

general agreement as to the significantly larger size of the Na-N₂ cross sections, as compared with the Na-H₂ value, which has been attributed to a relatively easy formation of the Na-N₂ transition complex, caused by a potential unsaturation in the N₂ molecules.^{2,9} The small differences between the cross sections for H₂, HD, and D₂ are of some interest for, although these molecules have identical electronic structures, their vibrational levels differ. The work of Karl and Polanyi⁹ suggests that, in a collision between an excited atom and a molecule in the $v=0$ vibrational state, about one-half of the total available atomic excitation and kinetic energy should be available for transfer to the vibrational levels in the case of H₂ and D₂, and between one-third and two-thirds in the case of HD. The NaD

⁹ G. Karl and J. C. Polanyi, *J. Chem. Phys.* **38**, 271 (1963).

levels are at 17 000 cm⁻¹ and kT at 127°C provides an additional 277 cm⁻¹, making a total of 8650 cm⁻¹ available for vibrational excitation in collisions with H₂ and D₂. This should be compared with the energy interval of 8070 cm⁻¹ between the most highly populated rotational levels of the ground vibrational state $v=0$ and the $v=2$ state in H₂. The appropriate figures for D₂ are 5860 cm⁻¹ for excitation of the $v=2$ state and 8620 cm⁻¹ for the $v=3$ state. In HD, either the $v=2$ or the $v=3$ states at 7070 cm⁻¹ and 10 350 cm⁻¹, respectively, might be excited. If the lower vibrational states were excited preferentially, the resonance would be closest in the case of H₂, while a smaller effect would be expected with D₂. It is doubtful whether these considerations can be used to account for the small differences in the cross sections until a considerably larger volume of experimental data becomes available.

Elastic Scattering of Lithium Ions in Helium and Hydrogen*

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The cross sections for elastic scattering of 50- to 800-eV Li⁺ ions in He and in H₂ have been measured using a method in which the energy-loss spectrum of the ions is observed as a function of the scattering path length. The experimental procedure yields directly the cross section for scattering outside a given angle which ranges from 10° to 160° in the center-of-mass system. From these data, the interaction potential was computed by a process which involves the numerical integration of the inverted orbit equation for a series of constant angular momenta. The potential so found may be represented by the Born-Mayer form within a few percent as $V(r) = 3.7 \times 10^2 e^{-5.1r}$ eV for Li⁺-He and $3.0 \times 10^2 e^{-11.0r}$ eV for Li⁺-H₂, with r in Å. The $V(r)$ for Li⁺-He has also been calculated using the two-center Thomas-Fermi-Dirac statistical model, yielding reasonably good agreement with the experimental result.

I. INTRODUCTION

THE elastic scattering of one particle by another provides the most direct experimental means of determining the interaction potential energy of the two particles. If, in particular, there is reason to believe that the force is a monotonic function of the internuclear separation, then the scattering can be interpreted unambiguously in terms of a force function.¹ Of particular interest, because of the simplicity of the electron configuration, is the scattering of He by He, or by systems of like configuration. A considerable amount of work has already been done experimentally by Amdur *et al.*² and theoretically by Phillipson, Ransil,

Slater and others³ on the determination of the interatomic potential for He-He. There exists, however, a fairly large discrepancy between experiment and theory for internuclear distances less than about 1.0 Å.

The scattering of Li⁺ in He as an experimental problem is much easier than He in He, for, the scattered ion is more readily detected and its energy thus measured. Since, in this case, the incident particle is heavier than the target atom, the angular distribution of the scattered ions will fold back on itself in the laboratory system; that is, for a given laboratory angle of scattering less than the maximum, there will be ions of two energies. Consequently, if an angular distribution is desired, either an energy distribution may be measured directly or the ions that are scattered at a given angle may be energy-analyzed. The energy retained by the ion is, however, a monotonic function of the angle of scattering in the center-of-mass system.

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¹ E. A. Mason and J. T. Vandarslice, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic Press Inc., New York, 1962).

² I. Amdur, *J. Chem. Phys.* **17**, 844 (1949); I. Amdur and A. L. Harkness *ibid.* **22**, 664 (1954); I. Amdur, J. E. Jordan, and S. O. Colgate, *ibid.* **34**, 1525 (1961).

³ P. E. Phillipson, *Phys. Rev.* **125**, 1981 (1962); B. J. Ransil, *J. Chem. Phys.* **34**, 2109 (1961); J. C. Slater, *Phys. Rev.* **32**, 349 (1928); P. Rosen, *J. Chem. Phys.* **18**, 1182 (1950).

