ON VARIOUS METHODS USED IN THE CALCULATIONS OF INELASTIC ELECTRON-ATOM AND ELECTRON-MOLECULE COLLISIONS

YUH-KANG PAN
Department of Chemistry, Boston College, Chestnut Hill, Massachusetts 02167

ABSTRACT. — Various approximate methods used in the calculation of inelastic electron-atom and electron-molecule collisions are classified into six different categories, namely, Born approximation, Born-Oppenheimer approximation distorted wave Born approximation, distorted wave Born-Oppenheimer approximation, the method of integral equation, and variational method. The nature of these six different methods are described and their advantages and disadvantages are presented. The difficulties in the calculations of inelastic electron-molecule collisions are discussed. Some recommendations are made for future progress in the calculation of inelastic electron-molecule collisions.

The theory of electron-atom and electron-molecule collision processes has been developed very rapidly in the last few years and has attained a very important practical meaning. This is because the best way to learn something about the forces acting between elementary particles is to observe their interaction with one another. Most of what we know about the microworld has been established by means of studying collision processes. Besides, the understanding of a great many facets of chemical kinetics, spectroscopy, the physics of gaseous discharges, astrophysics, radiative transfer in flames and in the atmosphere, atomic physics, physics of the upper atmosphere and solid state physics depends on our knowledge of the elementary interaction processes of electrons with atoms, molecules and other elementary particles. The calculations of inelastic electron-atom and electron-molecule collisions are highly desirable. Because for many applications it is necessary to have reliable information on the rates of the various processes involving excitation of atoms and molecules by electrons. Many of the processes concerned are not readily investigated experimentally, so it is essential to rely to a considerable extent on theoretical prediction. Various approximate methods have been used in the calculations of the inelastic scattering cross sections for electron-atom collisions. These methods can be roughly classified into six different categories, namely, Born approximation, Born-Oppenheimer approximation, distorted wave Born approximation (D.W.B.), distorted wave Born-Oppenheimer approximation (D.W.O.B.), the method of integral equations, and variational methods.

BORN APPROXIMATION

The Born approximation assumes that the coupling of the incident electron with the atom is weak (all matrix elements of the interaction between the electron and atom, whether diagonal or non-diagonal are small). Therefore the calculation of the scattering cross-section can be carried out by a first-order perturbation method. The effect of

electron exchange between the incident beam and the atom is ignored in this approximation. The cross section is then proportional to the square of the matrix element of the interaction between initial and finial states in which the free electron wave functions are plane waves and the overall wave function is simply an unsymmetrical product. The inapplicability of Born approximation for electron energies near the threshold is well known (Bates, Fundaminsky and Massey, 1950). In low energy collisions the processes become quite complicated owing to various threshold effects which arise during the excitation and ionization of atoms and ions. Some transitions which are quite strong near threshold become completely forbidden in this approximation, because the effect of electron exchange is ignored in the approximation.

Born-Oppenheimer Approximation

If we include the effect of electron exchange between the incident beam and the atom but still assumes that all matrix elements are small, then we obtain the so called Born-Oppenheimer approximation to the scattering amplitude or, in short, Born-Oppenheimer approximation (see, for example, B.L. Moiseiwitsch, Revs. Mod. Phys. *40*, 238, (1968). However, we should distinguish this approximation from the Born-Oppenheimer approximation to the separation of electronic and nuclear motions). The overall wave functions used to calculate the probability amplitude are properly summetrized combinations of plane wave and atomic wave functions of the form

$$\Psi_o(r_a)e^{ik_o r} \quad \Psi_n(r_a)e^{ik_n r}$$

where Ψ_o and Ψ_n are the wave functions of the initial and final atomic states respectively and r_a represents the aggregate of the coordinates of the atomic electrons. The relative motion of the colliding electron is represented by undisturbed plane waves of wave length $2\pi/k_o$ before the collision and $2\pi/k_n$ after the collision.

