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Final Report Report
on
Few Electron Transitions
in Atomic Collisions

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1 Work Completed

1.1 Introduction

During the past three years we have evaluated probabilities and cross sections for few and multiple electron transitions in atomic collisions. Our studies included interactions of atoms and molecules with incident protons, bare ions, electrons, positrons, anti-protons, ions carrying electrons and photons. We also studied the inter-relation between collisions with charged particles and collisions involving various processes with photons.

This work has complemented various studies of collisions of atoms with charged particles[1, 2, 3, 4, 5] and with photons[6, 7, 8] as well as more general efforts to understand the nature of multi-electron systems[9, 10, 11, 12, 13, 14, 15]. Our aim has been to begin with relatively simple two electron systems and to focus on fast processes in which there is too little time for complicated processes to occur. We have used a variety of computational techniques, but we emphasize those appropriate for fast collisions in which we hope to obtain insight into the physical nature of the process itself. We generally considered systems in which experimental data was available.

1.2 Calculations with incident charged particles and anti-particles

Techniques were developed[16] to include correlation in the double excitation of atoms. These techniques have been applied to various two-electron processes including excitation-ionization by projectile impact. The aim of our primary technique has been to represent multi-electron bound states with fully-correlated configuration-interaction (CI) wave-functions and to replace the time-ordering operator in the second-order term by its integral representation. Our method yields the scattering amplitude as a sum of analytical terms for the first-order and energy-conserving second-order contributions and a one-dimensional integral for the energy-nonconserving second-order contribution. Thus, the technique greatly reduces computer time.

We used pseudostates to represent high Rydberg and continuum states. Because these expansions have the same analytical character as hydrogenic orbitals, an exponential multiplied by a polynomial in the radius, the general analytic form found for hydrogenic transitions may be applied to transitions

to such states. This technique results in a one-dimensional integral for the energy-nonconserving second-order term and analytical expressions for the energy-conserving second-order and first-order terms in the many-electron transition amplitude.

1. Scattering Amplitude:

The probability amplitude for transition from an initial state $|i\rangle$ to a final state $|f\rangle$ may be written,

$$a_{if} = \langle f | T \exp[-i \int V(t) dt] | i \rangle , \quad (1)$$

where V is the interaction between the projectile and the electrons in the atom,

$$V(t) = \sum_j e^{-iH_0 t} V_j(t) e^{iH_0 t} , \quad (2)$$

in which

$$V_j(t) = -\frac{Z_p}{|\mathbf{R}(t) - \mathbf{r}_j|} + \frac{Z_p}{R} \quad (3)$$

and T is the time ordering operator[3, 17, 18]. The Born expansion of the amplitude is then given by

$$a_{fi} = a_{fi}^{(0)} + a_{fi}^{(1)} + a_{fi}^{(2)} \dots , \quad (4)$$

where $a_{fi}^{(0)} = \langle f | i \rangle$, which will be zero for the problems under consideration.

2. First order amplitude:

The first order amplitude is

$$a_{fi}^{(1)} = -i \int_{-\infty}^{\infty} dt \langle f | e^{iH_0 t} [V_1(t) + V_2(t)] e^{-iH_0 t} | i \rangle . \quad (5)$$

For initial and final states given as CI wave functions,

$$|i\rangle = \sum_{\alpha_1 \alpha_2} C_{\alpha_1 \alpha_2} |\alpha_1\rangle |\alpha_2\rangle \quad (6)$$

and

$$\langle f| = \sum_{\beta_1 \beta_2} \bar{C}_{\beta_1 \beta_2} \langle \beta_1| \langle \beta_2|, \quad (7)$$

one then obtains a weighted sum of one-electron scattering amplitudes

$$A_{n'\ell'm', n\ell m} = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle n'\ell'm'| V(t) | n\ell m \rangle \quad (8)$$

and overlap integrals $\langle n'\ell'm' | n\ell m \rangle$ as the fully correlated two-electron amplitude:

$$a_{fi}^{(1)} = \sum_{\beta_1 \beta_2} \bar{C}_{\beta_1 \beta_2} \sum_{\alpha_1 \alpha_2} C_{\alpha_1 \alpha_2} (-i) \left[A_{\beta_1, \alpha_1}^{\lambda' \lambda}(\omega) \langle \beta_2 | \alpha_2 \rangle + A_{\beta_2, \alpha_2}^{\lambda' \lambda}(\omega) \langle \beta_1 | \alpha_1 \rangle \right] . \quad (9)$$