While the electron configuration in the two systems $\text{Li}^+\text{-He}$ and He-He are similar, the unequal nuclear charges in the case of $\text{Li}^+\text{-He}$ removes the symmetry property of the molecular orbitals. In the $\text{Li}^+\text{-He}$ system, the Li^+ 1s electrons should become 1σ electrons in the molecule, while the He 1s electrons would be promoted to 2σ . This compares with He-He in which the molecular configuration is $(1\sigma)^2(2p\sigma)^2$. The united atom of $\text{Li}^+\text{-He}$ [$\text{B}^+(1s^22s^2)$] has an electronic energy of -24.0 atomic units (a.u.), while the united atom of He-He [$\text{Be}(1s^22p^2)$] has an energy of -14.4 a.u. Obviously, no conclusions can be drawn from this for a comparison of the interatomic repulsive energy at distances of ~ 0.5 Å except that the larger nuclear repulsion of $\text{Li}^+\text{-He}$ would tend to make the two potential energies more nearly the same.

A relatively simple way of measuring the cross section for scattering outside a given center-of-mass angle α is to observe the attenuation of the ion current with the scattering path length for a series of specific values of the energy retained by the ion. This can readily be done by an energy analysis of the scattered ions using a parallel and reversed electric field.⁴ Ions which have lost an energy greater than some minimum value are not measured as part of the ion current. Observation of this current as a function of the scattering path length yields the cross section for scattering outside the angle corresponding to the energy loss chosen. The method has the advantage of being insensitive to the size of the beam cross section and to small divergences in the beam, since the scattering is summed over the azimuthal angle. Further, uncertainties introduced by the rapid variation of the cross section at small angles of scattering are avoided in this method which, however, turns out to be insensitive for angles of scattering smaller than 10° in the center-of-mass system.

The choice of ion energies to be used is determined by the lower limit of experimental feasibility and an upper limit such that the inelastic cross sections are small compared to the elastic. When measurements by van Eck *et al.*⁵ of the cross sections for charge exchange and for ionization for Li^+ ions in He for 5–20 keV ion energy are extrapolated back to ion energies of 1 keV, these inelastic cross sections are found to be less than 0.1 Å². As will be shown later, the equivalent elastic cross sections are about 3.0 Å², so that the inelastic contribution is sufficiently small to be neglected.

In the following sections, the apparatus and the experimental method are first described, followed by the measured scattering cross sections for 50–800 eV Li^+ ions in He, and, as well, Li^+ ions in H_2 . The method for deducing the interatomic potential function $V(r)$ from the scattering data is next outlined and the results

discussed. Finally, the $V(r)$ for the $\text{Li}^+\text{-He}$ system is calculated using the two-center Thomas-Fermi-Dirac statistical molecule developed by Abrahamson *et al.*⁶ This is then compared with the experimental result.

II. EXPERIMENTAL METHOD

The Li^+ ions were produced by thermionic emission from a hot W ribbon coated with spodumene ($\text{Li}_2\text{OAl}_2\text{O}_3\text{SiO}_2$). Total emission currents as high as 10^{-4} A were obtained from a surface area of 0.15 cm². With the pure spodumene as the emitting coating, there occurred a gradual increase in the potential drop through the coating with time and a concurrent decrease in the ion beam energy for a constant accelerating potential. This was remedied by the addition of fine W powder to an equal amount of spodumene before the vacuum fusing of the coating on the W ribbon.

The ions were accelerated by shaped electrodes,⁷ and the focused beam was then mass analyzed by a double focusing 90° mass spectrometer. The design followed Cross⁸ and Bainbridge.⁹ Resolution was such that the Li isotopes (6.02 and 7.02 amu) were separated at the exit aperture by 10 half-widths of the isotope peaks for an entrance aperture of 2.0 mm. After being made plane parallel the ion beam was collimated by double orifices and entered the scattering chamber. The ion detector (see Fig. 1) was a stainless-steel flat plate 12 cm in diameter with a grid of 0.0051 cm stainless-steel wire on 0.0585 cm centers and placed 0.955 cm in front of the plate. The transparency of the grid was about 91%. The analyzer system could be moved along the axis of the scattering chamber about 7 cm, and the diameter of the detector was such that it intercepted the total scattered ion cone for all positions. A carefully aligned way and a screw drive ensured parallelism and accurate positioning throughout the motion.

The detector current was amplified and recorded on an x - y recorder with the x coordinate controlled by the detector position. In order that single scattering dominate, the scattered ion current was usually kept to less than 10% of the incident beam. Since the detector receives the unscattered, as well as the scattered ion current which has sufficient energy to reach it, the current change with path length is small compared to the total current. It was advantageous, therefore, to suppress a large part of the amplifier output. Both the recorder amplification and the current suppressor were adjusted so that maximum resolution was always obtained.

A considerable effort was directed toward obtaining

⁶ A. A. Abrahamson, R. D. Hatcher, and G. H. Vineyard, *Phys. Rev.* **121**, 259 (1961); A. A. Abrahamson, *ibid.* **123**, 538 (1961); **130**, 693 (1963); **133**, A990 (1964).

⁷ M. von Ardenne, *Tabellen zur Angewandten Physik* (VEB Deutscher Verlag der Wissenschaften, Berlin, 1962).

