FIZIKA 9 (1977) Supplement 4, 707–720
(Proceedings of the Int. Symp. on Nuclear Collisions and
Their Microscopic Description, Bled, September 1977)

A SURVEY OF NEW DEVELOPMENTS IN THE MICROSCOPIC THEORY OF COLLISIONS IN ATOMIC PHYSICS

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1. Introduction. - My objective in this brief survey of recent developments in the theory of collisions involving atomic particles such as electrons, positrons, atoms and molecules, including their respective ions, is to indicate the methods which are currently being used to derive formulae and calculate values of quantities such as the scattering length, phase shifts, scattering amplitudes and, in the general case, the elements of the scattering matrix, which enable differential and total cross sections for various collision processes to be evaluated. In the present short survey it is necessary to be very selective in the choice of topics which we shall discuss and so many most interesting researches have been omitted. A more detailed and extensive review of the subject has been given by Moiseiwitsch 1).

2. Collisions between electrons or positrons and atoms. - An important method for calculating the scattering length a and phase shifts η_l is Kohn's variational method which is based on the variational principle of Hulthén. Using suitable trial functions depending on a large number of adjustable parameters c_i , accurate values for a and η_l have been calculated in the case of the elastic scattering of low energy electrons e^- by hydrogen atoms, allowance being made for the Pauli exclusion principle, and thus electron exchange, by using symmetrized wave functions. The elastic scattering of positrons e^+ by H has also been studied in detail taking account of virtual positronium $e^- e^+$ formation. The values obtained for the scattering length are necessarily upper bounds to the exact values of a in the case of atomic hydrogen as target, but for complex atoms such as He this is not true owing to the inexact knowledge of the atomic wave function, which produces singularities for certain values of the parameters 2). This difficulty has been overcome to some extent by Drachman 3) who introduced a model Hamiltonian $\overline{H}_0$ to replace the exact Hamiltonian H_0 of the target atom chosen so that the approximate wave function is an eigen function

of $\overline{H}_c$. Further information on the use of variational methods can be found in the review by Moiseiwitsch4).

Although we have been concerned above with the elastic scattering of $e^{\pm}$ by atoms in a given state, usually the ground state, the influence of the other states of the target has been taken into account by introducing terms depending on the distances r_{1i} between the incident particle 1 and the atomic electrons i .

An interesting way of calculating elastic scattering phase shifts is the Fredholm method introduced by Reinhardt and his coworkers5) in which the Fredholm determinant $D(z)$ is approximated by using a basis set of square integrable functions. $D^{\text{approx}}(z)$ is then fitted to a rational fraction $R[N,M](z)$ at $N+M+1$ points in the upper half of the complex z plane away from the poles of $D^{\text{approx}}(z)$. The phase shift $\eta(E)$ can then be calculated by evaluating $R[N,M](z)$ at $z=E+i\epsilon$ using the formula $D(E+i\epsilon)=|D(E+i\epsilon)|e^{-i\eta(E)}$ where E is the energy of the incident electron.

Dispersion relations have been used to analyze experimental data on collisions between electrons and inert gas atoms by Bransden, McDowell and their coworkers. Discrepancies were found which are believed to arise from the presence of singularities in the exchange amplitude along the negative real axis6). Such a discrepancy does not appear for positron scattering since there does not exist an exchange amplitude in this case.

The usual procedure for investigating excitation collisions and complex target systems at low incident particle energies is the close coupling (cc) approximation which expands the total wave function Ψ of the system of incident particle and target atom in terms of a finite number of states ν of the atom:

$$\Psi(\underset{\sim}{r_1},\underset{\sim}{r_2}) = \sum_{\nu} F_{\nu}(\underset{\sim}{r_1})\,\psi_{\nu}(\underset{\sim}{r_2}) \qquad (1)$$

This yields a finite set of coupled integro-differential equations which can be solved by several different techniques7).

Nesbet and his coworkers8) have developed a matrix variational method in which the trial function is written as a linear combination of analytical functions with variable coefficients, yielding a set of linear matrix equations, and has been applied to the scattering of electrons by the alkali metal atoms and by C, N, O atoms.

A different method which converts the cc equations into a system of linear algebraic (LA) equations has been introduced by Eissner and Seaton[9)] and allows the use of accurate configuration interaction wave functions representing the target complex atom at the expense of a certain small loss of accuracy arising from the coarse net of integration points which is used. The excitation of the O^{2+} atomic ion has been studied extensively employing this approach.