3. Second order amplitude:

The second order amplitude may be put in the form of pair-products of one-electron transition amplitudes (8) if the time-ordered intermediate-state propagator is replaced by its integral representation,

$$\frac{T}{2} e^{-iE_n(t-t')} = \int_{-\infty}^{\infty} d\Omega e^{-i\Omega(t-t')} \left[\frac{1}{2} \delta(\Omega - E_n) + \frac{i}{2\pi} P \frac{1}{\Omega - E_n} \right] . \quad (10)$$

It is

$$a_{fi}^{(2)} = \sum_n \int \sum_{\beta_1 \beta_2} \bar{C}_{\beta_1 \beta_2} \sum_{\alpha_1 \alpha_2} C_{\alpha_1 \alpha_2} \\ \times \left\{ \frac{(-i)^2}{2} \left[\sum_{\nu_1} \sum_{\nu_2} \hat{C}_{\nu_1 \beta_2} \hat{C}_{\alpha_1 \nu_2} A_{\beta_1, \nu_1}^{\lambda' \lambda}(E_f - E_n) A_{\nu_2, \alpha_2}^{\lambda' \lambda}(E_n - E_i) \right] \right\}$$

$$\begin{aligned}
& + \sum_{\nu_2} \sum_{\nu_1'} \hat{C}_{\beta_1, \nu_2} \hat{C}_{\nu_1', \alpha_2} A_{\beta_2, \nu_2}^{\lambda' \lambda} (E_f - E_n) A_{\nu_1', \alpha_1}^{\lambda' \lambda} (E_n - E_i) \Big] \\
& - \frac{i}{2\pi} P \int_{-\infty}^{\infty} \frac{d\Omega}{\Omega - E_n} \\
& \times \left[\sum_{\nu_1} \sum_{\nu_2'} \hat{C}_{\nu_1, \beta_2} \hat{C}_{\alpha_1, \nu_2'} A_{\beta_1, \nu_1}^{\lambda' \lambda} (E_f - \Omega) A_{\nu_2', \alpha_2} (\Omega - E_i) \right. \\
& \left. + \sum_{\nu_2} \sum_{\nu_1'} \hat{C}_{\beta_1, \nu_2} \hat{C}_{\nu_1', \alpha_2} A_{\beta_2, \nu_2}^{\lambda' \lambda} (E_f - \Omega) A_{\nu_1', \alpha_1}^{\lambda' \lambda} (\Omega - E_i) \right] \Big\} , \quad (11)
\end{aligned}$$

where $\sum_n$ extends over bound and continuum intermediate states.

The projectile-charge dependence of cross sections for excitation-ionization in many-electron atoms may be calculated using a technique that greatly reduces the computer costs of multi-electron calculations. The first-order amplitude is given in analytic form and may be made as exact as desired. The second-order amplitude contains an analytic energy conserving term (correlated generalization of the IEA) and an energy nonconserving (time-ordered) one-dimensional integral that interferes with the first-order term. Additional detail is given in Section 5.

1.2.1 Time ordering

In our analysis the role of time ordering is emphasized. The time ordering operator, T , is defined in Eqs.(1) and (10). This operator enforces causality in the evolution operator, $U(t_2, t_1)$ by restricting $U(t_2 < t_1) = 0$. If this restriction is not enforced, then T may be replaced by its average value, $T_{av} = 1$ in Eq.(10). Thus, the effect of time ordering is carried by the operator $T - T_{av}$.

Various features of time ordering have been noted[3, 18]:

1. T_{av} is a factor of i out of phase with respect to $T - T_{av}$, as may be seen from Eq.(10).
2. Correlation in time may be ascribed to $T - T_{av}$.

3. The $T - T_{av}$ contributions may be ascribed to non-energy conserving fluctuations about intermediate state energies, as may be seen from Eq.(10).
4. In a calculation second order in the projectile charge, Z , the phase of $T - T_{av}$ in the Z^2 amplitude is the same as the phase of the entire first order term in Z . Consequently the Z^3 term in the probabilities and cross sections comes from the effects of time ordering as well as the electron-electron effects in the first order term.
5. Nagy and McGuire (unpublished) have recently shown that there are in general no odd order Z effects in observable transition probabilities and cross sections without the effects of time ordering, i.e. contributions from $T - T_{av}$.