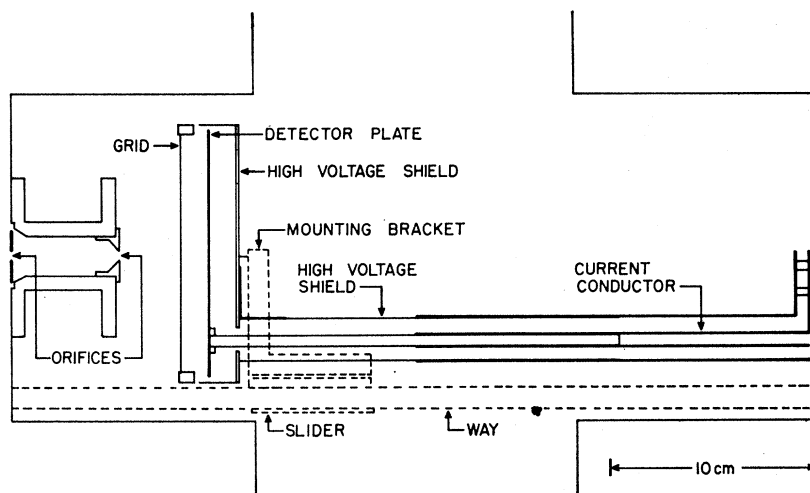
⁸ W. G. Cross, *Rev. Sci. Instr.* **22**, 717 (1951).

⁹ K. T. Bainbridge, in *Experimental Nuclear Physics*, edited by E. Segré (John Wiley & Sons, Inc., New York, 1953).

⁴ W. J. Ham, *Phys. Rev.* **63**, 433 (1943); H. Gummel, M. S. thesis, Syracuse University, Syracuse, New York, 1950 (unpublished).

⁵ J. van Eck, F. J. de Heer, and J. Kistemaker, in *Ionization Phenomena in Gases*, edited by H. Maecker (North-Holland Publishing Company, Amsterdam, 1962).

FIG. 1. Scale drawing of the scattering chamber showing the ion detector in cross section.



as monoenergetic an ion beam as possible. A large part of the energy spread that was found was traced to the source. The addition of the W powder and the heating of the emitter with half-wave rectified current with the acceleration on the off half-cycle reduced the spread to a value that was considered satisfactory. Measurements of the unscattered beam energy distribution were made for each set of scattering data. The distribution was approximately Gaussian with a value at half-height of less than 1.0% for the 50-eV beam and decreasing to less than 0.2% for beam energies of 300 eV and above. The midpoint of the Gaussian distribution was used as the corrected beam energy. The departure of the equipotential surfaces of the retarding field from flatness at the grid surface was also considered as a source of a spurious energy spread. The potential distribution was studied by both an electrolytic tank model and by a theoretical analysis. Calculations done to find the error in the energy distribution introduced by the bulging field for different points of incidence of an ion between the grid wires showed a maximum fractional loss of kinetic energy in the direction normal to the detector surface of 0.045% at the edge of the grid wires and going to zero at the midpoint. Consequently, this source of error was ignored.

The maximum angle of divergence of the ion beam entering the scattering chamber was 4.6° based solely on the geometry of the entrance apertures. However, a measurement of the beam cross section showed no measurable increase in a distance of 24 cm from the entrance aperture. Assuming a 4.6° divergence in the ion beam cone averaged over the azimuthal angle of scattering, the maximum error introduced into the component of energy normal to the detector, however, would be about 0.4%. Any actual divergence would have been much smaller than this because of other geometrical constraints preceding the entrance aperture. These would reduce the maximum error from this cause to about 0.1%.

The gas pressure in the scattering chamber was measured by a Schulz-Phelps¹⁰ ionization gauge which is extremely linear in the region of 10^{-4} – 10^{-1} Torr.¹¹ This gauge was calibrated against a precision McLeod gauge for three different base lines on the closed tube with average slopes which differed by less than 3%, and with a deviation from linearity of less than 1%. Also, care was taken in the design of the liquid-N₂ cold trap and of the connecting tubing¹² to ensure negligible pressure differential. The background gas in the scattering chamber was of the order of 10^{-3} of the scattering gas pressure.

III. EXPERIMENTAL RESULTS

The data taken consisted of a series of curves of the ion current as a function of path length for a given value of the beam energy and for some 10–15 values of the retarding potential for both increasing and decreasing path length. With retarding potentials corresponding to values greater than the maximum energy loss possible for an elastic collision of Li⁺ in He, there should be no attenuation of the ion current with path length if only single scattering occur and if there are no other sources of loss of ions or of ion energy in excess of the maximum. Processes such as charge exchange, excitation, and ionization as well as multiple scattering would lead, however, to such an effect. Thus a measure of the attenuation for energy losses greater than the maximum provides a means of observing the relative importance of such collisions. Generally, these were too small to measure with sufficient accuracy and were, moreover, independent of the retarding voltage. When warranted, these cross sections were subtracted out.

For single scattering the ion current as a function of the path length is given by

$$I = I_0 \exp(-S_a N x), \quad (1)$$

¹⁰ G. J. Schulz and A. V. Phelps, Rev. Sci. Instr. **28**, 1051 (1957).

¹¹ P. H. Carr, Vacuum **14**, 37 (1964).