Another valuable procedure for solving the cc equations is the R-matrix method employed by Burke and his collaborators[10)]. This method separates configuration space into an inner region $r \leq b$ where r is the relative distance between the incident particle and the target system, in which the interaction between the particles is strong, and an outer region $r > b$ in which the interaction is weak and electron exchange can be neglected. The wave function in the inner region is expanded in terms of a set of eigenfunctions $u_i(r)$ with eigenvalues k_i^2 obeying logarithmic boundary conditions at $r = b$ and gives

$$R = \frac{1}{b} \sum_i \frac{\{u_i(b)\}^2}{k_i^2 - k^2} \tag{2}$$

where k is the wave number of the incident particle. This quantity, known as the R-matrix for the case of multichannel scattering, enables the K-matrix, or tan η_λ in the case of single channel scattering, to be determined since the wave function for $r \leq b$ must fit smoothly to the asymptotic form of the function for $r > b$ It can be shown that the value of η_λ at a pole $k = k_i$ of R provides a lower bound to the exact value of η_λ. The R-matrix method has been applied with considerable success to the scattering of electrons by H, He, N, Mg atoms and N^+,O^+ ions.

The close coupling approximation does not take into account higher states of the target atomic system. This defect has been overcome in various ways. For example the correlation function expansion method may be used which expands the excluded states in terms of square integrable functions such as $r_1^{n_1} r_2^{n_2} r_{12}^{n_{12}} \exp\{-\lambda(r_1+r_2)\}$

where n_1, n_2, n_{12} are positive integers or zero. An alternative way of dealing with the higher states is the pseudo-state expansion method. Here the total wave function of the system is expanded in terms of so-called pseudo-states which make allowance for the various polarizabilities of the atom. Another procedure is the second-order potential method of Bransden and Coleman[11)] in which the closure formula

$$\sum_q \overline{\psi_q(\mathbf{r}')}\,\psi_q(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}') \qquad (3)$$

is used to sum over all the states of the atom, assuming an effective average eigenenergy $\bar{E}$, to produce an optical potential possessing the correct long range behaviour $-\alpha/2r^4$ where α is the dipole polarizability of the atom. A different procedure which has been used with some success by Callaway and his coworkers[12)] is the polarized orbital method of Temkin which writes the total wave function in the symmetrized form

$$\Psi^{\pm}(\mathbf{r}_1,\mathbf{r}_2) = F(\mathbf{r}_1)\{\psi(\mathbf{r}_2)+\psi^{pol}(\mathbf{r}_1,\mathbf{r}_2)\} \pm F(\mathbf{r}_2)\{\psi(\mathbf{r}_1)+\psi^{pol}(\mathbf{r}_2,\mathbf{r}_1)\} \qquad (4)$$

where $\psi^{pol}(\mathbf{r}_1,\mathbf{r}_2)$ is an extra term added to the atomic wave function $\psi(\mathbf{r}_2)$ coming from the polarization produced by the incident charged particle represented by $F(\mathbf{r}_1)$.

The distorted waves method was used in the past to approximate the solution of the cc equations assuming that only the initial and final states of the atom need to be included in the expansion and that back-coupling can be neglected. In this method the wave function of the scattered electron represents the motion of the free particle in the static field of the final state of the atom. However recently it has been shown by calculation and by using the random phase approximation (RPA), equivalent to the time dependent Hartree-Fock approximation, that better results can be seemingly obtained by replacing the final state static field by that of the initial state but this leads to the violation of time-reversal invariance. The RPA method has been used to study the scattering of electrons by atoms by Taylor and his collaborators[13)] and also by Amusia, Cherepkov and their coworkers.

Now directing our attention to higher energy incident electrons we find that the methods which have been used are based on the Born series. The first Born approximation has, of course, been applied extensively. Also a number of investigations using the second Born approximation have been carried out on collisions between $e^{\mp}$ and H and He atoms, the summation over the infinite set of intermediate states being accomplished by using the closure formula (3) and a suitable choice of average atomic eigenenergy $\bar{E}$ 14,15). This energy $\bar{E}$ must not be taken as the ground state energy since this gives rise to a spurious logarithmic singularity in the imaginary part of the elastic scattering amplitude in the limit as the momentum change vanishes. The second Born approximation is of restricted value since the third order Born approximation term is important. This term has been taken into account by Joachain and his coworkers16) by using the eikonal-Born series (EBS) which takes a combination of the second Born approximation and the Glauber approximation for the third order term. The unmodified Glauber approximation has also been applied quite successfully but is based on the use of the closure approximation taking the ground state energy as an average energy $\bar{E}$, which produces a logarithmic divergence for small momentum change.