However, the Born-Oppenheimer approximation, apart from the inclusion of the possibility of electron exchange, is still only a first-order perturbation formula. From an analysis of the observed data it appears that this approximation often overestimates the importance of exchange to a very serious extent. This failure is particularly serious in the calculations of the cross section near the threshold of excitation of one level from another if both belong to the same electron configuration and in other cases in which there is no change of azimuthal quantum number of the atomic electron concerned in the process (e.g. when an s-s transition is involved). Marriott (Marriott, 1958) has shown that the Born-Oppenheimer approximation cannot be relied on at all at low electron energies whether the coupling between initial and final states is weak or not. Unfortunately, for many applications it is the cross-section near the threshold which is required. Ochkur (Ochkur, 1963) thinks that the deficiencies of the calculations using the Born-Oppenheimer formula primarily result from an incorrect extrapolation into the domain of low-energies. By using the Born-Oppenheimer formula as a basis, Ochkur obtains a new simple formula. The excitation functions have been calculated for the 2^3S and 2^3P level in helium by using this new formula. The results are in reasonably good agreement with the experimental data. Rudge (Rudge, 1965)

pointed out that Ochkur's formula is not rigorous in the sense of being obtainable from a variational principle and gave an alternate expression obtainable from a variational principle. Nevertheless, Ochkur's formula has been successfully used in several other inelastic atomic collision calculations and has been applied to the excitation of the hydrogen molecule by Khare (Khare, 1966a, 1966b, 1967). Khare's results are in fair accord with experimental results and other theoretical estimates.

Distorted Wave Born Approximation

The distorted wave Born approximation assumes that only the non-diagonal matrix elements are small. The plane waves which represent the initial and final free electron wave functions are then replaced by waves distorted by the mean interaction with the atom in the initial and final states respectively. It was first pointed out by Mott (Mott, 1932) that the contribution to the cross section for an inelastic collision between two interacting systems which arises from impacts in which their relative angular momentum is $\{l(l+1)\}^{1/2}\hbar$ can never exceed $(2l(l+1)\lambda^2/_4$ where λ is the wavelength of the initial relative motion. Bates et al. have shown that the calculations for $O(2^3P, 2^1S)$, O^+ $(2^4S, 2^2D)$ and $O^{2+}(2^3P, 2^1D$ and $2^1S)$ using D.W.B. approximation yields cross sections in excess of the possible maxima (Mott, 1932). So it is also not a good method for the calculation of inelastic cross sections for electron-atom collisions.

Distorted Wave Born-Oppenheimer Approximation

The distorted wave Born-Oppenheimer approximation also assumes that only the non-diagonal matrix elements are small. The plane waves which represent the initial and final free electron wave functions are then replaced by waves $F_o(r)$, $F_n(r)$ distorted by the mean interaction with the atom in the initial and final states respectively. $F_o(r)$ is the wave function which represents a plane wave $e^{ik_o r}$ and an outgoing spherical wave scattered by atom in its ground state, not allowing for the possibility of any inelastic collisions but including exchange effects as far ts they effect elastic scattering. $F_n(r)$ is the corresponding wave function representing a plane $e^{ik_n r}$ and an outgoing spherical wave scattered by the atom in the nth excited state. The effect of electron exchange in producing distortion is allowed for in this approximation. Erskine and Massey (Erskine and Massey, 1952) first applied this approximation to the excitation of the 2S level of hydrogen from the ground state. They find that for electron energies near the threshold the cross section for the excitation is given by

$$Q = 4_{\cdot} k_1 |\beta|^2 / k_o^3 \qquad (1)$$

k_o and k_1 are the wave numbers of the initial and final motion of the election relative to the atom. $|\beta|$ arises from requiring the solution of a pair of integro-differential equations have the asymptotic form

$$f \sim \beta \exp(ik_1 r) \qquad (2)$$

Since the maximum possible value (Mott, 1932) for Q is π/k_o^2, we may call $4\pi k_1 |\beta|^2 k_o$ the probability of the particular inelastic collision concerned.

The integro-differential equation expressed in atomic units is of the form

$$[\frac{d^2}{dr^2} - 2V_{oo}(r) + k_o^2]f_o + \int_o^\infty K_{oo}(r,r')f_o(r')dr' = 2V_{o1}(r)f_1(r) - \int_o^\infty K_{o1}(r,r')f_1(r')dr$$

$$[\frac{d^2}{dr^2} - 2V_{11}(r) + K_1^2]f_1 + \int_o^\infty K_{11}(r,r')f_1(r')dr' = 2V_{o1}(r)f_o(r) - \int_o^\infty K_{1o}(r,r')f_o(r')dr' \quad (3)$$

and the solutions must be proper functions satisfying the asymptotic conditions (2) and

