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INNER SHELL COULOMB IONIZATION BY HEAVY CHARGED PARTICLES STUDIED BY THE SCA MODEL.

A Condensed Status Review by Johannes M. Hansteen.

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by

Johannes M. Hansteen

Abstract:

A sketch is given of the development of and some achievements hitherto gained from the semi-classical approximation (SCA) model of atomic Coulomb excitation by heavy charged particles. A few very recent results (1975-1975) are incorporated in the discussion.
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References.
Preface.

The research project to be outlined and discussed in the present status review has been carried out for the most part at the Department of Physics, University of Bergen, in the period 1971 - 1976, whereas the founding work was done in Copenhagen in the late 1950's. The discussion will mainly concentrate on the following six papers, to be mentioned in the text below by their ascribed Roman numerals:


Nuclear Physics A201 (1973) 541-560.


IV. J.M.Hansteen, O.M.Johnsen and L.Kocbach: Coulomb Ionization of the L Sub-Shells by Heavy Charged Projectiles.  
V. J.M. Hansteen, O.M. Johnsen, and L. Kocbach: Predictions of Inner-Shell Coulomb Ionization by Heavy Charged Projectiles. 
Atomic Data and Nuclear Data Tables 15 (1975) 305-317.

VI. Johannes M. Hansteen: Inner Shell Ionization by Incident Nuclei.

It should be emphasized that an intense and steadily increasing international research effort is going on at present in connection with the atomic Coulomb excitation and related phenomena occurring in the general ion-atom collision. The author has therefore deemed it necessary to include in the discussion references to several reports and review lectures presented by himself in the above period, as well as some brief and hopefully fair mention of pertinent research efforts by research collaborators. All responsibility for interpretations, comments and tentative predictions, however, solely rests with the author.

During the period spent working on this research project, considerable new insight has been gained. Hence some of the viewpoints, results and conclusions presented in Papers I - V have rather naturally been subject to modifications at the present state of knowledge and development. The views presented in Paper VI are presumably to be considered as the more well-balanced and correct ones.
Moreover, attempts have been made to incorporate in the present expose a few ideas and experimental findings appearing only after the final editing of the review article VI (i.e. autumn 1975). This, however, only strengthens the principal claim that the emerging, near-quantitative picture of the atomic Coulomb ionization phenomenon, partially obtained from an extensive application of the SCA model, by now appears to be rather firmly established.

The main impetuses to write the present expose were the several positive reactions to the review article VI and the inspiring occurrence of the Second International Conference on Inner Shell Ionization Phenomena in Freiburg in March-April 1976. Both these factors, together with strong urgings from various colleagues, seemed to indicate the time to be ripe for the present undertaking.

My sincere thanks are due to the Department of Physics, University of Bergen, under the auspices of which the majority of the present researches have been performed.

To O.P. Mosebekk, L. Kocbach, O.M. Johnsen, P.A. Amundsen, and O. Aashamar I am greatly indebted for innumerable inspiring and thought-provoking discussions and highly fruitful collaboration.

The Norwegian Research Council for Science and the Humanities (NAVF) and Nordisk Institut for Teoretisk Atomfysik (NORDITA), Copenhagen, have on various occasions contributed financially to the furthering of the present researches. My deepfelt thanks are offered to both institutions.
1. Introduction.

1.1 Brief_historical_remarks.

The inner shell Coulomb ionization induced by heavy charged particles has for a long time been investigated from the point of view of atomic as well as nuclear physics. A rather broad treatment of the historical aspects connected with this process is given in the Introduction of Paper VI. In the present and the following subsection we stress a few extra points relevant to the understanding of the specific development of the SCA model.

In historical context we note that the interest in inner shell vacancy production caused by various types of collisions is still (summer 1976) on the rise \cite{1}. One reason for this is obviously the continued exploitation of experimental techniques developed in low and medium energy nuclear physics \cite{2,3}.

As a more specific fact we mention that, at least to the knowledge of the author, the first more elaborate attempts to investigate the heavy particle induced inner shell Coulomb ionization in this country, were made already in the middle of the 1950's, cf. refs. \cite{4,5}.

1.2 The_origin_of_the_semi-classical_approximation
model_for_atomic_Coulomb_excitation.

In nuclear Coulomb excitation induced by heavy charged particle impact the primary objects under study are the
γ-rays of nuclear origin. In the region of low γ-ray energies the characteristic X-radiation originating from the inner shell Coulomb ionization of the target atom may constitute an important and sometimes highly annoying background to the nuclear radiation. This intermixing of radiation of nuclear and atomic origin is instructively illustrated in several contributions from the Copenhagen group, see for instance ref. 6) and references quoted therein. Factors as these were decisive for the working out of a semi-classical theory for atomic Coulomb excitation by heavy charged particles, cf. Paper I. (This last mentioned publication will in the following text most often be referred to as B.H., in accordance with common usage in this particular branch of collision physics.) The said semi-classical model is based on a first-order, time-dependent perturbation treatment, advantageously given in impact parameter form.