To conclude this section it is worthy of note that classical theory has been used to investigate the scattering of electrons by atoms under suitable circumstances17). This can be done by employing correspondence principles or by solving the classical Newtonian equations of motion choosing the initial state at random, known as the Monte Carlo method.

3. Collisions between electrons and molecules. - Electron-molecule collisions are rather more difficult to treat than electron-atom collisions and thus various approximations necessarily have to be made. The simplest model is the fixed-nuclei approximation in which the nuclei are supposed to be at a fixed displacement $\underset{\sim}{R}$ apart. A static potential is obtained by using single-centre orbitals to construct the molecular wavefunction $\chi(\underset{\sim}{r}_i, \underset{\sim}{R})$ where $\underset{\sim}{r}_i$ denotes the position vector of the electron i of the molecule and to this is added a polarization potential. The function $F(\underset{\sim}{r}, \underset{\sim}{R})$, representing the motion of the incident electron with position vector $\underset{\sim}{r}$, is expanded in terms of spherical harmonics and the radial functions determined by solving coupled differential equations. This procedure has been applied by

Burke and Chandra[18] to the case of N_2 molecules. R-matrix theory can also be used for electron-molecule collisions. A transformation between the space-fixed and molecule-fixed frames in the outer region is required, a complication which does not arise in electron-atom collisions.

So far we have not included the possibility of molecular vibrations. This can be achieved by using a close coupling expansion for $F(\underset{\sim}{r},\underset{\sim}{R})$ in terms of vibrational eigenfunctions and assuming that the rotational energy is small compared with the vibrational energy. Then making an expansion using spherical harmonics leads to coupled differential equations for the radial functions which may be solved by standard procedures.

An improvement over the fixed-nuclei scattering amplitudes can be made by integrating them over vibrational and rotational wave functions. This is called the *adiabatic-nuclei approximation* and is valid as long as the scattering delay-time is small compared with the time of vibration. A further improvement introduced by Chandra and Temkin[19] and called the *hybrid theory* uses a close coupling approximation for vibration and an adiabatic-nuclei approximation for rotation. Chandra and Temkin have applied the hybrid theory to the scattering of electrons by N_2 molecules, finding that vibrational close coupling was needed only for the ${}^2\Pi_g$ partial wave.

Another approach to the vibrational excitation of the N_2 molecule by electrons assumes that an unstable state of N_2^- is formed during the collision. The nuclear wave function ξ representing the N_2^- state is a superposition of an outgoing wave and a single reflected wave originating at the first turning point and for this reason the approximation was called the *boomerang model* by Birtwistle and Herzenberg[20]. Oscillations in the vibrational excitation cross section as a function of energy are produced as the nodes of ξ drift across the nodes of the final vibrational state wave function of the N_2 molecule.

4. *Collisions between atomic systems.* - In the case of low energy heavy particle collisions the total wave function Ψ is usually expressed as an expansion in terms of molecular orbitals χ_s . Such a molecular orbital approach is the foundation of the *perturbed stationary state* (PSS) method. To see what this involves we consider a collision between a target H atom and an incident proton H^+ and denote the respective nuclei by A and B .

If $\underset{\sim}{R}$ is the position vector of B referred to A and $\underset{\sim}{r}$ is the position vector of the electron referred to an origin O on the internuclear line AB we write

$$\Psi(\underset{\sim}{r},\underset{\sim}{R}) = \sum_{s} F_s(\underset{\sim}{R})\,\chi_s(\underset{\sim}{r},\underset{\sim}{R}) \tag{5}$$

and substitute (5) into the time-dependent Schrodinger equation for the whole system. A partial waves expansion using symmetric-top wavefunctions characterising the rotation of the molecular system then gives rise to a set of coupled differential equations for the radial functions.

