

THE PHYSICAL REVIEW

A Journal of Experimental and Theoretical Physics Established by E. L. Nichols in 1893

VOL. 60, No. 5

SEPTEMBER 1, 1941

SECOND SERIES

Scattering of Protons by Magnesium and Aluminum

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(July 14, 1941)

A new type of nuclear scattering camera utilizing photographic emulsions to determine number and energy of scattered protons at many sharply defined angles is described and compared with earlier experimental arrangements. A survey of the effects of various factors in producing straggling of the scattered particles is presented. The angular distributions of elastically and inelastically scattered proton groups are presented, and the former compared with Rutherford scattering. Excited states of magnesium nuclei are found to occur at 1.37 Mev, 2.80 Mev, and 4.07 Mev.

INTRODUCTION

IT has been recognized that much valuable experimental information concerning the fields of force about atomic nuclei of the lighter elements can be gained by a direct study of the scattering of protons, deuterons and alpha-particles by such nuclei.¹ Yet relatively few experimental results have been published in this field in recent years,²⁻¹⁵ and the majority of these were obtained only with alpha-particles.

Published results have appeared in two general forms. In one procedure the ratio of observed to expected or classical yield of particles scattered through a selected scattering angle has been measured as a function of the energy of the bombarding particles. Another procedure has included measurement of the same ratio as a function of the angle of scattering for bombarding particles of constant incident energy. The expected or classical yield is that predicted by Rutherford's theory¹⁶ for scattering of particles by an inverse square field of force. Where the scattering of large numbers of particles has been studied, no publications have, until recently,^{8,10,11,14} contained measurements of the energy distribution of the scattered particles.

* Because of the untimely death of Professor T. R. Wilkins this work has been completed and presented by Gerald A. Wrenshall, McMaster University, Hamilton, Canada.

¹ H. A. Bethe, *Rev. Mod. Phys.* **9**, 69 (1937).

² E. S. Bieler, *Proc. Roy. Soc.* **A105**, 434 (1924).

³ E. Rutherford and Chadwick, *Phil. Mag.* **50**, 889 (1925).

⁴ Reizler, *Proc. Roy. Soc.* **A134**, 154 (1932).

⁵ Reizler, *Ann. d. Physik* **23**, 198 (1935).

⁶ G. Brubaker, *Phys. Rev.* **54**, 1011 (1938).

⁷ S. Devons, *Proc. Roy. Soc.* **A172**, 127 (1939).

⁸ T. R. Wilkins and G. Kuerti, *Phys. Rev.* **55**, 1134A (1939).

⁹ G. Kuerti and T. R. Wilkins, *Phys. Rev.* **57**, 1081 (1940).

¹⁰ T. R. Wilkins and G. Kuerti, *Phys. Rev.* **57**, 1083 (1940).

¹¹ T. R. Wilkins and G. Kuerti, *Phys. Rev.* **57**, 1083 (1940).

¹² Powell, May, Chadwick, and Pickavance, *Nature* **145**, 893 (1940).

¹³ Kanne, Taschek, and Ragan, *Phys. Rev.* **58**, 693 (1940).

¹⁴ A. J. Ferguson and L. R. Walker, *Phys. Rev.* **58**, 666 (1940).

¹⁵ T. R. Wilkins and G. Wrenshall, *Phys. Rev.* **58**, 758 (1940).

¹⁶ Schultz, Davidson, and Ott, *Phys. Rev.* **58**, 1043 (1940).

¹⁷ E. Rutherford, *Phil. Mag.* **21**, 669 (1911).