The effects of time ordering have been recently studied by Stolterfoht et al.[17] and by Vegh et al.[18] using an energy shift due to the electron-electron interaction in the intermediate states of an interaction.

1.2.2 Results for ionization excitation

We have recently used our calculations to evaluate cross sections for ionization plus excitation in helium by the impact of fast protons and anti-protons. These are the first calculations for ionization excitation by the impact of fast heavy charged particles and anti-particles. They have been recently submitted to Physical Review as a rapid communication.

1.3 Calculations with photon impact

1.3.1 Use of MBPT

Study of two electron transitions stimulated by interaction of a single photon is perhaps the simplest way to probe the dynamics of the electron-electron interaction, since such processes are dominated by the dynamics of the electron-electron interaction. A few years ago in collaboration with the group of Takeshi Ishihara in Tsukuba, Japan, we studied[20] the double ionization of helium by the annihilation of a single photon (i.e., photoionization). Our theoretical study came at the same time that the first data at photon energies above 1 keV was taken by Levin et al.[21, 22]. These studies made it

clear that the correct ratio for double to single ionization was 1.7%, lower than the value of about 4% extrapolated from earlier data at lower photon energies.

Our calculations were done using standard many body perturbation theory (MBPT) using a V^{N-1} mean field potential[23]. The MBPT amplitudes may be obtained by expanding the fully correlated theory described above in an expansion in the electron-electron correlation interaction. These calculations were done to first order in the $\vec{p} \cdot \vec{A}$ interaction in the dipole limit. Thus both Compton[24, 25, 26] and resonant Raman scattering were not included. Our results were in agreement with both observation and with other calculations[28, 29, 30, 31] at high photon energies which gave an asymptotic high energy value of 1.6 - 1.7% for the ratio of double to single ionization.

As data was evaluated at energies near and above 6 keV, it became evident that Compton scattering, where the incident photon is inelastically scattered from the target, becomes dominant over photoionization, where the incident photon is annihilated. It was a surprise that our theory for photo-annihilation was in good agreement with data for Compton scattering. Some debate ensued as to whether these two different processes give the same value of the high energy limit for the ratio of double to single ionization. Along with others[25, 26], we argued that we expected different ratios for Compton scattering than for photoionization. Recent observation tends to confirm our prediction, although the experimental situation is not entirely clear[27].

1.3.2 Gauge dependence of MBPT amplitudes

Another point of conflict arose over the issue of the relative importance of the various MBPT contributions in double ionization. In particular there was clear disagreement over the importance of the so called two-step 1 (TS1) contribution where one electron interacts with the other electron on the way out of the collision. In single ionization this problem does not arise if central potentials are used since there is one MBPT amplitude in lowest order which is identical in the L, V and A forms of the calculation. However, for double ionization there are three MBPT contributions to lowest order, namely shakeoff (SO), ground state correlation (GSC) and TS1. Some authors believed that the TS1 contribution dominated the total cross section, while others claimed that the contribution was negligible[6]. Surprisingly, both groups obtained similar numbers for their cross sections in agreement with observation. The

resolution to this paradox was given by Dalgarno and Sadeghpour[7] who pointed out that the TS1 contribution is different in the length (L), velocity (V), and acceleration (A) forms of the dipole matrix element. Dalgarno and Sadeghpour correctly explained that while TS1 was important in the L form, it went to zero at high energies in the A form.

Explicit calculations of the MBPT amplitudes were done by our group in collaboration with Ishihara's group[20]. The individual contribution of each of the three leading order MBPT diagrams was explicitly evaluated in each of the L, V and A forms. It was further shown that the sum of the SO and GSC and TS1 amplitudes is independent of the L, V and A forms.

More recently we have been able to demonstrate that the L, V and A forms of the dipole operator correspond to different electromagnetic (and quantum) gauges[32]. The specific gauge transformations from V to L and V to A have been identified in the dipole approximation. This means that the MBPT amplitudes, which are often used to define collision mechanisms are gauge dependent, although the sum of the lowest order terms is gauge invariant. Consequently, MBPT amplitudes have no consistent meaning as mechanisms of double ionization by photo-annihilation unless one defines the form of the dipole operator. This raises the question: What do we mean by the term 'scattering mechanism'? This issue is at present unresolved.