These coupled equations can be solved conveniently by using <u>semi-classical theory.</u> The easiest situation to treat occurs when we make a two-state approximation. However a difficulty arises from the fact that the two classical turning points differ considerably, but this has been overcome by Bates and Crothers[21)] by forcing a <u>common-turning point.</u> Another approach is based on the fact that scattering at large angles is determined by the interaction potential at small internuclear distances so that the motion of the nuclei can be adequately described by an average potential. This leads to the <u>mean trajectory method</u> used by Gaussorgues et al[22)] for $H^+ - H$ scattering.

The straightforward molecular orbital expansion (5) discussed above leads to difficulties with regard to the translational motion of the nuclei since the PSS equations for charge transfer collisions lead to dependence on the position of the origin O on the internuclear line AB which is clearly undesirable. However this defect has been corrected by Bates and McCarroll[23)] by means of the introduction of <u>travelling molecular orbitals</u> having a translation factor

$$\exp\left(\frac{i m \underset{\sim}{v}\cdot\underset{\sim}{r}}{2\hbar} f\right) \exp\left(-\frac{i}{\hbar}\int_{-\infty}^{t}\{\epsilon_s(R) + \tfrac{1}{2}m(v/2)^2\}\,dt\right) \tag{6}$$

where $\underset{\sim}{v}$ is the velocity of relative motion of the nuclei, assumed constant, $\epsilon_s(R)$ is the eigenenergy of the molecular state s , and $f \to -1$ and $+1$ according as the electron attaches to nucleus A or B respectively after the collision. Although O has been chosen for convenience here to be at the mid-point of AB , the charge transfer cross section is actually independent of the choice of origin when travelling molecular orbitals are used. It should be noted that even though the molecular orbitals χ_s are orthogonal, the above travelling molecular orbitals are not, since f has different values depending on whether the electron becomes bound to A or B for large R. However if the factor $\exp\left(\frac{i m \underset{\sim}{v} \cdot \underset{\sim}{r}}{2\hbar} f(\underset{\sim}{r}, \underset{\sim}{R})\right)$ possesses the same function $f(\underset{\sim}{r}, \underset{\sim}{R})$ for all travelling molecular orbitals then they will be orthogonal. Various suitable functions f have been used, the most recent being determined variationally by Crothers and Hughes[24] as a function of $Z = \underset{\sim}{R} \cdot \hat{\underset{\sim}{v}}$ yielding very satisfactory results for the case of $H^+ - H$ charge transfer collisions.

In order to interpret the behaviour of the colliding atomic particles in a scattering process it is necessary to possess a detailed knowledge of the potential energy curves connecting the initial and final states of the atomic systems involved. For example in the case of the elastic scattering of $He^+(1s)$ by $He(1s^2)$., the ungerade scattering amplitude f^- is determined by the attractive $^2\Sigma_u$ potential energy curve of He_2^+ which correlates unambiguously with the $1s^2 2p\ ^2P$ state of Be^+ for small R. On the other hand the gerade scattering amplitude f^+ is determined by the repulsive $^2\Sigma_g$ curve which connects adiabatically with the $1s^2 2s\ ^2S$ state of Be^+ for small R. However the motion of the atomic systems is actually too swift for adiabatic behaviour and it was shown by Lichten[25] that the appropriate repulsive curve to use corresponds to a diabatic state which correlates with the $1s\,2p^2\ ^2D$ state of Be^+ in the united atom limit and does not satisfy the von Neumann and Wigner non-crossing rule, and in fact crosses the $^2\Sigma_g$ potential curve which dissociates into $He^+(1s)$ and $He(1s2s)$ for large R. Smooth oscillations in the differential cross section for elastic scattering resulting from the interference between the g and u states of He_2^+ are found. Also in the case of $^4He^+ - {}^4He$ elastic scattering, a secondary pattern of oscillations is seen arising from interference due to the identity of the He nuclei. This secondary pattern is not present in the case of $^3He^+ - {}^4He$ elastic scattering since the nuclei are different here[26].

Oscillations in the electron capture probability for $H^+ - H(1s)$ collisions as a function of energy E for a given scattering angle Θ are also found. Using the two-state theory based on the $1s\sigma_g$ and $2p\sigma_u$ states of H_2^+, the oscillations are discovered to be very nearly π radians out of phase with those observed for large $E\,\Theta$. This occurs as a consequence of rotational coupling between the $2p\sigma_u$ state and $2p\pi_u$ state of H_2^+ in close encounters which is neglected in the two state theory.