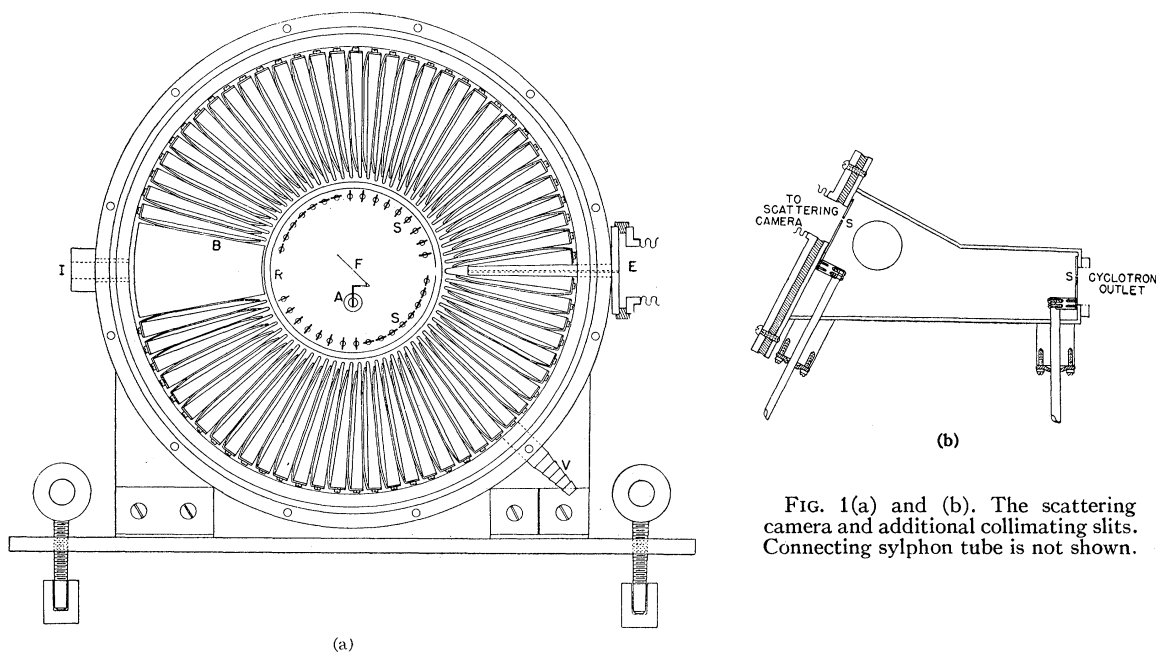


FIG. 1(a) and (b). The scattering camera and additional collimating slits. Connecting syphon tube is not shown.

The general lack of intense sources of protons, deuterons and alpha-particles until recent years, and of suitable means of faithfully registering scattered particles for long periods of time, has forced investigators in this field to use poorly defined scattering angles in order to obtain results. This lack of precision has rendered theoretical analyses of experimental results somewhat inconclusive.¹⁷ Both of these deficiencies have been improved upon in the present analysis, in which measurement of the yield of scattered particles at a series of sharply defined angles is attempted. A cyclotron is used to produce a sufficiently intense and homogeneous source of bombarding particles (protons). The yield and energy of scattered protons at the selected scattering angles are measured from the number and length of the discrete tracks produced in suitable photographic emulsions by the passage of these particles.

EXPERIMENTAL

A scattering camera consisting of a flat cylindrical container made of brass 0.9 cm thick, and of about 30 cm outside diameter and 5.0 cm depth has been employed. It contains a

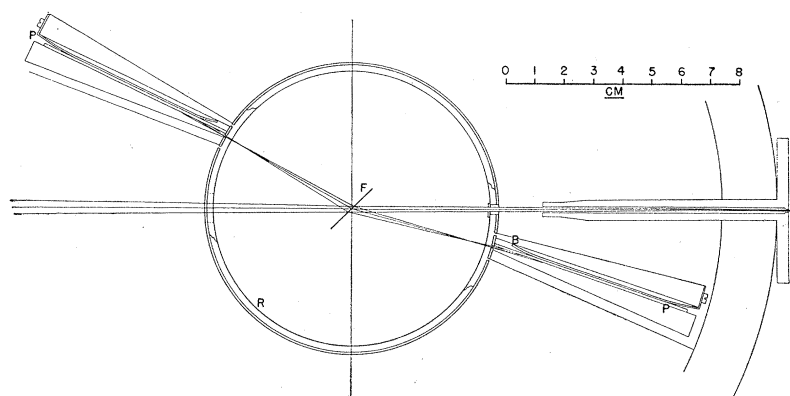
series of sixty-six photographic plateholders set fan-wise at five-degree intervals about a central scattering foil *F* (Fig. 1(a)) so that angular scattering over the range 15° to 170° can be studied. The plateholders are arranged so that particles entering the camera at *E* and scattered by *F* enter the emulsion surface of each ($1'' \times 3''$) photographic plate at a grazing angle of 4° . The ensemble of plateholders is milled from a single disk of brass. Each photographic plate is held firmly in position by a flat bow spring *B*.

