DIFFRACTION THEORY OF SCATTERING BY HYDROGEN ATOMS*

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(Received 19 February 1968)

Diffraction theory is applied to elastic and inelastic scattering of charged particles by hydrogen atoms. At small momentum transfers the calculated intensities for elastically scattered electrons are significantly greater than those calculated by the first Born approximation.

In recent years considerable theoretical interest has been focused upon electron-atom collisions, with particular emphasis on electron-hydrogen (e-H) scattering. Many of the techniques developed have been restricted, for practical purposes, to low incident momenta, where the important phase shifts are small in number. An interesting exception is the analysis of Akerib and Borowitz,[1] who have applied the impulse approximation to inelastic e-H scattering. A more current approach, which in some aspects resembles the impulse approximation, is mainly due to Vainshtein, Presnyakov, and Sobelman,[2] who have calculated cross sections for several inelastic e-H collisions. In both methods the interaction of the incident electron with the proton is considered negligible. In the first Born approximation (FBA) for inelastic collisions, its contribution, in fact, vanishes.

In this note we present a theoretical analysis of collisions of charged particles with hydrogen atoms which is applicable to both elastic and inelastic scattering. The technique we utilize is based upon the Glauber approximation,[3] which is a diffraction approximation that has been applied to a number of problems in nuclear and particle physics.[4-6] In particular, its application to scattering by deuterons is extensive.[5,6] It differs from the eikonal approximation which applies to scattering by a fixed potential in that it includes a number of other dynamical approximations. It differs from the ordinary impulse approximation for scattering by deuterons in that it explicitly treats the effects of double collisions, i.e., collisions in which the incident particle interacts with both target nucleons. In the analogous problem of scattering by hydrogen, we explicitly treat the interaction of the incident particle with both the target electron and the target proton. The approximation is applicable at high energies and is expected to be most useful in the energy domain for which the FBA is inaccurate and detailed phase shift analyses are too laborious. For e-H collisions we expect the approximation to apply at kinetic energies $E \gtrsim 100$ eV, but even at lower energies the method will yield improvements over other approximations.

In the present analysis we treat the target proton as being infinitely heavy and neglect exchange scattering (which is generally quite small at energies above ~100 eV for e-H scattering). The amplitude $F_{fi}(\vec{q})$ for collisons in which the hydrogen atom undergoes a transition from an initial state i with wave function φ_i to a final state f with wave function φ_f and the incident particle imparts a momentum $\hbar\vec{q}$ to the target is identical in form to the amplitude for corresponding collisions involving strongly interacting incident particles and deuterium targets. These latter collisions have been studied in some detail,[5,6] and we shall therefore not discuss here the derivation of the general form of the scattering amplitudes.

Let the origin of coordinates be placed at the proton, and let $\vec{b}$ denote the impact-parameter vector relative to the origin. If $\vec{r}$ denotes the position vector of the target electron, the amplitude for scattering of a particle of momentum $\hbar k$ by hydrogen takes the form[5]

$$F_{fi}(\vec{q}) = (ik/2\pi)\int \varphi_f^*(\vec{r})\Gamma(\vec{b},\vec{r})\varphi_i(\vec{r})\exp(i\vec{q}\cdot\vec{b})d^2b\,d\vec{r}, \tag{1}$$

where the two-dimensional integration over impact-parameter vectors is over a plane perpendicular to the direction of the incident beam. The function $\Gamma(\vec{b},\vec{r})$ depends upon the integral, along the direction of the incident beam, of the instantaneous potential between the incident particle and the target. If we write $\vec{r}=\vec{s}+\vec{z}$, where $\vec{s}$ is the projection of $\vec{r}$ onto the plane of impact parameters, Γ

may be expressed as

$$\Gamma(\vec{b},\vec{r}) = 1-\exp((-iZe^2/\hbar v)\int_{-\infty}^{\infty}\{(b^2+\zeta^2)^{-1/2}-[(\vec{b}-\vec{s})^2+(\zeta-z)^2]^{-1/2}\}d\zeta)$$
$$= 1-\exp[-2i(Ze^2/\hbar v)\ln(|\vec{b}-\vec{s}|/b)], \tag{2}$$

where Ze is the charge of the incident particle and v its velocity.