$$f_o \sim \text{Sin } k\ r + \alpha \exp(ik_o r) \quad (4)$$

In these equations V_{oo} and V_{11} are the interactions between the electron and the atom arranged over the initial and final states of the atom, K_{oo} and K_{11} are interaction kernels which represent the contribution of electron exchange to the mean interaction in each case, V_{o1} is the non-diagonal matrix element of the interaction and K_{o1}, K_{1o} are the corresponding contributions from exchange effects. If V_{o1}, K_{1o} and K_{1o} are zero the probability of the transition vanishes. If equation (3) is solved exactly the resulting cross section should be accurate, provided that the wave numbers k_o and k_1 are sufficiently small so that incident electrons with angular momenta greater than zero can be ignored and provided that the influence of other excited states is also negligible. It is quite clear that almost all of the violations of the conservation law (Mott, 1932) occur for electron energies near the threshold in which case the main contribution comes from head on collisions. The neglect of excited states is equivalent to ignoring dynamic polarization effects. At the election energies concerned these are probably not very important, although it is difficult to estimate their order of magnitude. In any case the exact solution of equation (3) will certainly give cross sections which obey the conservation laws. It is only when the equation is solved by approximate methods that violation of these laws can occur. All previous methods solve equation (3) by successive approximations on the asumption that V_{o1}, K_{o1} and K_{1o} are small. The distorted wave Born-Oppenheimer method makes no further assumptions, but the Born-Oppenheimer approximation assumes that V_{oo}, V_{11}, K_{oo} and K_{11} are also negligible and the Born approximation neglects K_{1o} and K_{o1} as well. It is to be expected that the D.W.B.O. method will give accurate results if V_{o1}, K_{o1} and K_{1o} are small but this is not sufficient to justify the Born-Oppenheimer approximation. In fact, for excitation of atoms by electrons with energy near the threshold the distortion introduced by V_{oo} and V_{11} is very marked. Erskine and Massey found their results for the excitation of the 2s level of atomic hydrogen were considerably different from those obtained by use of the Born-Oppenheimer approximation in which distortion is neglected. Whereas the latter approximation gives cross-sections at energies close to the threshold which are greater than the maximum possible value, the D.W.B.O. method gives values always less than this. Nevertheless, it approaches within 30% of this value at low energies. The coupling between the motion in the initial and final states is quite strong in this case. The D.W.B.O. approximation, which depends on this coupling being weak, cannot be expected to yield very good results under these conditions. Further evidence in support of this was obtained in a calculation, by a variational method, carried out by Massey and

Moisewitsch (Massey and Moisewitsch, 1953), which did not require the coupling to be weak.

The next application of the D.W.B.O. method was to the excitation of the 2^3S and 2^1S states of helium by Massey and Moiseiwitsch (Massey and Moiseiwitsch, 1954). In the 2^3S calculation they found a resonance effect very close to the threshold, leading to a sharp peak in the cross section, and the absolute magnitude was much smaller than given by the Born-Oppenheimer approximation. This was due to the fact that the distortion effectively annihilated the partial cross-section for excitation by incident electrons of zero angular momentum. Their results are in agreement with the experimental data, and represent an important success of the method. It is noteworthy that in this case the cross sections are all well below the maximum possible values showing the coupling to be weak. In the 2^1S state, experimental results show that a sharp peak in the excitation function near the threshold also occurs. This does not appear according to their calculations probably because the close coupling between the 2^3S and 2^1S state is ignored. Evidence for this has been afforded by accurate numerical calculations by Marriott on the cross-section for the deactivation of 2^1S helium atoms by slow electrons which produce transitions to 2^3S states. The first application of the D.W.B.O. method to an s-p transition was made by Khashaba and Massey (Khashaba and Massey, 1958) for the excitation of the 2p level of hydrogen. They calculated the total cross-section and the polarization of the radiation excited by the impact. Their results did not differ very much from those given by the Born-Oppenheimer approximation either for the total cross-section or for the polarization, but this was partly coincidental. Thus the distortion virtually annihilates the partial cross-section q_0 (for scattered electrons with zero angular momentum) but largely compensates this by increasing q_1 (for scattered electrons with angular momentum $\sqrt{2}\hbar$). The usual tests of coupling indicate that it is not very strong (the distorted wave partial cross-section q_1 never exceeds one-quarter of the maximum possible value $3\pi/k^2$). Massey and Moiseiwitsch carried out a calculation of the cross-section for excitation of the 2^3P state of helium by D.W.B.O. method on similar lines to those of Khashaba and Massey (Khashaba and Massey, 1958) for the 2p of hydrogen. The triplet state calculation is of great interest because excitation can only come through exchange which limits the significant contributions to the first two partial cross-sections for which the effects of distortion are much more marked. In other words, there is less dilution of these effects from the higher order partial cross-sections which are little affected by distortion. Their results have been compared with the corresponding results given by the Born-Oppenheimer approximation. Although there are considerable differences at electron energies below 100eV, these are much less marked than for the excitation of the 2^3S state (Massey and Moiseiwitsch, 1954). The D.W.B.O. method gives cross-sections in closer agreement with observation but substantial discrepancies still remain. The coupling between the 1^1S and 2^3P states is nowhere as strong as judged by the ratio of their results for the partial cross-sections to the maximum possible value. Thus their calculated values for either q_0 or q_1 is never as great as 0.25 of the