Between scattering foil and photographic plates there is a brass ring *R* in which are drilled the series of 0.09-cm diameter beveled holes which, with the scattering foil and the apertures through which the incident beam enters, define the angles through which the scattered particles pass to the photographic plates. The particles thus scattered produce flat parallel tracks in the photographic emulsion distributed over a very restricted area (1.0×0.1 cm), so that tracks produced by extraneous particles are easily recognized and eliminated from records.

Shutters *S* make it possible to block any of the apertures in *R* during a run if exposures of differing amounts are desired for different angles. Varying exposures are clearly very necessary, especially at smaller scattering angles, if the

¹⁷ P. Seligmann, Phys. Rev. **58**, 492 (1940).

FIG. 2. Degree of angular definition of scattering camera shown at two characteristic angles. Representative photographic plates P are shown.



distribution of scattered particles varies in approximate accordance with Rutherford's theory. Each shutter consists of a brass plate fastened to a tapered rotatable brass plug situated in the removable side of the camera, and serves to cover two adjacent apertures in R . To measure exposures, a current integrator at I , attached to an ionization chamber registers the beam after it has passed through the camera, so that suitable relative exposures of the photographic plates can be measured. A vacuum is maintained throughout the entire camera system by means of a pumping system attached at V .

Stopping foils of aluminum inserted between scattering foil and photographic plates reduce the ranges of scattered particles by known amounts to lengths suitable for registration in the plates, and also reduce an effect which is roughly equivalent to additional straggling which shall be referred to as apparent straggling, caused by the inequality in stopping power of the component parts of the photographic emulsion. The stopping foils are located in a rectangular ring trough cut on the inner side of R . The scattering foil F is placed at 45° to the beam, allowing simultaneous exposure of thirty-three plates distributed over diametrically opposed forward and backward quadrants of the camera. F can be rotated out of the beam, and accurately returned to its original position by a tapered brass arm A by which it is supported. A extends through the back of the camera, and can be adjusted during an experimental run. It may be replaced during a run by a second similar scattering foil arrangement not shown in Fig.

1(a) by which the remaining two quadrants of the camera can be used.

The angular definition of the camera proper is shown in Fig. 2 in terms of the camera's geometry. The individual scattering angles thus defined cannot vary from their mean value by more than about $\pm 1.2^\circ$. However, in addition to this definition, the beam is further restricted as it leaves the cyclotron by two 1.0 mm wide slits S (Fig. 1(b)) spaced 16 cm apart, after which it passes through an evacuated sylphon tube for a distance of 122 cm before reaching the camera. If it be assumed that the paths of the particles in this section are rectilinear, their maximum angular spread on scattering to a given photographic plate is reduced to about $\pm 0.5^\circ$. From these considerations it is felt that the maximum angular variation does not exceed $\pm 1^\circ$.

Throughout the present series of experiments, a single lot of Eastman Kodak "fine-grain alpha-particle" photographic plates have been used. The relative stopping power of these plates was obtained primarily by measuring the lengths of alpha-particle tracks of known energy. The emulsion sensitization, processing, and microscope techniques used have been described elsewhere.¹⁸ However, certain refinements have been made. To permit systematic counting of tracks and to have a check on the magnification of the microscope, each plate was marked photographically with a series of straight lines perpendicular to the direction of the emulsion tracks, and spaced 0.25 mm apart. These lines

¹⁸ T. R. Wilkins, J. App. Phys. 11, 35 (1940).

were prevented from penetrating deeply into the body of the emulsion by making the necessary exposure with ultraviolet light. This permits emulsion tracks located deep in the emulsion to be resolved more readily than if more penetrating illumination were used. The necessity for using depth focusing in emulsion track work is really an advantage in that it usually permits an observer to distinguish between the ever-present "fog" particles in the emulsion and the true ends of particle tracks. However, it makes impractical the publication of a clear photograph of emulsion tracks in this experiment.

Because of the considerable eyestrain and fatigue caused by long periods of close examination with a microscope, the microscopic image of the tracks was projected onto a vertical ground glass screen, with ground side toward the microscope. In contact with this side was mounted a frame carrying a series of twelve fine taut steel wires, spaced 0.8 cm apart, which crossed the track images at right angles and permitted the accurate measurement of emulsion track lengths. A large plano-convex lens mounted on the observer's side of the ground glass screen converges the light so that all parts of a track image can be viewed simultaneously. This arrangement has been found to be much less tiring to operate than the usual binocular or monocular microscope with eyepiece scale. Depth focus and the mechanical stage of the microscope are operated by the left hand, leaving the right hand free to record measurements.