Quite recently Hino et al.[33] have shown that in the first order approximation for Compton scattering where only the A^2 term is used, the individual MBPT amplitudes vary under mathematical transformation from V to L and V to A using commutator definitions. It is not clear at present what relation these transformations have to gauge transformations. It is also unclear whether one should transform only the A^2 term or more generally the $(\vec{p} - e\vec{A}/c)^2$ term. Furthermore, there is some dispute over the definition of the V form when the A^2 term is used.

1.4 Relation between charged particle and photon interactions

Both charged particles and photons interact with matter via electromagnetic fields. Thus, in principle, it should be possible to relate interactions with charged particles and interactions with photons. Doing this enables one to relate quite different data to each other and provides relatively stringent tests

on the self consistency of both the data and the analysis.

In practice the data are quite different. The natural scale of the cross sections may differ by many orders of magnitude, as we shall see in the comparison of Compton scattering to charged particle scattering below. Even ratios of double to single ionization may differ by more than a factor of five. For example, the ratio of double to single ionization by photon impact has an asymptotic high energy value of 1.7% while the corresponding ratio for total cross section ratios by impact of charged particles and anti-particles is 0.26% - a difference of a factor of 6.3.

These high energy limits are of interest for several reasons:

- The ratios tend toward constants asymptotically in many cases.
- The constants are different for different processes.
- The values of these constants depend on the dynamics of the electron-electron correlation interaction.
- the high energy limit is relatively simple and provides a good starting point for understanding the dynamics of the electron-electron interaction.

Understanding the nature of these ratios has been accomplished by determining which regions of momentum transfer, Q , contribute in various cases. Transitions at small Q (which occur at large distances from the target nucleus) are dominated by dipole matrix elements, while transitions at large Q (corresponding to distances close to the nucleus) are usually dominated by non-dipole matrix elements.

1.4.1 Dipole terms

If the momentum transfer, Q , is small, then $\langle f | e^{i\vec{Q} \cdot \vec{r}} | i \rangle \approx i \langle f | \vec{Q} \cdot \vec{r} | i \rangle$, and the generalized oscillator strength reduces to the standard dipole optical oscillator strength. In this limit the matrix elements reduce to the dipole matrix elements used for photo-excitation and ionization. For charged particle impact, if the Born cross section is expanded in inverse powers of the projectile energy, E , then $\sigma_Z(E) \simeq A \frac{\ln E}{E} + B/E$. The leading $\frac{\ln E}{E}$ (or $\frac{\ln v^2}{v^2}$) contribution to the cross section for charged particles may be expressed in terms of the cross section for photo-excitation or ionization[29], namely,

$$\frac{d\sigma_Z}{d\epsilon} = \frac{Z^2}{2\pi\alpha} \frac{\ln v^2}{v^2} \frac{\sigma_\gamma(\epsilon)}{\epsilon} \quad (12)$$

where v is the velocity of the projectile, ϵ is the energy transfer, and α is the fine structure constant. If Q is near Q_{min} , then $Q \approx Q_{min} = K_i - K_f = \Delta E_{if}/2v \approx (I + \epsilon)/2v$, where I is the atomic binding energy. Using this limit, it is straightforward to express the ratio for double to single ionization by charged-particle impact as an integral over the cross section ratio for photoionization[34, 35], namely,

$$R_Z = \int R_\gamma(\epsilon) \rho_Z^+(\epsilon) d\epsilon \quad (13)$$

where $\rho_Z^+(\epsilon) = \frac{1}{\sigma_Z^+} \frac{d\sigma_Z^+(\epsilon)}{d\epsilon}$ is the density of states for single ionization by a charged particle. This relation has been recently used by us in collaboration with Steve Manson[35] to obtain the observed ratio of double to single ionization in helium by charged particle impact, $R_Z \approx 0.26\%$, from the observed ratios for photoionization.

There are two notable difficulties. Using the values quoted in the literature for R_γ , the asymptotic value obtained for R_Z using the above relation is 0.32% somewhat above the observed value of $0.26\% \pm 0.03\%$. Also, the high-energy shape of $R_Z(E)$ given by Eq.(13) differs somewhat both from experiment and the Forced Impulse Method calculation of Reading and Ford[36]. We shall see below that these may be resolved by sensible inclusion of non-dipole contributions.