maximum and is usually much less. Effects due to coupling between 2P and 2S states are likely to be smaller than for atomic hydrogen owing to the larger energy differences. The cross-section for excitation of the 2p state of hydrogen by electron impact, calculated by Khashaba and Massey (Khashaba and Massey, 1958) using the exactly similar D.W.B.O. method, is in considerably closer agreement with the observations of Fite and Brackmann (Fite and Brackmann, 1958). On the other hand, in the hydrogen case, the atomic wave functions are accurately known and no account has to be taken of the coupling between 2^3P and 2^1P states. It is difficult to judge how important these two factors are. It is also difficult to estimate the accuracy of Massey and Moiseiwitsch's results with any certainty because there are inconsistencies in the observed data. In any case, one would have expected the D.W.B.O. method to give very good results if the coupling between the motion in the initial and final states is weak.

The Method of Integral Equations

The method of integral equations had been developed by Drukarev (Drukarev, 1953). Using this method, the excitation of the sodium atom by slow electrons has been calculated (Veldre, 1956). In this calculation only the s-wave of the incident beam was taken into account. For a certain value of incident electron energy the exchange and strong coupling have been included. The elastic scattering of slow electrons by lithium atoms with the inclusion of exchange was calculated by the Drukarev approximation (Veldre, Gailitis, Damburg and Stepinsh, 1956). In the incident beam only the s-wave was taken into account. The question of the choice of radial wave functions of atomic electrons was investigated (Veldre, 1959) and it was shown that the behavior of the radial wave function near the zero does not have an important influence of the magnitude of the effective cross-section. In the inelastic cases the main advantage of the method of integral equations is that it can obtain analytical expressions for the desired atomic wave functions of different states for all r, and not merely their asymptotic forms. This feature can be used to obtain appropriate classes of variation functions associated with the calculation of electron scattering by variational methods. Matora (Matora, 1960) applied the Drukarev method to calculate the elastic s-scattering of electrons and the excitation functions of the 2^3S and 2^1S states of helium by electrons with energies from 0 to 40 eV. However, Massey and Moiseiwitsch's (Massey and Moiseiwitsch, 1954) result for 2^3S calculated by D.W.B.O. methods corresponds more closely to the experimental data than the result obtained by Matora using the method of integral equations. Damburg et al., pointed out that the method of integral equations has slow convergence. The effective cross-section for the elastic scattering of electrons by hydrogen atoms, calculated by the second approximation of the method of integral equations, agrees with the effective cross-section calculated by the second Born approximation. However, calculations by the second Born approximation are less complicated than the method of integral equations.

Variational Method

As mentioned before, it seems D.W.B.O. method is a reasonably good approximation in inelastic scattering of electrons by atoms and molecules. Owing to the labor involved in calculating the distorted waves F_o and F_n the method cannot be applied widely. However, variational methods greatly facilitate D.W.B.O. calculations, for both the functions F_o and F_n may be obtained in a convenient analytical approximation for both the antisymmetric and symmetric cases.