¹² M. Rusch and O. Bunge, Z. Tech. Physik **13**, 77 (1932).

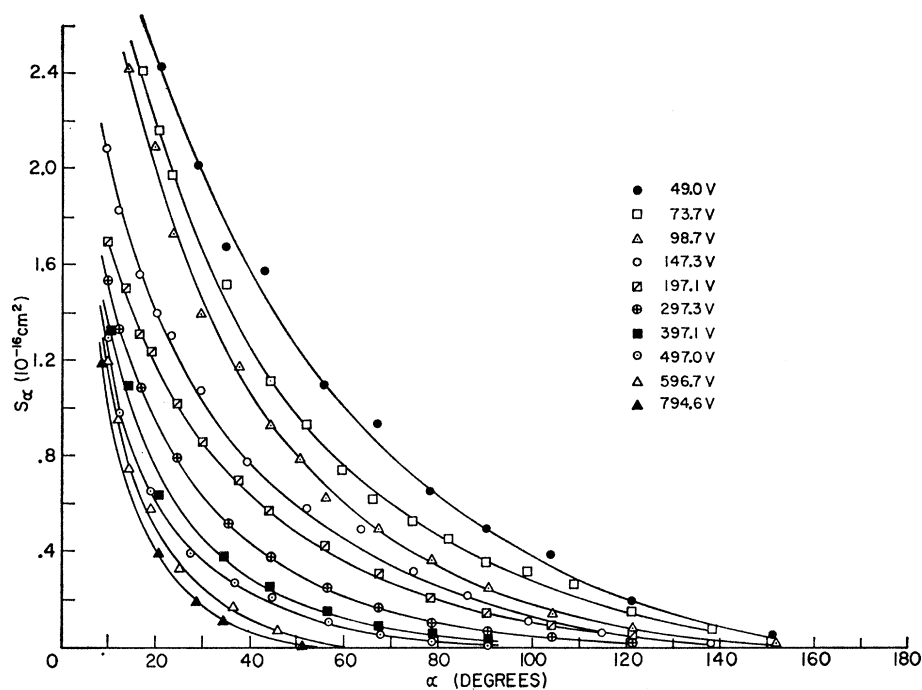


FIG. 2. The cross sections S_α for scattering outside the center-of-mass angle α as a function of α for Li^+ in He. The number on each curve is the ion energy in eV.

where I_0 =initial ion current, S_α =cross section for scattering outside the center-of-mass angle α , N =number of scattering centers per unit volume, and x =scattering path length. The scattering angle is related to the retarding voltage by

$$\alpha = \cos^{-1}[-m_1/m_2 + (m_1/m_2 + 1)(V_1/V_0)^{1/2}]. \quad (2)$$

V_1 and V_0 are the retarding and the accelerating potentials respectively, and m_1 and m_2 the target atom and beam ion masses. In this formula, the retarding potential is only that part of the ion energy associated with the velocity normal to the detector surface. Consistent with the conservation laws, the maximum angle of scattering in the laboratory system is given by $\alpha_{\max} = \sin^{-1}(m_2/m_1)$. For ${}^7\text{Li}^+$ in He this is 34.6° .

Ten values of the Li^+ ion beam energy between 50 and 800 eV were used. For retarding voltages close to the accelerating voltage, the difference was measured directly, and this along with the correction to the beam energy found from the energy distribution was used to determine the corrected ratio of the retarding voltage to the accelerating voltage. The estimated maximum uncertainty in the scattering angle arising from the uncertainty in this voltage ratio was about 1.5° . This occurred for the 50-eV beam and a retarding voltage of 44.8 V, but for most of the data this uncertainty was much less than 1° .

The two ion-current curves, one for increasing and one for decreasing path length, were used if they were essentially duplicates. For some 10 different values of x , the decrease in the beam current was obtained and from these the slope of the $\log(I/I_0)$ versus x was evaluated numerically and so the cross section S_α .

Semilogarithmic plots of the ion current versus x were examined occasionally for linearity as a check on single scattering. Fig. 2 shows the cross section S_α for 10 different beam energies of Li^+ in He. Since the experimental method used is relatively inaccurate for scattering angles less than 10° , and since the analysis to be used does not need the complete angular range, no data were taken for small angles. Figure 3 shows the corresponding results for Li^+ in H_2 . In reducing these data, the assumption was made that the scattering particle has the mass of the H_2 molecule. Evidence for this is shown in Fig. 4 where S_α versus $(V_1/V_0)^{1/2}$ is plotted. The maximum energy loss observed (minimum V_1/V_0) is definitely that expected for a target particle with the mass of H_2 for the low-energy ion beams, but less conclusively so for the 600- and 800-eV ion.