Already in the original B.H. publication considerable effort was put into elaborate evaluations of that particular model. The main text as well as the appendices in that work contain details and suggestions which even today (i.e. in 1976) have proven to be unexpectedly fruitful in current investigations. It is probably fair to state that much of the later results and recent developments in the field of atomic Coulomb excitation are in some sense present in embryo in the B.H. paper. Thus, the Paper II represents a natural extension of the ideas
in the B.H. work with due regard to newly acquired experimental insight.

The semi-classical approximation model has for reasons of practicability been denoted as \(7,8\) the SCA model. This abbreviation seems by now to be generally accepted in the literature, e.g. the representative references \(1,2a,3\).

2. **Selected details connected with the SCA treatment.**

2.1 **Comments on kinematical criteria.**

In the SCA picture the impinging projectile is ascribed a classical path. The necessary and sufficient condition for a classical description of the naked, ionizing projectile in the Coulomb field of the target nucleus is given by \(9\), with standard notation \((B.H.)\),

\[
\kappa = \frac{2Z_1 Z_2 e^2}{\hbar v_1} \gg 1 ,
\]

where the indices 1 and 2 refer to the projectile and target nucleus, respectively. In general, a hyperbolic path is introduced for the impinging particle, as described in detail in the Papers B.H., II and VI, where also other conditions for the validity of the model are discussed. Thus, the current version of the SCA model is valid when

\[
\frac{\Delta E}{E_1} \ll 1 ,
\]
where
\[ \Delta E = E_B + E_f, \] (3)

with \( E_B \) being the binding energy of the electron in its initial bound state and \( E_f \) the final energy of this electron.

A rigorous proof has been given of the equivalence between the straight-line SCA expression for the differential cross section for Coulomb ejection of an atomic electron and the corresponding one arrived at from the plane wave Born approximation treatment (Papers B.H., II, and VI). Mathematically this may be formulated as
\[
\left( \frac{d\sigma}{dE_f} \right)_{\text{str.l.}} = \left( \frac{d\sigma}{dE_f} \right)_{\text{SCA}} = \left( \frac{d\sigma}{dE_f} \right)_{\text{PWBA}},
\] (4)

which again implies a justification for the use of the SCA model at higher energies of the incoming particles. As tentatively elucidated in Paper VI, this appears paradoxical in view of the inequality in eq. (1), which relation should exclude the high energy region where the opposite inequality \( \kappa \ll 1 \) is valid. The statement that the Coulomb ionization cross sections from a complete SCA treatment are correct for all \( \kappa \) values as long as no projectile scattering angles are involved, may appear reasonable (VI). Nevertheless, a more thorough analysis on this point might be desirable, also to promote the understanding of the relations between
the various theoretical models in use for the description of the atomic Coulomb excitation.

At sufficiently high projectile energies, the ionizing projectile may well experience the influence of the nuclear potential. This implies deviations from the classical Kepler orbits and thus limitations to the validity of the SCA calculations as performed up till now, cf. B.H. and ref. 10. Valuable information on the nuclear surface region may well be obtained from the study and interpretation of such deviations.

2.2 Impact parameter dependences, ionization probabilities, and multiple ionization phenomena.

A great advantage of the impact parameter formulation of the SCA model is the inherent possibility to predict projectile angular dependences of the Coulomb ionization cross sections. Such predictions were given back in 1959 (B.H.). The importance of these predictions has been repeatedly stressed in various reports and lectures, cf. refs. 8,11-15) and Papers II - VI. Predictions of this kind, combined with measurements of angular correlations between the scattered projectile and the emitted characteristic X-rays, represent highly sensitive tests of the collision models for inner shell ionizations.

It is an historical fact that the early SCA predictions on impact parameter dependences initiated studies of
X-ray production from fission fragment collisions in matter \[16,17\). These researches led to the important discovery of completely new types of X-ray producing phenomena combined with the expected direct Coulomb ionization effect \[16\), i.e. inner shell vacancy formations at least qualitatively explainable within the frame of the molecular orbital (MO) model \[18\).