The application of variational methods to bound state problem has proved to be very fruitful, especially for obtaining approximations to the lowest eigenvalue of the energy. Although in principle still applicable to the approximate determination of the energies of excited states, the method becomes much less convenient because of the volume of analytical and computational work required. Variational methods for dealing with atomic collision problems were first proposed by Hulthen (Hulthen, 1944). Hulthen proposed a method, based on his variational principle, for the approximate calculation of the radial function and its phase, and verified his method on the simplest examples. In 1947, Schwinger (Schwinger, 1947) developed a variational method, different from Hulthen's method, which was based on an integral equation for the wave function. In 1948, Kohn (Kohn, 1948) geenralized Hulthen's formulation, extending it to the general case of scattering. Following on his work, a series of papers appeared (see for example, Newton, 1966) in which new variational methods were proposed. However, all these methods do not differ essentially from the two basic methods: the Hulthen-Kohn method based on Schrödinger's differential equation and Schwinger's method based on an integral equation. These variational methods are similar to those used for bound state problems but they differ in certain important respects. In both cases the aim is to obtain expressions involving wave functions describing the state of systems which remain correct to the first order when a variation is imposed on one or more of these functions. The bound state energies are found to be true minima with respect to the variational calculations under the imposed conditions while this is not true for problems of unclosed states which described collision processes. This has the consequence that greater flexibility in the choice of trial functions may even lead to less satisfactory results, a situation which can never arise in bound state problems. Much greater care has to be taken therefore in applying variational methods under these circumstances and it is usually difficult to estimate the accuracy of the results. The application of variational methods of scattering problems has also been limited by the complexity of the integration required in the use of the Schwinger formulation even for the simplest trial functions, and the difficulty of finding adequate trial functions in the relatively simple Kohn formulation. In spite of the difficulty of applying variational methods to collision problems, extensive development of the theory of elastic (Massey and Moiseiwitsch, 1950; Moiseiwitsch, 1953) and inelastic scattering of electrons by atoms using the variational methods of Hulthen and of Kohn has been carried out. The distorted wave functions used in Erskine and Massey's (Erskine and Massey, 1952),

Massey and Moiseiwitsch's (Massey and Moiseiwitsch, 1953), Khashaba and Massey's (Khashaba and Massey, 1958), and Massey and Moiseiwitsch's calculations (Massey and Moiseiwitsch, 1960) are determined by Hulthen's and Kohn's variational methods. The results obtained have been encouraging. The generalization of Hulthen's variational method to the inelastic scattering of electrons by atoms was first derived by Moiseiwitsch (Moiseiwitsch, 1951) by using the integral $L = \Psi^*(H-E)\Psi d\tau$ where H is the hamiltonian of the system. The complex parameters a, d, $c_1, \ldots, c_n$ in the trial function are determined through the conditions

$$L_t = 0 \qquad (5)$$

$$\frac{\partial L_t}{\partial a} + 2i\frac{k_1}{k} d^* \frac{\partial L_t}{\partial a} = 0 \qquad (6)$$

$$\frac{\partial L_t}{\partial C_i} = 0, \ (i=1, \ldots, n) \qquad (7)$$

where $L_t = \int \Psi_t^*(H-E)\Psi_t d\tau \qquad (8)$

and a and d are complex. In contrast to Hulthen's variational method applied to the elastic (Moiseiwitsch, 1953) scattering of electrons, the condition L=0 does not imply that a=0. A correction to the parameter may be obtained by considering the integral

$$L' = \int \Psi(H-E)\Psi d\tau \qquad (9)$$

For it can be shown that

$$\delta L' = 4\pi k \delta a \qquad (10)$$

therefore the corrected value of the parameter a is given by

$$\lambda = a - L'/4\pi k \qquad (11)$$

This variational method can be extended to include any order partial wave, and excitation to any state of the atom. Massey and Moiseiwitsch (Massey and Moiseiwitsch, 1953) first applied this method to the calculation of the 1s–2s electron excitation cross-section of hydrogen. Their results are qualitatively more in accord with those of the accurate numerical method of Marriott (Marriott, 1958) than either of the other methods. The poor quantitative agreement is probably a consequence of the use of an over-simplified trial function in the variational calculation. It is apparent that this variational method does not require the coupling between the motion in the initial and final states to be weak and the results of this method are better than those of other approximations. However, the great difficulty in applying this variational procedure is the complexity of the calculations involved even when using the simplest trial functions. For this reason, in Massey and Moiseiwitsch's calculation of the 1s–2s electron excitation cross-section of hydrogen, detailed numerical work was confined to trial functions of the form

$$f_+ = \sin kr + (A + be^{-r})(1 - e^{-r}) \cos kr \qquad (12)$$

$$f_1 = (1 - e^{-r}) d \exp(ik_1 r) \qquad (13)$$

b being the additional variable parameter. These wave functions suffer from the defect that they do not allow for mixing between the incident and scattered waves. Even for such over-simplified trial functions the analysis involved, is very extensive and the determination of "a" from the equations (5) to (7) was quite involved.