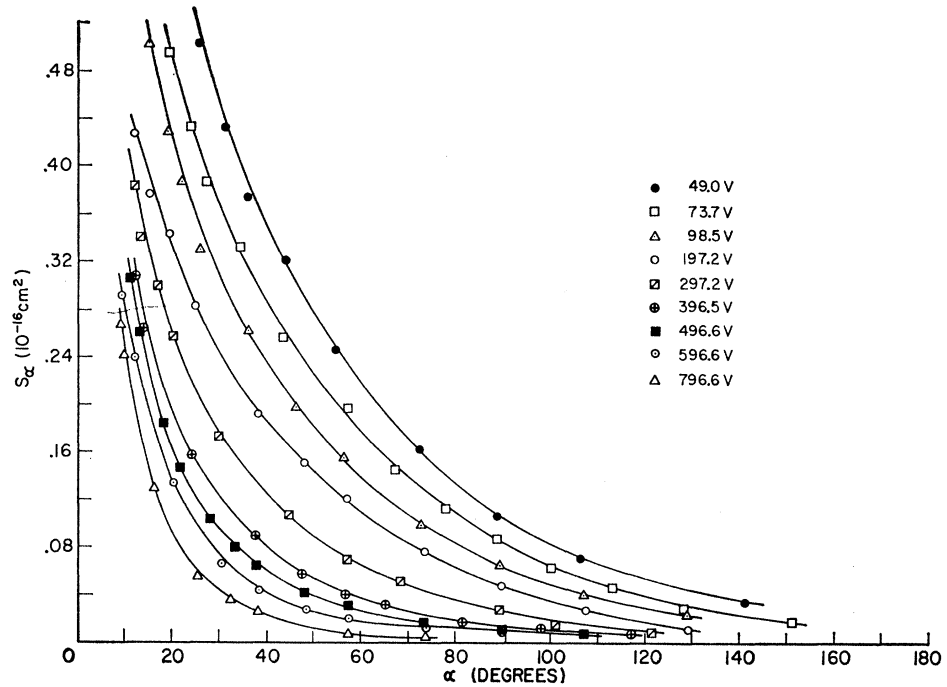
IV. INTERPRETATION OF THE DATA

For the ion beam energies used in this experiment, there is general agreement that classical methods of analysis suffice.^{1,13} On assuming a form for the interatomic potential $V(r)$, one can calculate the expected scattering distribution, or, in reverse, one may use the experimental distribution to determine numerical values of $V(r)$. There are two methods of calculation of the potential function assuming a monotonic dependence on the internuclear separation. One such method by Hoyt¹⁴ requires a number of cross-section curves for different collision energies, but not neces-

¹³ N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, London, 1965), 3rd ed., p. 110.

¹⁴ F. C. Hoyt, *Phys. Rev.* **55**, 664 (1939).

FIG. 3. The cross sections S_α for scattering outside the center-of-mass angle α as a function of α for Li^+ in H_2 . The number on each curve is the ion energy in eV.



sarily over the complete angular range. A second method by Firsov¹⁵ and also by Keller *et al.*¹⁶ needs only a single beam energy but measured values of a cross section over essentially the complete angular range. The Hoyt method is better suited to the results here.

The cross section for scattering outside the angle α is

$$S_\alpha = 2\pi \int_{b(\pi)}^{b(\alpha)} b db = b^2(\alpha), \quad (3)$$

where $b(\alpha)$ is the impact parameter corresponding to the angle of scattering α . The angle of scattering in terms of the interaction potential energy $V(r)$ is

$$\alpha(b, E_0) = \pi - 2b \int_{r_0}^{\infty} [1 - b^2/r^2 - V(r)/E_0]^{-1/2} r^{-2} dr, \quad (4)$$

where r_0 is the distance of closest approach of the two particles and E_0 is the initial energy of the impinging particle in the center-of-mass system. Following Hoyt, if

$$U = V(r) + L^2/2\mu r^2, \quad (5)$$

where L is the angular momentum of the system and μ the reduced mass, and if $\phi(E_0)$ is defined as $\pi/2 - \alpha/2$, then

$$\phi(E_0) = -[L/(2\mu)^{1/2}] \int_{\infty}^{r_0} r^{-2} (E_0 - U)^{-1/2} dr. \quad (6a)$$

Now, if $f(U) = r^{-1}$ so that $dr/r^2 = -f'(U)dU$, then Eq. (6a) becomes

$$\phi(E_0) = [L/(2\mu)^{1/2}] \int_0^{E_0} (E_0 - U)^{-1/2} f'(U) dU. \quad (6b)$$

This is an integral equation of the Abelian type and as solved by Klein¹⁷ yields

$$r^{-1} = f(U) = [(2\mu)^{1/2}/\pi L] \int_0^U \phi(E_0) (U - E_0)^{-1/2} dE_0. \quad (7)$$

The infinity in the integrand at the upper limit can be removed by rewriting the integral in two parts as

$$\int_0^U \phi(U) E_0 U^{-1} (U - E_0)^{-1/2} dE_0 - \int_0^U (U - E_0)^{-1/2} [\phi(U) E_0 U^{-1} - \phi(E_0)] dE_0 \quad (8)$$

where $\phi(U) = \text{constant}$. The left-hand term can be integrated directly and the expression becomes

$$\frac{4}{3} [U^{1/2} \phi(U)] - \int_0^U (U - E_0)^{-1/2} \times [\phi(U) E_0 U^{-1} - \phi(E_0)] dE_0. \quad (9)$$

As E_0 approaches U , both numerator and denominator approach zero, but this indeterminate ratio is also zero. Rewriting the expression in terms of the ratio $x = E_0/U$

¹⁵ O. B. Firsov, Zh. Eksperim. i Teor. Fiz. (USSR) **24**, 279 (1953).