1.4.2 Non-dipole terms

We have also studied Compton scattering in collaboration with Joachim Burgdörfer[37] of Oak Ridge. Photoionization and ionization by Compton scattering are different processes. In photoionization (i.e., the photo effect first described by Einstein), the photon is annihilated, while in Compton scattering the photon is inelastically scattered (and not annihilated). At present there is some disagreement as to what the high-energy limit is for the ratio R_C , of double to single ionization for Compton scattering and how

it is related to photoionization. It is widely agreed, however, that total ionization cross sections for photoionization are well described by the dipole approximation for the interaction operator with the photon even at high photon energies where $k_i r > 1$. In Compton scattering, on the other hand, the contributions are mostly non-dipole.

For Compton scattering the cross section for inelastic scattering from an arbitrary initial state $|i\rangle$, to an arbitrary final state, $|f\rangle$, may be expressed[37] in first order (in both the fine structure constant, α , and $1/c^2$) as,

$$\begin{aligned} \frac{d\sigma_C}{d\Omega_f} &= r_d^2 \frac{k_f}{k_i} |\vec{\lambda}_i \cdot \vec{\lambda}_f^*|^2 |\langle f | A^2 | i \rangle|^2 \\ &= r_d^2 \frac{(1 + \cos^2 \theta_f)}{2} |\langle f | e^{i\vec{Q} \cdot \vec{r}} | i \rangle|^2 \end{aligned} \quad (14)$$

where r_d is the classical radius of the electron, $\vec{k}_{i,f}$ is the initial or final photon momentum, $\vec{\lambda}_{i,f}$ is the polarization vector of the initial or final photon, $\vec{A}$ is the vector potential and $(\vec{Q})^2 = (\vec{k}_i - \vec{k}_f)^2 = k_i^2 + k_f^2 - 2k_i k_f \cos \theta_f \approx 2k_i^2(1 - \cos \theta_f)$. The expression in the second line above is for unpolarized light.

For the impact of a high velocity particle of charge Z the cross section in the plane-wave Born approximation is given by,

$$\begin{aligned} \frac{d\sigma_Z}{d\Omega_f} &= a_0^2 \frac{K_f}{K_i} \frac{\mu^2}{4\pi^2} |\langle f | \frac{Z}{|\vec{R} - \vec{r}|} | i \rangle|^2 \\ &= a_0^2 \frac{4\mu^2 Z^2}{Q^4} |\langle f | e^{i\vec{Q} \cdot \vec{r}} | i \rangle|^2 \end{aligned} \quad (15)$$

where a_0 is the radius of the ground state of hydrogen, $\vec{K}_{i,f}$ is the initial or final photon momentum, now $\vec{Q} = \vec{K}_i - \vec{K}_f$ is again the momentum transfer of the projectile and μ is the reduced mass of the system. We note that in this approximation no momentum is transferred to the projectile by the target nucleus, so that the momentum transfer, $\vec{Q}$, is the momentum transferred to the electron(s).

From Eqs.(14) and (15) it is apparent that both the Compton and the charged particle cross sections above are proportional to the generalized oscillator strength, $f_{fi}(Q) = \Delta E_{fi}/Q^2 | \langle f | e^{i\vec{Q}\cdot\vec{r}} | i \rangle |^2$. Consequently, the cross section for Compton scattering may be expressed in terms of the first Born cross section for scattering by charged particles. Using $1 + \cos^2\theta_f = 1 + (\frac{k_i^2 + k_f^2 - Q^2}{2k_i k_f})^2$ and $K_i^2/\mu^2 = v^2$ where v is the velocity of the incident charged particle, we obtain from Eq(1) and Eq(2) a useful relation[37], namely,

$$\frac{d\sigma_C}{dQ} = \frac{r_d^2}{a_0^2} \frac{v^2}{8k_i^2 Z^2} \left(1 + \left(\frac{k_i^2 + k_f^2 - Q^2}{2k_i k_f} \right)^2 \right) Q^4 \frac{d\sigma_Z}{dQ}. \quad (16)$$

This relation is valid for arbitrary final states, $|f\rangle$, including both single and double ionization. This relation could be tested experimentally by observing differential cross sections for Compton scattering and comparing them to existing data for differential cross sections by charged particle impact weighted by the factors in the above relation. This relation may also be used to evaluate cross sections for Compton scattering by modifying existing computer codes for single and double ionization by charged-particle impact.