Electron-Molecule Collision Problems

Although the scattering of slow electrons by atoms has been extensively studied theoretically, comparatively little theoretical work has been done on the elastic and inelastic scattering of slow electrons by diatomic or polyatomic molecules. This is undoubtedly due to the mathematical complexity of the problem. We cannot apply Born's approximation, because it is least reliable in the low energy domain. Thus we have to solve the Schrödinger equation for the incident electron directly. This problem is fairly simple in the case of atoms on account of the sperical symmetry of the potential field, but in the case of molecules, the molecular potential (force) is not spherically symmetric, so the Schrödinger equation is not separable and the analysis becomes very complicated. Under certain conditions, however, it is possible to treat the individual atoms in the molecule as independent scattering centers so that the amplitude for scattering by the individual atoms in the molecule can be obtained by adding the amplitudes for scattering by the individual atoms with proper allowance for phase differences. The resulting cross sections must then be averaged over all molecular orientations to give observable data. This appoximation will only be valid if multiple scattering of an electron within the molecule is negligible and if the distortion of the atomic fields by the valence forces is also unimportant. Both these conditions are likely to be well satisfied for impacts with fast electrons for which Born's first approximation gives an adequate representation of the atomic scattering (Massey, 1956). It is not so obvious that when Born's first approximation is inadequate the assumption of independent scattering will always be satisfactory, but there is evidence that it does have a range of validity extending to scattering of electrons with velocities much too slow for Born's first approximation to be applicable. On the other hand, for very slow electrons, with wave-lengths comparable with the atomic separations in the molecule, there is no doubt that the independent scattering approximation is no longer valid and the calculation of the scattering presents much greater difficulties.

According to our discussions in the above sections, it seems more flexible to use the variational method for inelastic scattering of the electrons by diatomic or polyatomic molecules. The behavior of phases at small energies, the relation between the discrete and the continuous spectrum are directly or indirectly connected with variational principles. Besides, it is well known that the basic equations of stationary perturbation theory for bound state can be derived from a variational principle. Similar results can also be obtained in collision theory for the scattering amplitudes and the phases if one starts from the stationary property of appropriate functionals. As regards numerical calculations, it seems as if only variational methods allow one to take into account effectively and rigorously such phenomena as the polarization of an atom by an incident electron and obtain results of the same degree of accuracy as is attained in the evaluation of atomic and molecular energy levels. However, in order to generalize Moiseiwitsch's variational method for inelastic scattering of electrons by molecules, first we have to solve the difficulties of the variational meth-

od (such as the complexity of the calculations involved and the question of choosing trial functions). As to the trial functions, the Hulthen's, Kohn's and Moiseiwitsch's criteria for selection of the "best" values of the parameters are reasonable, but of course not essential or necessarily the best to choose. Hulthen's and Kohn's criteria merely make the trial function simulate one property of the exact wave-function. We shall examine various alternative procedures and look for the possibilities for finding the best criteria. The special feature of the method of integral equations as mentioned before shall be studied and the applicability to obtaining appropriate classes of variation function associated with calculation of electron inelastic scattering by the variational method shall be examined. For diatomic molecule calculations, the difficulty due to the distortion of a two-center field also should be overcome. For inelastic scattering of electrons by the hydrogen molecule, Huzinaga's (Huzinaga, 1957) and Hoyland's (Hoyland, 1966) one-center wave functions shall be used for both the initial and final states of the molecule. This will allow all the integrals to be evaluated exactly and with little labor. Calculations on this line are now in progress in our laboratory.

Acknowledgments

The author is indebted to Herschel Rabitz of Harvard University for reading the manuscript.

Literature Cited

Bates, D. R., A. Fundamisky, J. W. Leech and H. S. W. Massey, 1950. Excitation and Ionization of Atoms by Electron Impact. Phil. Trans. 243A: 93-143.

Damburg, R. and V. Kravchenko, 1960. The Scattering of Electrons By Alkali Metal Atom. V. Latv. PSR Zinat. Akad. Vest. 1:73-81.