Bates and Sprevak[27] have calculated the probability of exciting the $2p_{\pm1}$ states in $H^+ - H(1s)$ collisions as a function of scattering angle Θ and found that it is given closely by $\frac{1}{2}\sin^2\Theta$. A simple explanation of this result is provided by the realization that the orientation of the $2p\sigma_u$ orbital remains fixed in close fast collisions and that the probability that the $2p\pi_u$ state is occupied when the particles recede is $\frac{1}{2}(2S^2)$ where $S = \frac{1}{\sqrt{2}}\sin\Theta$ is the overlap integral for the $2p\sigma_u$ wave function oriented along the direction of incidence and the $2p\pi_u$ function oriented along the direction of scattering.

The pseudo-crossing, or avoided crossing, of potential energy curves provides a very useful concept for understanding certain types of collision processes. The original theory was developed by Landau and Zener. If ϕ_1, ϕ_2 are approximate wave functions corresponding to potential energy curves given by $H_{11}(R) = (\phi_1, H\phi_1)$, $H_{22}(R) = (\phi_2, H\phi_2)$ which cross at $R = R_c$, where H is the Hamiltonian operator, Landau and Zener assumed that $H_{11} - H_{22}$ changes rapidly and depends linearly on $Z = vt$, and that $H_{12} = (\phi_1, H\phi_2)$ is constant in the interaction region. If P is the probability that the system makes a transition from one curve to the other for a single passage through the pseudo-crossing point R_c, the total probability for a transition from state 1 to state 2 is $2P(1-P)$ since the system traverses R_c both on the incoming and outgoing passages. The Landau-Zener formula gives the wrong decay of transition probability with energy since it involves a transition zone width which increases with velocity as $v^{1/2}$ whereas the actual width is bounded.

Perturbationsin cross sections can be produced by pseudo-crossings, an interesting example being provided by the avoided crossing of $^2\Sigma_g$ curves of He_2^+, the upper curve dissociating into $He^+(1s)$ and $He(1s2s\ ^{1,3}S)$, giving rise to perturbationsin the elastic differential cross section for $He^+ - He$ collisions.

Demkov[28] has introduced a different but.related approximation for dealing with charge transfer collisions based on transitions between potential energy curves. For large R, where $|H_{12}| \ll |H_{11} - H_{22}|$, the wave function of the quasimolecular system is $\psi_1(r_A)$ or $\psi_2(r_B)$, the atomic wave functions of the active electron attached to atoms A or B. For small R where $|H_{12}| \gg |H_{11} - H_{22}|$ the wave function becomes $\frac{1}{\sqrt{2}}\{\psi_1(r_A) \pm \psi_2(r_B)\}$ which is similar to the wave function occurring in symmetrical resonance charge transfer. The wave function changes its form in the non-adiabatic zone where $|H_{12}| \approx |H_{11} - H_{22}|$. Demkov assumes that $H_{11} - H_{22}$ is nearly constant in the non-adiabatic region and that H_{12} can be represented by an exponential model.

A more general analysis has been given by Nikitin[29)] which yields the Landau-Zener formula on replacing the exponential model by a linear model and also gives the Demkov formula as another special case.

An interesting approximation has been obtained by Crothers[30)] who gets the transition probability formula

$$\mathrm{sech}^2 \frac{y}{\hbar v} \sin^2 \frac{x}{\hbar v} \tag{7}$$

where

$$x + iy = \int_0^{Z_c} \left[4H_{12}^2 + (H_{11} - H_{22})^2\right]^{\frac{1}{2}} dZ, \tag{8}$$

the integral being taken over a suitable contour in the complex plane connecting the origin to the zero Z_c of the <u>integrand</u> lying closest to the real axis in the first quadrant, and $R = \sqrt{\rho^2 + Z^2}$ where ρ is the impact parameter. This formula yields the Demkov result, and also is exact for symmetrical resonance collisions as well as for the Rosen and Zener model $H_{12} = \frac{1}{4}\,\mathrm{sech}\,\alpha Z$, $H_{11} - H_{22} = \Delta E$ where ΔE is the constant energy splitting.