The intense illumination required for dark-field projection was obtained from an automatic feed arc lamp. Best results were obtained by using small diameter cored carbons to prevent wandering of the arc spot, and consequent fluctuations in the brightness of the projected images. The light beam was heat filtered by passage through a water solution of copper chloride.

ACCURACY OF OBSERVATIONS

(1) Factors affecting width of distribution peaks

It is of some interest to investigate the relative importance of the factors which contribute to the breadth of the distribution peaks obtained by plotting the frequency against length of

emulsion tracks, the peaks representing proton groups. The factors will include the normal straggling of the protons in the homogeneous stopping and scattering foils, apparent straggling, and error in measurement of track lengths due to least count and grain spacing along tracks in the photographic emulsion. Superimposed on these will be the effects of inhomogeneity of the proton beam as it arrives at the scattering camera, and, in the case of magnesium, the broadening of the peak produced by elastic scattering due to the inherent presence of the three important isotopes. In Table I are presented measurements made at four representative angles on the widths of the distribution peaks for 6.9-Mev protons scattered by magnesium using the scattering camera. All of the photographic plates were simultaneously exposed, and were analyzed by the same observer using the same microscope.

Examination of the scattering arrangements of the camera as shown in Fig. 2 shows that the mean straggling of a homogeneous beam of bombarding particles, scattered back through the same surface of foil through which they entered, will, to a fair approximation, be greater than for particles scattered through the opposite side by the air equivalent of the scattering foil. This statement refers specifically to the arrangement used and shown in Fig. 1, namely where photographic plates are exposed only in the diametrically opposed quadrants of the camera indicated by the normals to the scattering foil. For a homogeneous proton beam there would thus be a relatively large increase in the straggling of scattered particles for scattering angles greater than 90° , roughly proportional to scattering foil thickness. But when the other factors previously mentioned produce distribution curves of considerable average width, this effect is reduced in importance since it is not additive. For example, in this experiment the

TABLE I. Mean peak half-widths, in cm of equivalent air, of distribution curves produced by protons scattered elastically (E), and inelastically (I_1) by magnesium.

Scattering angle	60°	80°	125°	145°	Average
E peak half-width	2.32	2.35	2.26	2.57	2.38
I_1 peak half-width	1.69	2.04	2.07	2.15	2.00

average increase in straggling for scattering angles greater than 90° would have been ± 0.62 cm air for a homogeneous beam of bombarding protons, while actually for the representative results of Table I it produced a mean peak width increase of only $\pm(2.26-2.10) = \pm 0.16$ cm air straggling. Hence it would appear that this factor in broadening the large-angle scattering peaks is relatively ineffective in this experiment due to the presence of more important factors.

Because of the dependence of recoil energy of a scattering nucleus on its mass, a beam of homogeneous protons scattered by a mixture of the Mg isotopes would appear in the elastic scatter peak as three components slightly displaced relative to each other. A simple calculation shows that the displacement of the three isotope peaks would be slight in the present case, being of the order of 0.02 Mev. This would be scarcely detectable keeping in mind that Mg^{24} constitutes 80 percent of normal magnesium. It would at most produce a slight distortion of the elastic scatter peak on the high energy side, an effect which is not observed here.

An indication of the apparent straggling effect which the inhomogeneous photographic emulsion produces can be found by comparing the average widths of the two main scatter peaks in Mg. The elastic scatter peak should be the broader of the two due to the greater path of its particles through the photographic emulsion. This is seen to be true for the representative results in Table I. There is an average increase in the width of the elastic scatter peak over that of the inelastic scatter peak of $\pm(2.38-2.00) = \pm 0.38$ cm air. The corresponding increase in mean peak width for passage of the proton beam through a thickness of air equivalent in stopping power to the emulsion thickness between the peaks considered is ± 0.19 cm air. Thus the photographic emulsion inhomogeneity roughly doubles the straggling in our work.¹⁹

Uncertainties in measuring track lengths due to the finite spacing of silver grains defining the tracks, and by least count error in estimating track lengths, are of the same order of magnitude. The average grain spacing for protons was found

¹⁹ This measurement should be independent of all such factors as initial inhomogeneity of scattered beam, and characteristic errors in measuring track lengths.