¹⁶ J. B. Keller, I. Kay, and J. Shmoys, Phys. Rev. **102**, 557 (1956).

¹⁷ O. Klein, Z. Physik **76**, 226 (1932).

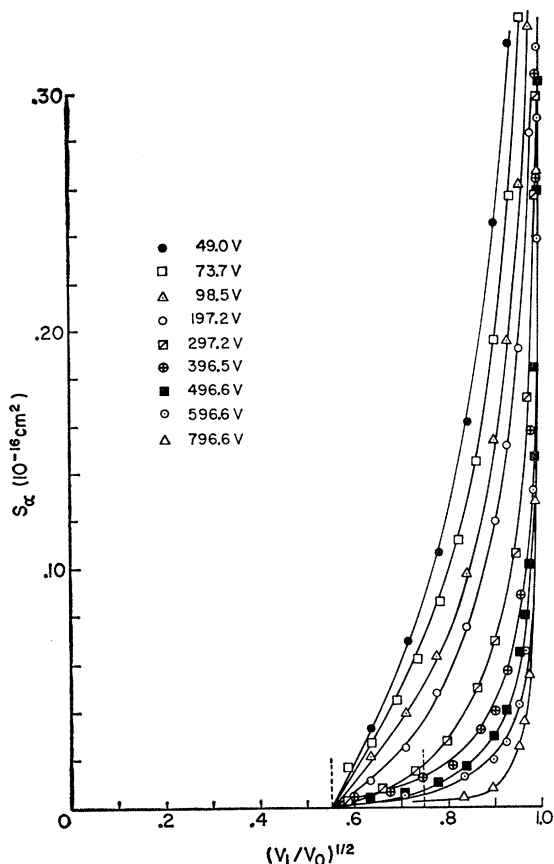


FIG. 4. The cross sections S_α as a function of the square root of the ratio of the retarding potential to the accelerating potential for Li^+ in H_2 . The minimum value of $(V_1/V_0)^{1/2}$ for elastic scattering of Li^+ by molecular hydrogen is 0.56.

and rearranging, we obtain

$$f(U) = r^{-1} = \frac{\phi(U) (2\mu U)^{1/2}}{\pi L} \times \left\{ \frac{4}{3} - \int_0^1 (1-x)^{-1/2} [x - \phi(E_0)/\phi(U)] dx \right\}. \quad (10)$$

With a judicious choice of L , a value of S_α is calculated and an α is found from the S_α versus α experimental results. The integral in Eq. (10) may then be evaluated numerically for a particular value of L and U . The interatomic potential energy $V(r)$ is then found from Eq. (5). This process can be repeated for a number of values of L within the limits imposed by the range of beam energies and the corresponding angles of scattering of the experimental data. Overlapping results obtained with different L and thereby arising from different sections of the S_α curves indicate, to some degree, the internal consistency of the measurements. The $V(r)$ so determined are shown in Fig. 5. Different values of L are indicated by the symbols of different shapes. The curve drawn represents the majority of the points to within about 2%; however, the accuracy

of the pressure and the ion current measurements lead to an estimated uncertainty of $\leq 5\%$. Figure 6 shows the corresponding curve evaluated from the scattering of Li^+ in H_2 . A semilogarithmic plot of $V(r)$ versus r approximates a straight line so that the interatomic potential may be represented by the Born-Mayer form within a few percent, viz., $V(r) = 3.7 \times 10^2 e^{-5.1r}$ eV for Li^+ -He and $3.0 \times 10^2 e^{-11.0r}$ eV for Li^+ - H_2 with r in \AA .

V. CALCULATION OF INTERACTION POTENTIAL

A number of recent calculations³ of the repulsive interaction between two ground-state He atoms have employed the molecular-orbital method. According to this approach two He atoms are considered to be an He_2 molecule with each of the four electrons assigned to a molecular orbital which is a one-electron wave function extending over the whole molecule. Such a calculation by Phillipson represents the most elaborate calculation to date. He employed the single configuration molecular orbital approximation in which the wave function was expressed as a single antisymmetrized spin-orbital product involving molecular-orbital factors taken as the sum and difference of Slater-type orbitals with the energy minimized in terms of the exponents. The results were further refined to account for the effects of electron correlation by a superposition of configurations treatment. The interatomic potential was computed for five internuclear separations over

TABLE I. Calculated values of $V(r)$ for Li^+ -He and He-He.