From the relations above we have shown that cross section ratios for Compton scattering and charged particle scattering at a fixed value of the momentum transfer, Q , are related in first order by,

$$R_C = \frac{\sigma_C^{++}}{\sigma_C^+} = \frac{\int (d\sigma_C^{++}/dQ) dQ}{\int (d\sigma_C^+/dQ) dQ} \approx R_Z(Q \approx \infty) = \left(\frac{d\sigma_Z^{++}}{dQ} / \frac{d\sigma_Z^+}{dQ} \right)_{Q \approx \infty}. \quad (17)$$

Here Q is the momentum transferred by the target electron(s) with no inter-nuclear momentum transfer.

1.4.3 Combined terms

Our group with the help of Joachim Borgdörfer has developed a relationship between charged particles that includes both dipole and non-dipole contributions[38]. The dipole contributions for charged particles are related to photo-annihilation cross sections and the non-dipole are related to Compton scattering. Treating these contributions separately one easily obtains,

$$R_Z = \int R_{\text{Annihilation}}(\epsilon) \rho_{\text{dipole}}^+(\epsilon) d\epsilon + \int R_{\text{Compton}}(\epsilon) \rho_{\text{non-dipole}}^+(\epsilon) d\epsilon. \quad (18)$$

In our calculations we used somewhat simple five-term Roothan-Hartree-Fock wave function for the initial state of He and the final state is a Coulomb wave. Also, we did not separate the $\ell = 1$ term from Compton scattering in our calculation. The density of states, $\rho(\epsilon)$, was calculated. The values of $R_{\text{Annihilation}}$ were taken from experiment and R_{Compton} was a fit to the best combination of theory and experiment then available.

Our results using Eq(13), which improperly includes all multipole terms in ρ is in agreement with Manson and McGuire[35] but has a magnitude and energy dependence which is not quite in agreement with observation. The dipole term alone is a bit small. But the sum of dipole and non-dipole terms, using Eq(18) is in good agreement with observation. A more complete calculation separating the $\ell = 1$ Compton contribution, using better wavefunctions and using more recent definitive data for Compton scattering, should give a result accurate well within present experimental errors.

1.5 Systems with electrons on more than one center

1.5.1 Projectile electrons

In recent years there has been growing interest in understanding the effects of projectile electrons[39, 40]. These effects have been represented by various names, including 'two center correlation', 'two center dielectric effects' and 'anti-screening'. Most of the analysis has been done in the wave picture. Recently, in collaboration with Eduardo Montenegro of Rio de Janeiro, we have developed an impact parameter representation for dealing with projectile electrons[41]. This is useful in cases where one may wish to employ a version of the independent electron approximation for multiple ionization of target electrons. Our work also has lead to a new physical picture of the role of projectile electrons, which we call the virtual impact parameter picture.

The probability amplitude, $a(B)$, in the particle picture may be related to the scattering amplitude, $f(Q)$, in the wave picture by

$$a(B) = \int d^2Q e^{i\vec{Q} \cdot \vec{B}} f(Q). \quad (19)$$

In the wave picture, which is correct for most scattering experiments, the first Born approximation gives[41] the simple result that

$$f(Q) = f_{proj} f_{target} . \quad (20)$$

We introduce the notion that f_{proj} may be regarded as $Z_{eff}(Q)$, and f_{target} may then be regarded as the scattering amplitude per unit charge. Then we define,

$$\bar{Z}_{eff}(B') \equiv \int d^2 Q e^{i\vec{Q} \cdot \vec{B}'} Z_{eff}(Q) . \quad (21)$$

Here $\bar{Z}_{eff}(B)$ is the projectile charge per impact parameter defined over a Gaussian cylinder.

Then, using the well known Faltung theorem,

$$\begin{aligned} a(B) &= \int d^2 Q f(Q) = \int d^2 Q e^{i\vec{Q} \cdot \vec{B}} Z_{eff}(Q) \int d^2 B' e^{-i\vec{Q} \cdot \vec{B}'} a_{target}(B') \\ &= \int d^2 B' a_{target}(B') \int d^2 Q e^{i\vec{Q} \cdot (\vec{B} - \vec{B}')} Z_{eff}(Q) \\ &= \int d^2 B' \bar{Z}_{eff}(B - B') a_{target}(B') . \end{aligned} \quad (22)$$

The resulting physical picture is easily understood. When an electron is added to a nuclear projectile of charge, Z , the effect of the projectile electron is to localize the net projectile charge, Z_{eff} , in Q space. and thus to spread the charge in B space. In Q space a constant Z is changed to Z_{eff} which decreases at small Q (and increases at large Q). In B space the localized charge density, $Z\delta(B - B')$, changes when an electron is added to a bare projectile to $\bar{Z}_{eff}$ which is spread out about $B = B'$.