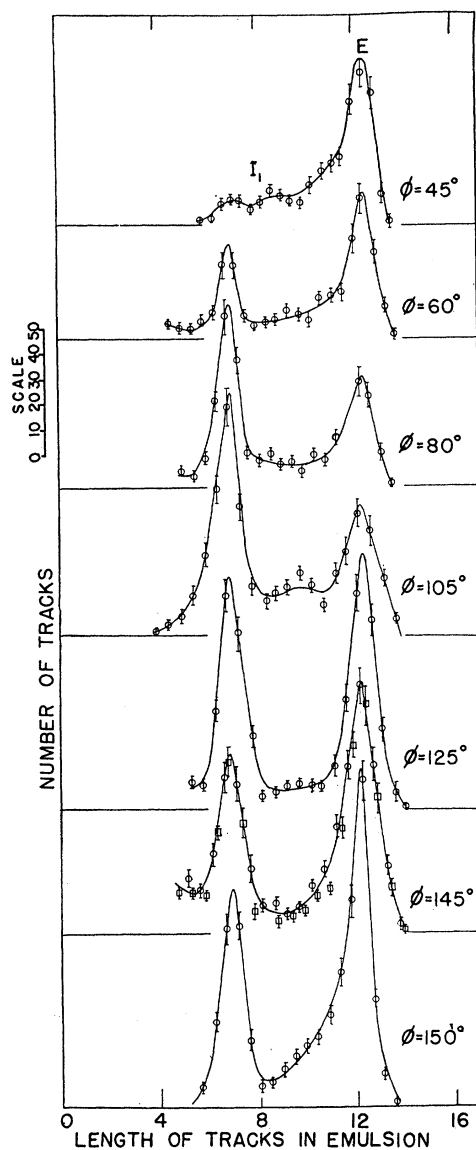


FIG. 3. Range distribution curves for protons scattered by magnesium through various angles ϕ . The curves have been shifted laterally to align the two main peaks, a slight shift being necessary since the recoil energy imparted to the scattering nuclei varies with the angle of scatter. One scale division = 19.6μ .

to be about 0.1 scale division in track length. Track lengths were measured to the nearest tenth of a scale division. It is estimated that, combined, these effects produce an average uncertainty in track range measurements of ± 0.6 cm of equivalent air.

Since protons were allowed to enter the photographic emulsion at a mean grazing angle

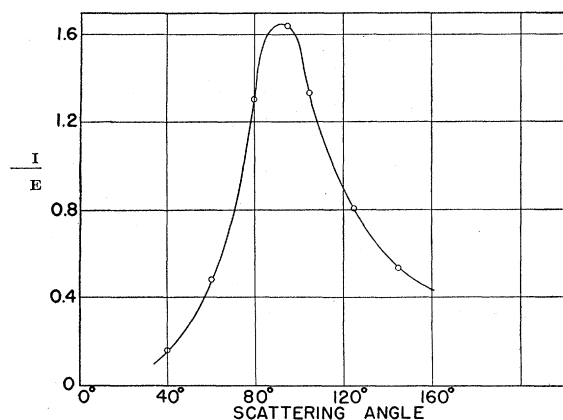


FIG. 4. Relative yield of elastically and inelastically scattered protons as a function of angle for magnesium (run No. III).

of 4° , it is important to know surface and depth conditions in the emulsion. Interference fringes were produced between the surfaces of samples of undeveloped emulsion plates and optically flat glass, using sodium yellow light. It was found that the emulsion surfaces were surprisingly flat except in the immediate vicinity of the natural edges of the plates. Edges along which glass cuts had been made showed no abnormal effects. From plate to plate the emulsion thickness varied between thickness of 30μ to 55μ . At the 4° entrance angle this permits corresponding tracks of maximum length between 400 and 750μ . The finite thickness limits the energy of the protons which can be successfully studied by this method, although considerably thicker emulsion plates are being developed for this purpose.

While it is difficult to estimate the homogeneity of the incident cyclotron beam from available experimental data, a minimum for the mean energy variation can be tentatively considered as ± 0.1 Mev, which is twice the peak voltage across the dees. This is undoubtedly a smaller variation than actually was obtained in the experiments, since variations in the field strength of the cyclotron magnet over the time required for a run are not allowed for.

(2) Precautions relative to scattering angle

To obtain accurately known and reproducible scattering angles care was taken to insure that the center of the ellipse defined by the inter-

section of the beam of incident protons and the scattering foil was located at the geometrical center of the camera. To prevent reduction in the accuracy of scattering angles due to the effect of the cyclotron's magnetic field on the scattered protons, the camera was located where the field was found to be effectively zero. As an added precaution, the plane of scattering of the camera was vertical, so that in any case any vertical magnetic field could not alter the direction of scattered particles in the plane of scattering.