Drukarev, G. F. 1953. Excitation of the Sodium Atom By Slow Electrons. Zhur. Eksptl. Theoret. Fiz. 25: 129-133.

Erskine, G. A. and H. S. W. Massey, 152. The Application of Variational Method to Atomic Scattering Problems II. Proc. Roy. Soc. 212A: 521-530.

Fite, W. N. and R. T. Brackmann. 1958. Collision of Electrons With Hydrogen Atoms II. Physi. Rev. 112: 1151-1156.

Hoyland, J. S. 1966. Single-Center Calculations on the Lowest-Lying π_u and π_s Excited States of H_2. J. Chem. Phys. 45: 3928-3933.

Hulthén, L. 1944. Neutron-Proton Scattering in the Region 0-5 Mev. Fysiogr. Sallsk. Lund. Forhandl. 14: 2-8.

Huzinaga, S. 1957. One-Center Expansion of Molecular Wave Function, II. Progr. Theoret. Phys. (Kyoto) 17: 162-168.

Kare, S. P. 1966a. Excitation of Hydrogen Molecules by Electron Impact. Phys. Rev. 149: 33-37.

————, 1966b. Excitation of Hydrogen Molecules by Electron Impact II. Phys. Rev. 152: 74-75.

————, 1967. Excitation of Hydrogen Molecule by Electron Impact III. Phys. Rev. 157: 107-112.

Khasaba, S. and H. S. W. Massey. 1958. The Excitation of the 2p State of Hydrogen by Slow Electrons — Distorted Wave Treatment. Proc. Phys. Soc. 71A: 574-584.

Kohn, W. 1948. Variational Methods in Nuclear Collision Problems. Phys. Rev. 74: 1763-1772.

————, 1949. Variation Scattering Theory in Momentum Space I. Phys. Rev. 84: 495-501.

Marriott, R. 1958. Calculation of the 1s-2s Electron Excitation Cross Section of Hydrogen. Proc. Phys. Soc. 72A: 121-129.

Massey, H. S. W. 1956. Theory of Atomic Collisions. Handbuch der Physik, 36: 232-408.

Massey, H. S. W. and B. L. Moiseiwitsch. 1950. The Application of Variational Methods to Atomic Scattering Problems I.

————, 1953. Calculation of 1s-2s Electron Excitation Cross Section of Hydrogen By a Variational Method. Proc. Phys. Soc. 66A: 406-408.

———, 1954. The Application of Variational Methods to Atomic Scattering Problems IV. Proc. Roy. Soc. 227A: 38-51.

———, 1960. The Excitation of the 2^3P State of Helium By Electron Impact. Proc. Roy. Soc. 258A: 147-158.

MATORA, I. M. 1960. The Scattering of Slow Electrons By Helium Atoms, With Excitation of the 2^3S and 2^1S Levels. Opt. i. Spectr. 9: 707-713.

MOISEIWITSCH, B. L. 1951. A Variational Method for Inelastic Collision Problems. Phys. Rev. 82: 753-753.

———, 1953. The Application of Variational Methods to Atomic Scattering Problems III. Proc. Roy. Soc. 219A: 102-109.

NEWTON, R. G. 1966. Scattering Theory of Waves and Particles. McGraw-Hill Book Company, New York.

MOTT, N. F. 1932. The Theory of the Effect of Resonance Levels on Artificial Disintegration. Proc. Roy. Soc. 133A: 228-240.

OCHKUR, V. I. 1963. The Born-Oppenheimer Method in the Theory of Atomic Collisions. Zhur. Eksptl. Theoret. Fiz. 45: 734-741.

RUDGE, M. R. H. 1965. The Calculation of Exchange Scattering Amplitudes. Proc. Phys. Soc. 85: 607-608.

SCHWINGER, J. 1947. A Variational Principle of Scattering Problems. Phys. Rev. 72: 742-742.

VELDRE, V. 1959. Excitation of Atoms by Electrons. Latv. PSR. Zinat. Akad. Vest. 5: 105-109.

———, M. GRAILITIS, R. DAMBURG AND STEPINSH. 1956. Elastic Scattering of Slow Electrons by Lithium Atoms. Latv. PSR. Zinat. Akad. Vest. 5: 73-81.

Manuscript received April 6, 1970