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Determination of the Li^+-He Interaction Potential from Low-Energy Experimental Differential Scattering Cross Sections*

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The Li^+-He experimental elastic differential cross sections of Aberth and Lorents in the 3.6- to 218-eV energy range have been analyzed and yield a simple repulsive potential. The potential may be parametrized as $V(R) = 2.95 \times 10^2 \exp(-4.30R) + 1.00 \times 10^3 \exp(-20.4R)$ in which R is in Å, and the energy is in eV. The estimated error is $\pm 25\%$ for $0.30\ Å < R < 0.80\ Å$. The potential is in fair agreement with recent *ab initio* quantum calculations and the potential of Zehr and Berry who analyzed the energy loss of Li^+ as a function of scattering path length.

INTRODUCTION

The measurement of low-energy differential cross sections provides a means of deducing the forces between atoms. Several techniques may be employed, each of which has its own attributes and limitations. The Firsov method,[1] which is convenient for obtaining a monotonic potential, requires a knowledge of the differential cross sections from 0 to 180° at some energy. Expansion methods[2] may also be employed with success if convergence is rapid. For some systems and (usually) low energies, iterative techniques[3] provide the easiest approach.

For the Li^+-He system, clustering[4] and mobility[5] data have allowed several analyses[6] to be made and information to be retrieved primarily about the forces at large internuclear separations. Quantum calculations[7] have been performed in this region and, recently, also at the small internuclear distances.[8,9] For separations of less than 1 Å, however, the only other experimental information about the internuclear forces has been that obtained from energy-loss spectra by Zehr and Berry.[10]

In this analysis, a semiempirical fit has been made to the structureless differential cross sections of Aberth and Lorents.[11] (The lack of structure, along with the inability to observe inelastic cross sections experimentally, indicates that inelastic effects were not of importance in this energy range.) The potential so retrieved from experiment was found to be in fair agreement with that of Zehr and Berry[10] and with the recent quantum calculations of Fischer,[8] and Junker and Browne.[9] With the potential obtained from the differential cross sections, the elastic total cross sections were also computed.

METHOD

A semiempirical fit has been made to the experimental data of Aberth and Lorents.[11] The usual classical formulas[12] have been used to calculate the deflection functions and the differential scattering cross sections.

Because of the high experimental collision energies and the weak attractive forces present for

this system, only information about the repulsive potential could be obtained. Two forms for the repulsive potential were initially chosen in this analysis. They are: the Born-Mayer potential, $V(R)=A\exp(-BR)$, and the shielded Coulomb potential, $V(R)=C/R\exp(-DR)$. Both forms contain only two disposable parameters.

The semiempirical analysis proceeded as follows: One of the above two potential forms was selected with estimates of the two parameters. The differential cross sections were calculated at each energy and compared to the experimental cross sections. With the aid of reduced plots of $E\theta$ versus $\theta\sin\theta\sigma(\theta,E)$ and the expansion formulas, [2a, 2c] changes of the parameters could be made by hand until a best fit was achieved over the complete energy range. For both forms it took approximately four cycles. The expansion formulas were not used directly because many terms of a series were needed for convergence. The formulas were utilized, however, so that qualitative changes could be made to the potential parameters and a rapid convergence attained.

In Figs. 1 and 2, the solid circles represent the experimental data of Aberth and Lorents[11] presented at fixed angles. The data were continuous but, to avoid confusion with the fit, they are presented this way.

Of the two potential forms, the Born-Mayer produced a much better fit than the shielded Coulomb potential. For energies, $E\lesssim 109$ eV, the potential was found to be best represented by

$$V(R)=2.95\times10^{2}\exp(-4.30R),$$

in which the energy is in eV and the internuclear distance is in Å. At the two highest energies an additional term was needed, however, to obtain a fit. This term produced a harder core and probably indicates the increasing dominance of the Coulomb forces. The potential form then became

$$V(R)=2.95\times10^{2}\exp(-4.30R)+1.00\times10^{3}\exp(-20.4R)\ .$$

The resulting fit to the data is shown by the solid lines in Figs. 1 and 2. A comparison can be made with the differential cross sections calculated from the potential of Zehr and Berry, $V(R)=3.7\times10^{2}\exp(-5.1R)$. Indications are, assuming no error in the experimental data, that their potential is too soft. However, it should be recognized that the experimental error in the absolute scaling is estimated to be ± 25%. The result is an approximate ± 25% uncertainty in the derived potential with a region of validity from about 0.30 Å to 0.80 Å. Zher and Berry's potential there is in agreement with these data. The retrieved potential and that of Zehr and Berry

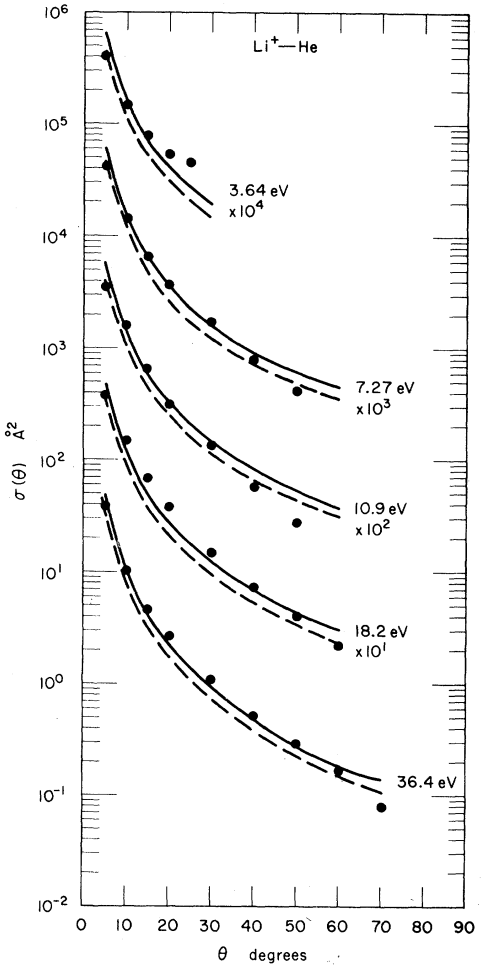

FIG. 1. Experimental elastic differential cross sections of Aberth and Lorents (summarized by solid circles) are compared to the differential cross sections calculated from the retrieved potential (solid line) and the potential of Zehr and Berry (dashed line). At each energy, the differential cross sections are displaced by an order of magnitude above those below it. Center-of-mass energies were used throughout.

are illustrated in Fig. 3.