Cross sections for elastic or inelastic collisions may be explicitly calculated by means of Eqs. (1) and (2). As an example, we consider elastic scattering of electrons by hydrogen in its ground state. For this case we have $\varphi_i=\varphi_f=(\pi a_0^3)^{-1/2}\exp(-r/a_0)$, where a_0 is the first Bohr radius. If we let $n=e^2/\hbar v$, we may express the five-dimensional integral (1) as

$$F_{ii}(q) = (ik/\pi a_0^3)\int\exp[-2(s^2+z^2)^{\frac{1}{2}}/a_0][1-(|\vec{b}-\vec{s}|/b)^{2in}]J_0(qb)bdbdzd^2s,$$

where the integration with respect to impact parameters b is over the interval $(0,\infty)$. Upon performing the z integration we obtain

$$F_{ii}(q) = (2ik/\pi a_0^3)\int sK_1(2s/a_0)[1-(|\vec{b}-\vec{s}|/b)^{2in}]J_0(qb)bdbd^2s,$$

where K_1 is the modified Bessel function of the third kind. If we write d^2s as $sdsd\varphi$ and carry out the angular integration we find

$$F_{ii}(q) = (4ik/a_0^3)\int_0^\infty\int_0^\infty s^2K_1(2s/a_0)[1-(2s/b)^{in}G(y)]J_0(qb)bdbds, \tag{3}$$

where $y=2bs/(b^2+s^2)$ and

$$G(y) = y^{-in}(1-y^2)^{\frac{1}{2}+in}F(\tfrac{1}{2}+\tfrac{1}{2}in, 1+\tfrac{1}{2}in; 1; y^2).$$

Here F is the hypergeometric function. The integral (3) may be evaluated by transforming to polar coordinates, with the result

$$F_{ii}(q) = 2ika_0^2\int_0^{\frac{1}{2}\pi}\sin^3\theta\cos\theta[\sin^2\theta-\tfrac{1}{2}(a_0q)^2\cos^2\theta][\sin^2\theta+\tfrac{1}{4}(a_0q)^2\cos^2\theta]^{-4}$$
$$\times[1-(|\cos2\theta|/\cos\theta)^{2in}|\cos2\theta|F(\tfrac{1}{2}+\tfrac{1}{2}in, 1+\tfrac{1}{2}in; 1; \sin^2 2\theta)]d\theta. \tag{4}$$

This integral may be easily calculated by numerical methods. The differential cross section for elastic scattering is obtained by means of the relation

$$d\sigma(q)/d\Omega = |F_{ii}(q)|^2. \tag{5}$$

The total integrated cross section for elastic scattering is given by the expression

$$\sigma_{\text{el}} = (2\pi/k^2)\int_0^{2k}[d\sigma(q)/d\Omega]qdq. \tag{6}$$

Equations (1), (2), and (4) bear a simple relation to the corresponding results of the FBA. If we expand $\Gamma(\vec{b},\vec{r})$ in powers of n, we find that the first term in the amplitude $F_{ii}(q)$ is real and is identical in form to the amplitude given by the FBA.

The second term in the expansion of Γ yields a purely imaginary contribution to the amplitude. Its contribution to the integrated cross section contains an additional factor of n^2 compared with the first (or Born) term and is negligibly small at high energies (where $n\approx 1/137$). However, the corresponding additional contribution to the intensity is quite significant at small momentum transfers. The quantity $(1-v^2/c^2)d\sigma/d\Omega$ behaves as $(2na_0\ln q)^2$ for small q. The angular distribution resulting from the inclusion of this second term is consequently considerably larger than that of the FBA for small-angle scattering. At a fixed scattering angle the influence of the second term decreases rapidly as the incident kinetic energy is increased.

The logarithmic singularity in the forward elastic-scattering amplitude would not be present in a more exact treatment of the collision process. The approximation we have used assumes that the target particles may be regarded as being frozen in their instantaneous positions during the passage of the incident particle through the force field or, equivalently, that the collision time is much shorter than the period of the target electron. Now at very large impact parameters the effective interaction potential between the incident particle and the hydrogen atom is proportional to the inverse fourth power of the incident-particle–proton separation.[7] For such a long-range force the assumptions we have used are not satisfied for collisions at large impact parameters or, equivalently, for small-angle scattering. The inaccuracy of the approximation in the elastic-scattering amplitude at large impact parameters is intimately related, via unitarity, to a corresponding inaccuracy in the total cross section for inelastic scattering, an inaccuracy which results from a neglect of energy transfers. Considerations of these various approximations show[8] that the validity of the present theory requires $(a_0q)^2 \gg (\frac{3}{4}ka_0)^2$. Despite this restriction there still exists a range of momentum transfers for which the scattering amplitude contains a logarithmic dependence on q, and consequently the intensities for scattering at small momentum transfers significantly exceed those calculated by the FBA.