For a point particle with no electrons, the charge of the projectile is represented by $Z\delta(B - B')$, and the convolution gives the usual result, $a(B) = Z a_{target}(B)$. Note that the width of the probability amplitude for the target, $a_{target}(B)$, is approximately equal to the size of the target's electron cloud. The effect of the n electrons on the projectile is to spread this distribution in coordinate (B) space, corresponding to a localization of $Z_{eff}(Q)$ in wave (Q) space. The width of this distribution is roughly equal to the size of the projectile's electron cloud. If the projectile is far from the target, corresponding to the peak of the charge distribution lying well outside

the probability distribution for the target, then the effective charge of the projectile is $Z - n$, corresponding to a projectile screened by n electrons. If the width of the projectile is much larger than the target, then the effective charge reduces to $\sqrt{Z^2 + n}$ when one sums over final states of the projectile[41].

In any experiment one may observe the square of $a(B)$, where $a(B)$ is the convolution of $a_{\text{target}}(B')$ with $\bar{Z}_{\text{eff}}(B' - B)$. That is, $a_{\text{target}}(B')$ and $\bar{Z}_{\text{eff}}(B' - B)$ are not observable. Since B' is a non-physical variable, B' is referred to as a virtual impact parameter (in contrast to the physical impact parameter, B).

This virtual impact parameter picture is valid only in first order perturbation theory. It is interesting to ask how this picture would be changed in a more complete higher order theory. We note that this impact parameter version may be used to evaluate cross sections for multiple ionization of target electrons in a target in which the electrons are uncorrelated so that the independent electron approximation may be applied to the target electrons. This opens the possibility of evaluating cross sections for double ionization of the target in coincidence with single ionization on the projectile. Experiments are now underway that can test the limitations of this theory. Of particular interest are experiments using the new COLDTRIMS technique developed by Schmidt-Böcking in Frankfurt, Germany and now in use by Lew Cocke at Kansas State University. In these experiments one may separate events in which the projectile electron is elastically scattered from those in which the projectile electron is inelastically scattered - i.e., separate the screening and anti-screening contributions..

1.6 Summary

During the past three years we have evaluated and analyzed transition probabilities and cross sections for few and many electron transitions. The emphasis was on two and three electron transitions occurring in fast collisions of atoms and molecules with charged particles and photons.

2 References

References

- [1] R.E.Olson, J. Wang and J. Ullich in the Invited Papers of ICPEAC XVIII (AIP Conf. Proc. 295, Ed. T. Andersen, B. Fastrup, F. Folkmann, H. Knudsen, and N. Andersen), 520 (1993).
- [2] S. Datz Book on Invited Talks XVI ICPEAC (NY) ed. by A. Dalgarno et al., 13 (1989).
- [3] J.H.McGuire, Adv. in Atomic, Molecular and Optical Physics **29**, 217 (1992).
- [4] J.S.Briggs and J. Macek, Adv. in Atomic, Molecular and Optical Physics **28**, (1991).
- [5] W. Fritsch and C.D.Lin, Rep. Prog. Phys. **202**, 1 (1991).
- [6] J.H.McGuire, N. Berrah, R.J.Bartlett, J.A.R.Samson, J.A.Tanis, C.L.Cocke and A.S.Schlachter, J.Phys. B **28**, 913 (1995).
- [7] A. Dalgarno and H.R. Sadeghpour, Phys. Rev. A **46**, R3591 (1992).
- [8] R. Grobe and J.H. Eberly, Phys. Rev. A **47**, RC1605 (1993).
- [9] C. Pan, A.F. Starace, and C.H. Greene, J. Phys. B **27**, L137 (1994).
- [10] F. Robicheaux and C.H.Greene, Phys. Rev A **48**, 4429 (1993).
- [11] J. Muller and J. Burgdörfer, Phys. Rev. Letters **70**, 2365 (1993).
- [12] J.M. Feagin, J. Phys. B **17**, 2433 (1984).
- [13] Y. Hahn, Z. Phys. D., in press (1995).
- [14] D.M.Homan, M.J. Cavagnero and D.A. Harmin, Phys. Rev A **50**, RC1965 (1994).
- [15] T. Brage, C. Froese Fischer, and G. Miecnik, J. Phys. B **25**, 5289 (1992).