ADVANTAGES AND DISADVANTAGES OF THE EMULSION TRACK TECHNIQUE

An excellent general survey of the basic advantages and limitations in the use of tracks of nuclear particles in photographic emulsions has been recently presented by Shapiro.²⁰ Powell and Fertel²¹ have demonstrated some of the marked advantages of the technique in the measurement of neutron energies. The undesirable effects of apparent straggling in emulsion track studies have been discussed by Taylor.²²

Outstanding advantages of the emulsion track technique in nuclear scattering experiments are: (1) Simultaneous exposures can be made at a large number of sharply defined angles in a minimum of time. (2) Both yield and energy distribution of scattered particles are obtained at each scattering angle with the simplest of apparatus. (3) Since the tracks can be seen, random "background" tracks such as those caused near a cyclotron by neutrons, can be recognized as such. (4) Scattered protons of energy as low as 0.8 Mev can be readily detected and their energy estimated. Nothing in the nature of an entrance window is required for emulsions, as in the case of most impulse counters and cloud chambers.

Because of the comparatively slow rate at which track lengths can be measured,²³ several observers have taken part in the track analysis, using three independent microscopes set to the same magnification. In order to make a check

²⁰ M. Shapiro, *Rev. Mod. Phys.* **13**, 58 (1941).

²¹ Powell and Fertel, *Nature* **144**, 115 (1939).

²² H. J. Taylor, *Proc. Roy. Soc.* **A150**, 382 (1935).

²³ About 200 tracks per hour can be accurately measured for a limited time.

on the personal error involved in such mixed analyses, two observers, working independently on different analyzers, in turn analyzed the same plate (scattering angle 145°). A comparison of these two analyses is included in Fig. 3 in which it is seen that no important variation in curve shape present in the one is absent from the other. The slight difference in total track number is believed due to the fact that one observer counted only those tracks appearing in the portion of the plate seen by the scattering foil, while the other examined the entire plate surface for additional stray tracks.

RESULTS AND DISCUSSION

(1) Yield of scattered protons as a function of scattering angle

As a preliminary test of the scattering camera, 6.6-Mev protons were scattered by 0.2-mil platinum foil (run No. I), and the relative numbers (yield) scattered through five different angles were measured. The variation in yield with scattering angle agreed with that predicted for Rutherford scattering, as was expected. Subsequently, the scattering of 6.9-Mev protons by 0.5-mil foils of aluminum and magnesium has been studied and preliminary results presented^{9, 10, 14} announcing the detection of inelastic scattering for both elements, and the variation in the relative amounts of inelastic and elastic scattering with angle for the latter.

The apparent straggling effect produced in the photographic emulsion was reduced in the aluminum run (No. II) and in one of the magnesium runs (No. III) by insertion of a suitable thickness of aluminum stopping foils between scattering foil and photographic plates. This had the effect of increasing the resolution between the higher energy groups of scattered protons while cutting off all scattered protons of less than 2.5-Mev energy from the photographic plates. It also shortened the resulting emulsion tracks to such a degree that they could be conveniently examined as units under a microscope using a $10\times$ eyepiece and a 4-mm objective.

Track numbers and lengths have been measured for seven selected plates of run III, and the series of distribution curves so obtained is shown in Fig. 3. The peaks appearing at 12.2 scale

divisions are believed to be produced by elastically scattered protons. This conclusion is based on a comparison of the energy of the group of scattered protons of highest energy, and the energy of the incident ones. By use of range energy graphs²⁴ and the measured lengths of emulsion tracks, the former were found to have a mean energy of 6.87 Mev minus nuclear recoil energy, while from air range measurements the latter were found to have 6.9-Mev energy. The peak at 6.9 scale divisions is seen to appear in all plates of run No. III which have been analyzed so far, and the marked variation with angle of its intensity N_I relative to the intensity N_E of the peak at 9.1 scale divisions is shown in Fig. 4. The ratio N_I/N_E appears to pass through a maximum value for 90° scattering.