On the basis of the SCA picture (B.H., II, VI) it has been suggested that the decisive radius for the Coulomb ionization process at low projectile energies should be the adiabatic radius

\[ r_{\text{ad}} = \frac{\hbar v_1}{\Delta E} , \] (5)

and not the specific electron shell radius as might offhand be expected. Furthermore, the maximum contribution to the total Coulomb ionization cross section in this picture is given for projectiles with impact parameters roughly equal to

\[ P_{\text{max}} \approx r_{\text{ad}} . \] (6)

In the case of the adiabatic distance being much smaller than the electron shell radius in question, one speaks about "close collisions". This in contrast to large projectile velocities \[ v_1 \] where the bulk of the excitation probability is expected to originate from impact parameters comparable to or larger than the shell radius, i.e. "distant collisions".
The experimental verifications of the mentioned predictions of the ionization probabilities $I_p$ as functions of the impact parameter are one of the major successes of the SCA model (II, IV, V, VI). Among several measurements we only refer to the pioneer work of the Århus Group for K-shell ionization in close collisions $^{19}$, and further to a most recent work by Schmidt-Bøcking and collaborators $^{14, 20}$ on the L sub-shell excitation of a lead target by protons. The predicted and observed bumps in the $I_p$ curves are connected with the nodes in the radial wavefunctions of the target electrons. The close agreement obtained between experiment and theory is the more satisfactory as there are no adjustable parameters in the theory $^{14}$.

The further investigation of the importance of distant collisions, either in comparison with the SCA or other ionization models, remains a task for the future $^{21}$. The predicted and observed $^{22}$ plateau in the total sub-shell ionization cross section $\sigma_{2s,2p}$ as a function of the projectile energy is in the same manner straightforwardly explained within the frame of the SCA model, cf. Papers II, IV, V, and VI. The interpretation also of this plateau as a manifestation of a node in the electron density distribution ought to be a fact of lasting interest (II, VI and ref. $^{14}$).

The great applicability of the SCA model is demonstrated by Paper V where the straight-line version of the SCA model together with known scaling properties (II, IV, VI) are used to give tables of ionization probabilities by
protons for inner electron shells. The numerical procedure is rather complicated*. These tables by now appear to be widely used, see e.g. refs. 20,21).

As stressed in Paper VI, the analysis of Bohr on the validity of the classical orbital treatment should be kept in mind 9). According to this analysis the degree of accuracy possible by a classical projectile description is given by

\[
\left( \frac{\Delta \theta}{0} \right)^2 = \frac{1}{\kappa},
\]

(7)

with \( \Delta \theta \) denoting the uncertainty in the projectile scattering angle \( \theta \). Considering the strong current interest in impact parameter dependences of inner-shell excitation processes 15), at least a word of caution seems advisable on an indiscriminate use of semi-classical collision models 24).

The SCA model has with encouraging results been applied to the investigation of multiple inner shell vacancy production by heavy charged particles (III, VI). These studies are only in their initial state, but have nevertheless demonstrated the great usefulness of the semi-classical

* Due to a programming error connected with exploitation of formulae in ref. 23), some numerical results given in Paper II for L sub-shell ionizations are incorrect, whereas total L-shell cross section values are in close agreement with corresponding corrected computations, as for instance those in Paper V.
approximation model. For detailed studies of X-ray satellites produced in collisions between heavy ions and atoms, extended studies along these lines might prove highly rewarding. We note in passing that most recently multiple ionizations induced by low energy cosmic rays (i.e. by projectiles such as protons, α-particles, C, N, O nuclei etc. with energies around and below 100 MeV per nucleon) in penetrating the interstellar medium have been treated in a preliminary way by the SCA methods indicated in Paper III, see further ref. 25). New and promising fields of applications of the SCA picture are obviously in the process of being opened up. (See further note added on page 12a.)

2.3 The Coulomb deflection effect.

The effect of the Coulomb deflection of the projectile in the field of the target nucleus is in principle obtainable from the SCA picture (B.H., II, VI). Such deflection effects have up till now only been calculated for electron transitions of the type $s_{1/2} \rightarrow s_{1/2}$ with non-relativistic hydrogenlike electron wavefunctions, see B.H. and ref. 26). For K-shell ionization and electronic $s \rightarrow s$ transitions an elaborate analytic SCA treatment yields the following approximate but simple result (B.H.):

$$\frac{d\sigma_{K}}{dE_f}^{\text{hyp.}} \text{SCA} = e^{-\pi \xi} \frac{d\sigma_{K}}{dE_f}^{\text{str.line}} \text{SCA},$$

(8)
Note_Added_in_Proof: Very recently R.V. Gentry and collaborators by study of proton-induced X-ray emission from monazite inclusions in mica may have provided evidence for the existence of primordial superheavy elements. The observed X-ray spectra appear to be consistent with the presence of a number of hitherto non-identified superheavy atoms. Possible L X-rays from several elements with charge numbers between $Z = 105$ and $Z = 134$ have been detected, this partially being due to the large cross sections for the presumed proton-induced L shell Coulomb ionizations involved (IV, V, VI). We stress that final confirmation of this possible evidence for superheavy elements is lacking at present.

where the upper index "hyp." denotes the appropriate hyperbolic path, and the adiabaticity parameter $\xi$ is given by

$$\xi = \left(\sum_{i} Z_i^2 e^{2} / 2E_1\right) \left(\Delta E / h \nu_1\right), \quad (9)$$

with $E_1$ denoting the kinetic energy of the projectile. We stress that various conditions have to be fulfilled for the above approximation to be reliable (B.H.). Under such circumstances, however, there are strong indications that the relation (8) is approximately valid for an arbitrary $s_{1/2} - s_{1/2}$ target electron transition, independent of the choice of wavefunctions 27).

