1975 *J. Phys.* **B8** 1851
Shelton W N, Baluja K L and Madison D H 1973 *Proc. Eighth Int. Conf. on Physics of Electronic and Atomic Collisions* (Belgrade Institute of Physics) Abstract p. 296
Singh C S, Rai S N, Srivastava R and Rai D K 1984 *Z. Phys.* **A319** 9
Singh C S, Srivastava R and Rai D K 1983a *Phys. Rev.* **A27** 302
Singh C S, Srivastava R and Rai D K 1983b *Can. J. Phys.* **61** 981
Stauffer A D and Morgan L A 1975 *J. Phys.* **B8** 2172
Thomas L D, Csanak G, Taylor H S and Yarlagadda B S 1974 *J. Phys.* **B7** 1779
Trajmar S 1973 *Phys. Rev.* **A8** 191
Vanden Bos J 1969 *Phys. Rev.* **181** 191
Vriens L, Simpson J A and Mielczarck S R 1968 *Phys. Rev.* **165** 7
Winters K H 1974 Ph.D. Thesis, University of Durham
Yagishita A 1978 (quoted in Fon *et al* 1979)
Yagishita A, Takayanagi T and Suzuki H 1976 *J. Phys.* **B9** L53