We have calculated the integrated elastic-scattering cross section $\sigma_{\rm el}$ as a function of incident energy by means of Eqs. (4)-(6), and in Fig. 1 we compare the results with the FBA. We note that the cross sections obtained by the two approximations are nearly identical for $E \gtrsim 100$ eV. (As we have observed earlier, the corresponding intensities at small momentum transfers are not at all nearly identical.) At energies below ~100 eV our calculated cross sections are significantly larger than those of the FBA. No data exist, to our knowledge, on elastic e-H collisions for $E \gtrsim 10$ eV. But even below ~10 eV, where the present theory is not expected to be accurate, the shape of the energy dependence of $\sigma_{\rm el}$ which we have calculated is in fair agreement with the measurements,[9,10] which we show in Fig. 1. The magnitudes of the measured cross sections in this energy range are ~50% greater than those we have calculated, whereas they are ~200 to ~400% greater than those calculated in the FBA.

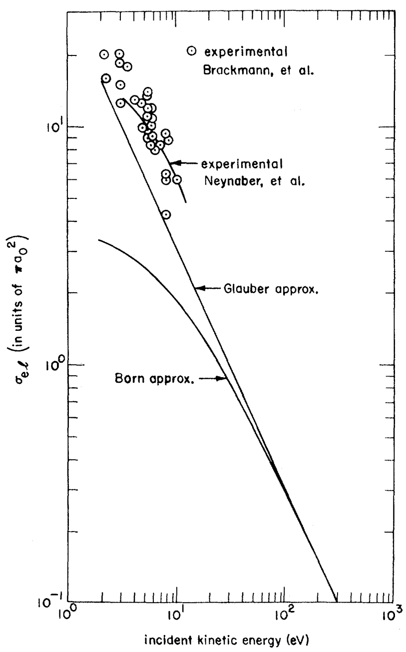

FIG. 1. Total (i.e., integrated) electron-hydrogen elastic-scattering cross sections, calculated as a function of the electron incident kinetic energy by means of the Glauber and the Born approximations. Measurements, which are available only below ~10 eV, are shown.

We have calculated the differential cross sections $(1-v^2/c^2)d\sigma/d\Omega$ by means of Eqs. (4) and (5), for various incident energies, as a function of q^2. In Fig. 2 the results are compared with the FBA, which is independent of energy. Although the theory we have employed may not be very accurate for large-angle scattering, we have calculated the intensities for a wide range of angles in order to compare them with the FBA. We note from Fig. 2 that the calculated intensities become very close to those of the FBA as the incident energy is increased, except in the small-momentum-transfer region where they are always larger than those of the FBA. The large intensities at small angles were first interpreted by Massey and Mohr[11] as a "polarization effect" which they calculated in a simplified second Born approximation. This effect has also been recently discussed by Bethe[12] as the atomic counterpart of "shadow scattering" in nuclear physics.

Unfortunately, measurements of e-H elastic scattering have, to our knowledge, been performed only below ~10 eV, which is not the

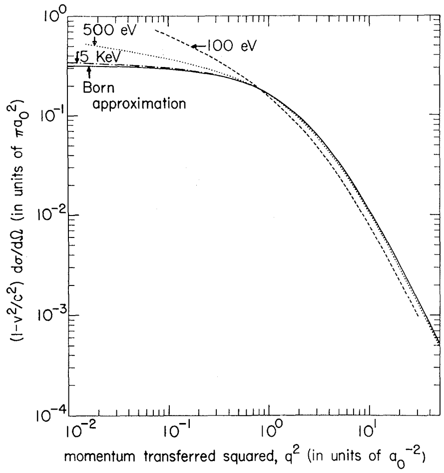

FIG. 2. Electron-hydrogen elastic-scattering intensities multiplied by $1-v^2/c^2$, calculated using Eq. (4) for 100-eV, 500-eV, and 5-keV electrons, compared with the results of the first Born approximation, which are energy independent. Our calculation for 5-keV electrons nearly coincides with the Born approximation results for $a_0^2q^2 \gtrsim 0.5$, and therefore is not shown separately in that region of q^2.

energy range of interest here. In view of the paucity of e-H data, it is perhaps noteworthy that the measured intensities of small-angle electron-helium elastic scattering at energies between 75 and 350 eV greatly exceed the predictions of the FBA.[13]

Without further discussion we note that the above analysis may be carried through with only minor modifications for incident charged particles other than electrons.

The author is extremely grateful to Professor R. J. Glauber for a helpful discussion concerning the validity of the theory at very small momentum transfers.

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*Work performed under the auspices of the U. S. Atomic Energy Commission.

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