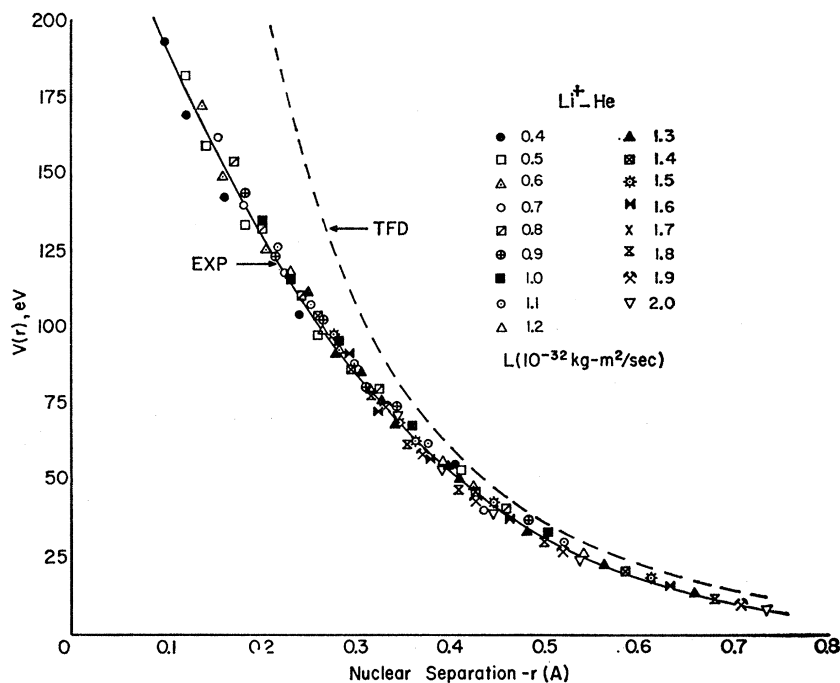
r (a.u.)	Li^+ -He $V(r)_{\text{TFD}}$ (eV)	He-He ^a $V(r)_{\text{TFD}}$ (eV)	He-He ^b $V(r)_{\text{M064}}$ (eV)
0.10	1319.3	899.92	
0.20	550.37		
0.30	310.84	217.67	
0.40	199.04		
0.50	136.63		
0.60	98.180	70.738	
0.70	72.568		
0.80	54.772		
0.90	41.949		
0.946	(37.29) ^c	(28.1)	27.76
1.0	32.445	24.713	
1.1	25.234		
1.18	(20.57)	(16.5)	17.33
1.2	19.671		
1.3	15.284		
1.4	11.804		
1.418	(11.26)	(10.0)	10.78
1.5	8.980	8.2688	
1.6	6.644		
1.7	4.728		
1.89	(2.004)	(3.80)	4.059
2.0		2.9145	

^a A. A. Abrahamson, Ref. 6.

^b P. E. Phillipson, Ref. 3.

^c Numbers in parentheses are interpolated.

FIG. 5. The interaction potential energy of $\text{Li}^+\text{-He}$ as a function of the internuclear separation. The different symbols indicate the different values of the angular momentum L used in the calculations. The dashed curve is the $V(r)$ from the two-center Thomas-Fermi-Dirac statistical model calculation.



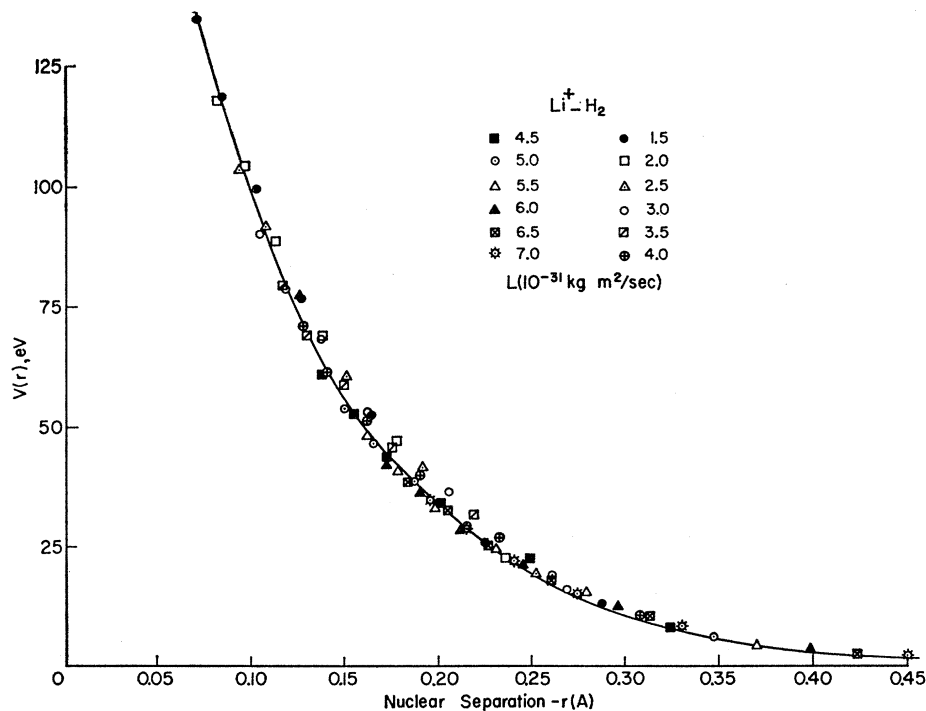
the range of 0.50–2.0 Å using various wave functions including 10–64 electron configurations, each of which was chosen to behave properly for an internuclear separation of 0 and ∞ . The results of Phillipson's 64-configuration calculation appear in Table I.