The angular distribution of protons scattered by aluminum (run No. II) differs greatly from that predicted for Rutherford scattering. (Fig. 5, curves *B* and *A*, respectively.) While curve *B* includes the total number of protons scattered by aluminum having energies between 3.0 and 6.9 Mev, it actually represents the yield for elastic scattering alone except at large scattering

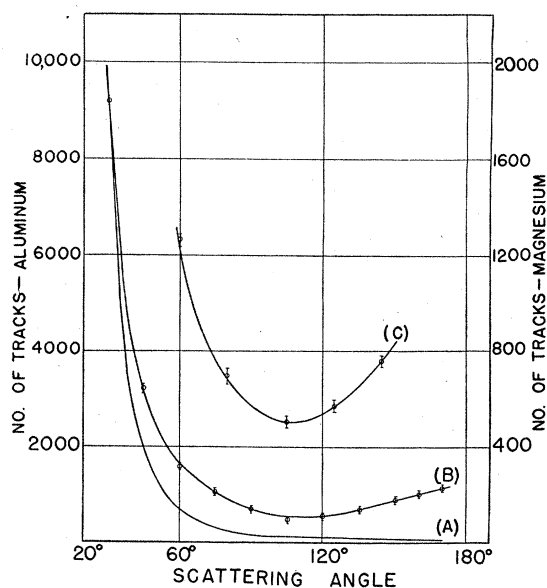


FIG. 5. Yield of elastically scattered protons from aluminum (curve *B*) and magnesium (curve *C*). Curve *A* represents the distribution predicted for Rutherford scattering, and is normalized to curve *B*.

²⁴ M. S. Livingston and H. A. Bethe, Rev. Mod. Phys. 9, 245 (1937).

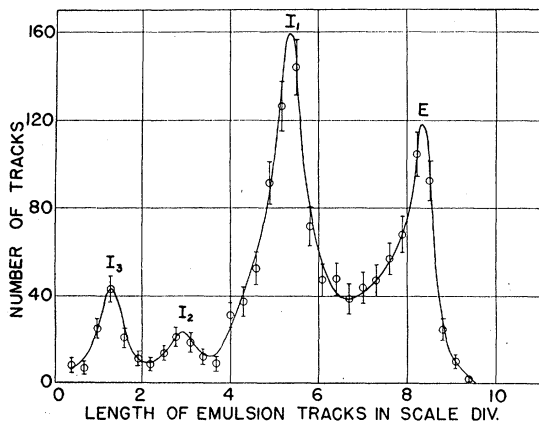


FIG. 6. Range distribution of protons scattered by magnesium for a scattering angle of 95° (run No. IV). One scale division = 39.2μ .

angles, since the one observed group of inelastically scattered protons is small relative to the elastically scattered group, and appears in this run only at scattering angles greater than 145° . The curve for magnesium (Fig. 5, curve C) is for elastically scattered protons alone. These curves demonstrate clearly that, exclusive of nuclear collisions in which the scattered particle gives excitation energy to the scattering nucleus, important deviations from Coulomb forces occur in the immediate neighborhood of the nucleus.

There is some evidence in Fig. 3 of unresolved proton groups of comparatively low intensity at about 9.5 and 11.0 scale divisions. An irregularity corresponding to the one at 11.0 scale divisions has been observed in a different experimental study now in progress²⁵ of proton scattering by magnesium.

In order to observe the distribution of emulsion track lengths over the largest possible energy range, another run (No. IV) was made in which no stopping foils were used between the magnesium scattering foil and the photographic plates. This allowed representative scattered protons of all available energies to reach the photographic emulsions. In Fig. 6 the distribution in emulsion track length of protons scattered through an angle of 95° and measured at one-half of the previous magnification, is shown. The two large peaks previously examined in run

No. III are at 5.37 and 8.35 scale divisions, while two further peaks are observed at 2.9 and 1.3 scale divisions. The presence of both of these peaks has been confirmed from the distribution curves of two other plates of the same run. Collection of information concerning their intensity variation with scattering angle is at present in progress.

(2) Excitation energies of magnesium nuclei

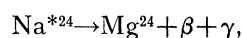
An explanation of the series of peaks obtained in Figs. 3 and 6 is that an effect analogous to that found in the Franck-Hertz experiment is occurring when the bombarding protons collide with atomic nuclei. While some of the protons undergo elastic nuclear collisions, others lose a discreet amount of energy to the nucleus. This energy may be considered as exciting the nucleus to a higher quantized energy state, from which it will subsequently revert to its normal state with the emission of gamma-radiation. Hence a measure of the decrease in energy suffered by the groups of inelastically scattered protons should represent directly the excitation energies of the struck nuclei; and these excitation energies and some of their differences should represent possible gamma-ray energies which the nuclei may emit.