- [16] Jack C. Straton, J. H. McGuire, and Zheng Chen, *Phys. Rev. A* **46**, 5514 (1992).
- [17] N. Stolterfoht, A. Mattis, D. Schneider, G. Schiweitz and B. Skovall, *Phys. Rev A* **51**, 350 (1995).
- [18] L. Vegh, B. Sulik and N. Stolterfoht, *Phys. Rev A* **51**, 3017 (1995).
- [19] S. Fuelling, R. Bruch, E.A. Rauscher, P.A. Neil, E. Traebert, P.H. Heckmann and J.H. McGuire, *Phys. Rev. Letters* **68**, 3152 (1992).
- [20] K. Hino, T. Ishihara, F. Shimizu, N. Toshima and J.H. McGuire, *Phys. Rev. A* **48**, 1271 (1993).
- [21] J.C. Levin, I.A. Sellin, B.M. Johnson, D.W. Lindle, R.D. Miller, N. Berrah, Y. Azuma, H.G. Berry, and D.H. Lee, *Phys. Rev. A* **47**, R16 (1993).
- [22] N. Berrah, F. Heiser, R. Wehlitz, J. Levin, S.B. Whitfield, J. Viefhaus, I.A. Sellin, and U. Bekker, *Phys. Rev. A* **48**, R1733 (1993).
- [23] A.F. Starace, *Handbuch der Physik*, Vol XXXI, 1 (1982).
- [24] J.A.R. Samson, C.H. Greene and R.J. Bartlett, *Phys. Rev. Lett* **71**, 201 (1993).
- [25] L.R. Andersson and J. Burgdörfer, *Phys. Rev. Lett* **71**, 50 (1993).
- [26] T. Suric, K. Pisk, B.A. Logan, and R.H. Pratt, *Phys. Rev. Lett.* **73**, 790 (1994).
- [27] J. Levin, private communication.
- [28] A. Dalgarno and R.W. Ewart, *Proc. Phys. Soc.* **80**, 616 (1962).
- [29] F.W. Byron and C.J. Joachain, *Phys. Rev.* **164**, 1 (1967).
- [30] Z. Tang and R. Shakeshaft, *Phys. Rev. A* **47**, R3487 (1993).
- [31] K. Meyer and C.H. Greene, *Phys. Rev A* **51**, (1995).

- [32] J.H.McGuire L. Nagy, J. Wang, K. Hino and M. Ya Amusia, Wigner Memorial Volume of Acta Physica Hungarica (1996), in press.
- [33] K. Hino, P. Bergstrom and J.H.Macek, Phys. Rev. Lett. **72**, 1620 (1994).
- [34] J.H. McGuire, J. Phys. B **17**, L799 (1984).
- [35] S.T.Manson and J.H.McGuire, Phys. Rev. A **51**, 400 (1995).
- [36] J.F. Reading and A.L. Ford, J. Phys. B **20**, 3747 (1987).
- [37] J. Burgdörfer, L.R.Andersson, J.H.McGuire and T.Ishihara, Phys Rev. A **50**, 349 (1994).
- [38] J. Wang , J.H.McGuire and J.Burgdörfer, Phys. Rev A **51**, June (1995), in press.
- [39] E.C.Montenegro, W.E.Meyerhof and J.H.McGuire, Adv. in Atomic, Molecular and Optical Physics **34**, 249 (1994).
- [40] P. Richard, in *X-ray and Inner-shell Processes*, AIP Conf. Proc. 215 (ed. T. Carlson, M.O. Krause and S.T. Manson), 315 (1990).
- [41] J. Wang, J.H.McGuire, and E.C.Montenegro, Phys. Rev A **51**, 504 (1995).
- [42] A.L. Godunov and V.A. Schipakov, J. Phys. B **26**, L811 (1993).
- [43] A. Dalgarno, private communication.
- [44] C.K. Au and Richard J. Drachman, Phys. Rev. A **37**, 1115 (1988).
- [45] Richard J. Drachman, A.K. Bhatia, and Abdulalim A. Shabazz, Phys. Rev. A **42**, 6333 (1990).
- [46] Private communication (1992).
- [47] Jack C. Straton, Phys. Rev. A **43**, 1381 (1991).