The Thomas-Fermi-Dirac (TFD) statistical model of the atom has been applied to a two-center system by Abrahamson *et al.*⁶ In the TFD model, the total

electron energy of the two interacting atoms may be written as a sum of the volume integrals as⁶

$$H = \kappa_b \int \rho^{5/3} dv + \frac{1}{2} e^2 \iint \frac{\rho(\mathbf{r}) \rho(\mathbf{r}') dv' dv}{|\mathbf{r} - \mathbf{r}'|} - e^2 \int \sum_i \frac{Z_i}{r_i} dv - \kappa_a \int \rho^{4/3} dv, \quad (11)$$

FIG. 6. The interaction potential energy of $\text{Li}^+\text{-H}_2$ as a function of the internuclear separation. The different symbols indicate the different values of the angular momentum L used in the calculations.



where a_0 =radius of the first Bohr orbit, ρ =electron density, $Z_i e$ =nuclear charge on the i th atom, and r_i =distance from the nucleus of the i th atom. The values of the constants are $\kappa_k = (3/10)(3\pi^2)^{2/3}e^2 a_0$ and $\kappa_a = (3/4)(3/\pi)^{1/3}e^2$. In order, the terms are the kinetic energy of the electrons, the electron interaction energy, the electron and nuclei interaction, and the electron correlation energy. By use of maximizing and minimizing conditions, Abrahamson *et al.* have obtained a form amenable to calculation with an error not exceeding 4% relative to the TFD approximation. The interatomic potential is in terms of H

$$V(r) = Z_1 Z_2 e^2 / r + H - H(\infty), \quad (12)$$

where Z_1 and Z_2 are the nuclear charges and $H(\infty)$ is the electronic energy at infinite separation. Again from Ref. 6, the reduced form of the potential is

$$V(r) = (Z_1 Z_2 e^2 / 2r) [\Psi(Z_1^{1/3} r / a) + \Psi(Z_2^{1/3} r / a)] \\ + \frac{1}{6} \iiint \{ \kappa_k [(\rho_{01} + \rho_{02})^{5/3} - (\rho_{01}^{5/3} + \rho_{02}^{5/3})] \\ - 2\kappa_a [(\rho_{01} + \rho_{02})^{4/3} - (\rho_{01}^{4/3} + \rho_{02}^{4/3})] \} dv, \quad (13)$$

where Ψ =TFD screening function, ρ_{0i} =exact undistorted electron density for the i th atom, and $a=0.8853a_0$. The integration is performed over the region of overlap of the electron clouds.

The TFD interaction potential $V(r)$ was calculated according to Eq. (13) for the system Li^+ -He on an

IBM 7074 digital computer. The values of the ionic and atomic radii and the corresponding electron densities ρ_{0i} were obtained from a set of tables computed by Thomas.¹⁸ A six-point Lagrangian interpolation procedure was used to obtain the radii, and a four point interpolation the electron densities for integral values of Z from the Thomas tables. The determinations of $V(r)$ was done for internuclear separations of $0.1a_0$ to $1.7a_0$, the latter determined by the TFD radii. These results are shown in Table I and also as the dashed curve in Fig. 5.

On comparing the TFD calculated $V(r)$ with the experimental, the agreement is seen to be fairly good, with the TFD value about 4 eV higher than the experimental for the range of separations down to about 0.35 Å. Below this the calculated $V(r)$ becomes increasingly too large. The work done by Abrahamson for various noble gas atom systems also shows such a disparity between the TFD values and experimental results for very small internuclear separations. The results of the TFD calculation by Abrahamson for He-He are also included in Table I for comparison with those for Li^+ -He.

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Electron-Impact Ionization Measurements of Surface-Ionizable Atoms*

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Total electron-impact ionization cross-section measurements are presented for calcium, strontium, barium, and thallium. These and previously determined cross sections for the alkali metals are compared with available techniques for calculating cross sections. Because of the difficulty of both the experimental measurements and the calculations, it is perhaps surprising to find agreement generally better than a factor of 2.

I. INTRODUCTION

THEORETICAL work by Rudge and Seaton¹ has aptly demonstrated the limited accuracy and difficulty of wave-mechanical calculations for predicting the ionization of atomic hydrogen by electron impact. Calculating other atomic-ionization probabilities by these methods is obviously more complex. In contrast, the semiclassical methods discussed by Gryziński² are sim-

ple and, while not completely understood, useful. Gryziński has shown the agreement between semiclassical calculations and experiment for the ionization of H, H₂, and He. In all instances the agreement was perhaps better than one might expect. Other theoretical work of classical or empirical origin includes that of Thomson,³ Elwert,⁴ Drawin,⁵ and Lotz.⁶ Stafford⁷

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