Diabatic potential curves have been used by Fano and Lichten[31)] to explain the <u>promotion</u> of inner shell electrons to higher states leading to <u>inner-shell excitation.</u> Thus, as an Ar^+ ion and Ar atom come together a $2p$ electron in the L shell may follow the diabatic $4f\sigma_u$ orbital taking it through crossings with other potential curves so that the electron finds itself in a highly excited orbital of Ar when the atomic systems move apart after the collision. Recent work on inner-shell excitation has been discussed by Fastrup[32] and by Briggs[33].

Another interesting effect, known as K-vacancy-sharing, comes about as a consequence of a vacancy created in a $2p\sigma$ orbital by electron promotion being transferred to the $1s\sigma$ orbital during a single passage through the transition zone. This has been examined by Meyerhof[34] using a similar analysis to that given by Demkov[28] in his treatment of charge transfer, and by Bøving[35] using the Nikitin[29] method. Good agreement with the Meyerhof formula has been obtained by Taulbjerg et al[36] using a three-state $1s\sigma-2p\sigma-2p\pi$ close coupling approximation approach.

So far we have been concerned with low energy collisions. In the case of heavy particles colliding at high energies we may use the first Born approximation and many such calculations have been carried out[37]. Greater accuracy may be achieved by using the close coupling approximation while considerable simplification can be introduced by taking rectilinear trajectories and using the impact parameter treatment which has been shown to be equivalent to the wave treatment at sufficiently high energies.

The first Born approximation has been used to discuss charge transfer at high impact energies. The simplest approach is the Oppenheimer-Brinkman-Kramers (OBK) approximation in which the nucleus-nucleus interaction is neglected. Omidvar[38] has carried out a detailed analysis of capture into excited states for hydrogenic systems obtaining an n^{-3} decay of the capture cross section with principal quantum number n at sufficiently high energies in accordance with the early work of Oppenheimer. Assuming that the main contribution to the charge transfer cross section comes from small angles of scattering the first Born approximation cross section falls off as E^{-6} with impact energy E but in the high energy limit the cross section is dominated by back scattering which yields an E^{-3} decay.

Drisco, and more recently Shakeshaft[39], have used the second Born approximation to evaluate the charge transfer cross section and have found that it falls off as $E^{-11/2}$ at high impact energies. This is in accordance with the classical model prediction of Thomas based on the classical impulse or binary encounter approximation (BEA) in which the capture process is assumed to occur as the result of two successive binary encounters, the first between the incident proton and the atomic electron and the second between the atomic electron and the proton to which it is bound both collisions producing scattering of the electron through 60°. The electron will then be moving parallel to the incident proton with the same speed and can be captured by it with a certain probability which can be derived in an analytical form. The theory of charge transfer has been discussed in detail by Mapleton[40] and Bransden[41].

The classical impulse approximation has been used by Bates and his collaborators to study a number of different types of suitable collision processes including electron detachment from H^- ions in collisions with various atoms and molecules[42] and electron loss from fast atoms[43]. Also the Monte Carlo method has been applied by Abrines and Percival[44] and Banks et al[45] to a classical three-body study of collisions between protons and H atoms including ionization and charge transfer.

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DISCUSSION

B. G. Giraud: I have a short comment and a question. The comment is that the perturbed stationnary state method you mentioned is equivalent to our nuclear generator coordinate method, but only in what I refered to as the Born-Oppenheimer limit in the third part of my talk. This is because adiabaticity is not always used in nuclear GCM at the early stage of the definition of the vector basis.

The question is, do you think that Padé approximants are very useful to improve the convergence in the kind of calculations you mentioned?

B.L. Moiseiwitsch: To obtain useful results using Padé approximants it is necessary to calculate the Born series up to the third order. Perhaps one could do this by using the third order Glauber term since third Born term is very difficult to determine.

M.A. Nagarajan: In the case of the closure approximation along with the use of an average excitation energy, you refered to the problem of a logarithmic divergence if the average energy was chosen equal to the ground state energy. Is this a special consequence of the long range Coulomb force occuring in atomic collisions?

B. L. Moiseiwitsch: This is probably the case but it may well be still a problem in nuclear collisions leading to poor results in the forward direction, although not a divergence.

M. Rosina: I was surprised that you discussed only the reactions between the lightgst atoms. Is there some basic difficulty to apply these method to heavier atoms?

B.L. Moiseiwitsch: I discussed light atomic systems only for the sake of simplicity. The main difficulty arises from the complexity of the atomic wave functions involved in heavy atomic systems although in certain situations a simple model may be used to overcome this problem.