The energies of the proton groups were calculated by determining the equivalent proton air ranges from their measured track lengths, and the known stopping powers of the photographic emulsion, stopping, and scattering foils. It is worthy of note, however, that it is incorrect to take the excitation energies as the direct differences between the energy of the elastically scattered group and the energies of the inelastically scattered ones as has been done with earlier results.^{10,14} A correction must be made since the recoil energy loss to the nucleus in the inelastic collisions differs from nuclear recoil loss in elastic collisions.²⁶ Referring to Fig. 6 the proton energies corresponding to peaks E, I_1 , I_2 , and I_3 are 5.94 Mev, 4.62 Mev, 3.25 Mev, 2.04 Mev, respectively, and the excitation energies corresponding to peaks I_1 , I_2 , I_3 are 1.37 Mev, 2.80 Mev, 4.07 Mev, respectively, in satisfactory agreement with values of Dicke and Marshall.²⁵

²⁵ R. H. Dicke and J. Marshall, Phys. Rev. **59**, 917 (1941).

²⁶ I wish to thank Mr. Dicke for developing the necessary correction equations which were used here.

It is only possible with the information available to offer a partial indication as to which of the proton groups I_1, I_2, I_3 is associated with which of the nuclei $Mg^{24}, Mg^{25}, Mg^{26}$. It is reasonably certain, however, that the group I_1 is produced by Mg^{24} , since at a scattering angle of 90° it is nearly 1.7 times as large as the E group and could scarcely be produced by the other two rarer isotopes. This observation is supported by Henderson's²⁷ measurement of the gamma-ray energy of radio-sodium in the proposed reaction,

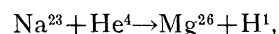


in which he finds, by the absorption coefficient method, that the gamma-ray energy has an approximate value of 1.3 Mev which compares with our value of 1.37 Mev. However, from a

²⁷ M. C. Henderson, Phys. Rev. **48**, 855 (1935).

number of published results, Livingston and Bethe²⁴ list gamma-rays for this reaction of energies 0.95 Mev, 1.93 Mev, and 3.08 Mev, none of which is closely comparable with the excitation energies or their differences as reported here.

From published studies of the proton groups from the reaction



Livingston and Bethe²⁴ have assigned excitation energies to Mg^{26} of 2.2 Mev, 4.0 Mev and 5.0 Mev. Of these, the first mentioned is not observed in our results, while the last value quoted is not in the range of our experiment. However, the group I_3 of measured excitation energy 4.07 Mev might perhaps correspond to the remaining proton group, thus associating this group with Mg^{26} .

Correction for Nuclear Motion in H_2^+

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(Received June 30, 1941)

The forced separation of variables usually employed in the quantum-mechanical treatment of molecular problems introduces certain small errors into the wave function. If the exact Hamiltonian is used, energy values can be computed very accurately because first-order errors in a wave function give rise to second-order errors in the energy. The energy of H_2^+ is ordinarily computed by using a separable, approximate Hamiltonian instead of an exact one. From a consideration of the terms which must be added to the approximate Hamiltonian to make it exact, Van Vleck has derived the correction terms needed to reduce the first-order error in the computed energy to a

second-order error. The correction term is a function of R , the internuclear distance, and its calculation requires a knowledge of the wave function. In this paper the ground state wave function of H_2^+ is accurately determined over values of R from 1.20 to 2.75 atomic units and a table of the wave function coefficients is given, along with the corresponding energy values. Then, correction terms are calculated for a set of values of R . Including the proper correction term, the total negative energy of H_2^+ for the equilibrium internuclear distance is found to be $1.20472 \pm 0.00001 E_H = 132,132 \pm 10 \text{ cm}^{-1}$. This result is compared with the consequences of certain experimental data.

1. THE PROBLEM

THE usual quantum-mechanical treatment of molecular problems is based upon a forced separation of variables.¹ This introduces certain small errors into the wave function, which, as such, is still as accurate as necessary.

¹ Cf. A. S. Coolidge and H. M. James, J. Chem. Phys. **6**, 730 (1938).

Since energy values are subject to much closer check by experimental data, it is desirable to determine energies as accurately as possible. They can be computed very accurately in some cases because first-order errors in a wave function give rise to second-order errors in the energy if the *exact* Hamiltonian is used in calculating the energy. The energy of H_2^+ is computed in the ordinary way by using, not the exact Hamil-