It is instructive to note the considerable amount of additional research work that has been inspired by the simple Coulomb deflection correction factor $\exp(-\pi \xi)$, see for instance refs. 28, 29).

The effect of the projectile Coulomb deflection is difficult to evaluate in the cases of L-, M-, and higher shell ionizations. A tangential approximation procedure ("tilting method") has been adopted to simulate the deflection effect in such cases, cf. ref. 23) and Paper II where further justification for this method is given. Improvements to the method have been suggested and applied with informative outcome up to the present day 30, 31, 32). However, the tangential approximation becomes poor in particular for large scattering angles, cf. e.g. ref. 10),
indicating the necessity for future extensive computations with complete hyperbolic paths (VI).

2.4 Remarks on choices of target electron wavefunctions.

Until quite recently most SCA computations have been based on non-relativistic hydrogenlike electron wavefunctions (II - VI). Only in the B.H. paper a rough estimate was given of the effect of using relativistic wavefunctions for the K-shell target electrons (B.H., p.25).

A most important development has taken place very recently in this direction. By use of relativistic Coulomb wavefunctions in the straight-line version of the SCA model and with a refined tilting correction, excellent agreement has been obtained with experiment for K- as well as L-shell ionization by protons \(10,27,33-35\). Such calculations represent an improvement in comparison with the non-relativistic SCA calculations (V), in particular for target elements in the upper half of the periodic table. It is gratifying to note that corrections for relativistic effects in the K-shell Coulomb ionization is not badly reproduced by the rough B.H. estimate in comparison with more refined approximation formulae developed recently \(36\), which formulae are connected with the above mentioned SCA computations with relativistic wavefunctions \(33,34\).
3. Other approximation schemes for inner shell Coulomb ionization.

A survey of the existing methods for the treatment of inner shell Coulomb ionizations has been given in the review paper VI. An instructive illustration of the regions of validity of some of the various approximation schemes for inner shell vacancy productions in ion-atom collisions is provided by the following figure adapted after Madison and Merzbacher, ref. 2a), p. 1.

Fig. 1. Approximate regions of validity for various models connected with inner shell vacancy productions in ion-atom collisions. The ordinate axis represents the ratio $\frac{Z_1}{Z_2}$ of the projectile and target charge numbers, and the abscissa the collision velocity $v_1$ measured in units of the target K-shell velocity $v_{2K}$. Shaded regions are indicated for the plane wave Born approximation (PWBA), the semiclassical approximation (SCA) and the quasi-molecular model (MO). (Figure adapted after Madison and Merzbacher, ref. 2a), p. 1.)
The shaded regions in the figure indicate regions of validity of the various approximation schemes. As to the lower region in the figure, i.e. the Coulomb excitation region, it could be safely stated that the situation is fairly well under control in view of the most recent developments.

For some time it has been a clearly stated goal to close the gap between the simple Coulomb excitation region and that of the molecular orbital (MO) model of Fano and Lichten. This is an important step on the road to a hopefully complete description of the general ion-atom collision.

4. Future aspects and brief conclusion.

In the preceding sections the development of the SCA model has been roughly sketched, the discussion in particular being based on the series of Papers I - VI, but also with other relevant works being brought into consideration.

The SCA model has by now reached a mature state. Hence it seems reasonable to regard the atomic Coulomb excitation phenomenon as part of the extremely complicated excitation mechanism being operative in the general ion-atom collision. In Paper VI, section VI, a discussion is given on future aspects of researches on inner-shell vacancy productions by heavy charged projectiles. Not much is at present to add to that chapter. At least some
statements have already been proven to be well-founded. Thus, the need of general interpretations of observed impact parameter dependences of inner shell vacancy productions outside the region of validity of the SCA picture, e.g. united atom phenomena \(^{37}\), has been strikingly demonstrated \(^{38}\). A clear understanding of the complicated X-ray producing mechanisms in such heavy-ion-atom collisions is lacking at present \(^{39}\). Despite these facts, the conceptually simple SCA model has furthered our understanding far beyond initial expectations. Moreover, this model has at the same time provided a well-founded starting point for continued researches in this rapidly expanding field of physics.
Remark to the reference list.

Please note that references by the author related to Papers I - VI have been written with full title, whereas most other references are given in the customary abbreviated form.
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