The elastic total cross sections may now be calculated over the same energy range. Because of the exponential nature of the interaction potential, it was possible to fit them over the 10–200-eV energy range by the following form:

$$Q^{1/2}(\text{Å})=5.636-0.668\log_{10}E(\text{eV})\ ,$$

where E is the c. m. energy.

DISCUSSION AND CONCLUSIONS

A simple repulsive potential has been retrieved from the experimental differential cross sections

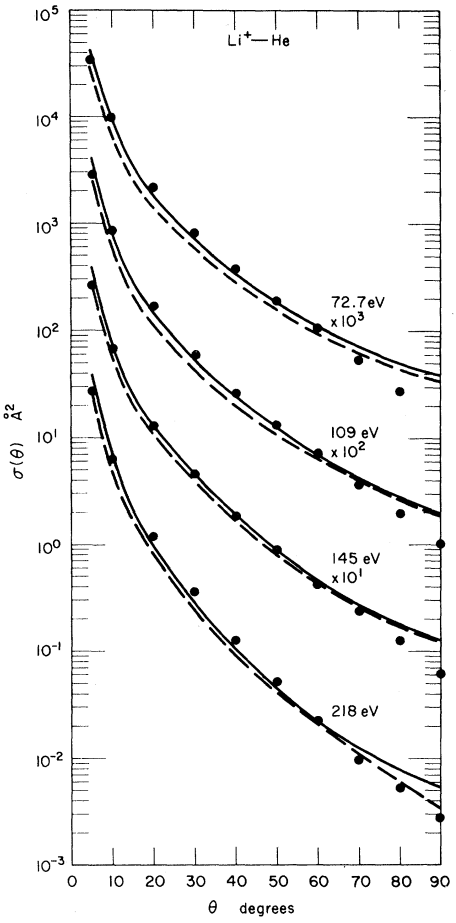

FIG. 2. Experimental elastic differential cross sections of Aberth and Lorents (summarized by solid circles) are compared to the differential cross sections calculated from the retrieved potential (solid line) and the potential of Zehr and Berry (dashed line). At each energy, the differential cross sections are displaced by a factor of 10 above those below it.

of Aberth and Lorents.[11] The error is estimated to be ±25% for 0.30 Å $< R <$ 0.80 Å. It arises primarily because of the uncertainty in the absolute scaling of the experimental cross sections. This potential is in fair agreement with that of Zehr and Berry.[10] At small internuclear separations, however, a trend to a harder core is noticeable. Fair agreement is also obtained with the calculations of Fischer,[8] and Junker and Browne.[9]

The potential of Fischer,[8] which is similar to that of Junker and Browne,[9] has also been used to calculate the differential cross sections. At all but the large angles at the highest energies the results are within experimental error. At these large angles there are experimental difficulties that preclude any comparison.

In the fit to the differential scattering cross sections, two effects stand out. One is that the calculated cross sections are larger than the experimental ones at the smallest angles. This effect is to be expected since the angular spread accepted by the detector increases at small angles, which yields measured cross sections that are less than the "true" cross sections.[13] The other effect is that the measured cross sections are less than the calculations at the large angles for each energy. One can only ascribe this behavior to some unknown experimental deficiency, since it corresponds to scattering from different impact parameters in each case. A possible explanation may be that, since at large angles the energies of the scattered ions are small, the detector efficiency is being reduced because of surface charging. A result of this large-angle die-off is that the potential is not accurately tested for impact parameters less than 0.3 Å.

The elastic total cross sections were also calculated and may be compared with the computations of Weber and Bernstein.[14] One finds their total cross sections to be much too large in this energy range. This discrepancy is not surprising, however, when one considers that their potentials were derived from low-energy mobility measurements and quantum calculations pertaining to large internuclear distances. At lower energies, their total cross sections are probably accurate.

As an estimate of the binding energy of Li$^+$-He, the derived repulsive potential was combined with the long-range attractive terms of Dalgarno and Kingston.[15] The well depth was found to be 0.053 eV, and its position was found to be 2.0 Å. The almost perfect agreement with the potential well parameters obtained from mobility measure-

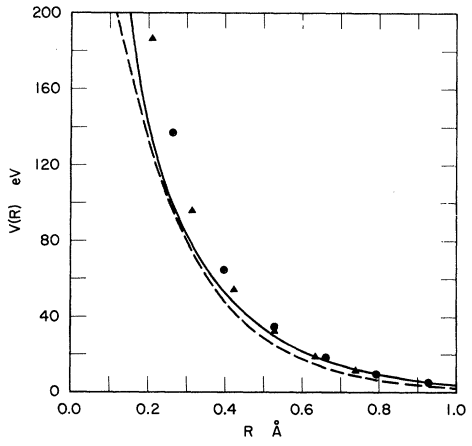

FIG. 3. Comparison of the retrieved potential (solid line) to that of Zehr and Berry (dashed line). The calculations of Fischer (Ref. 8) (solid triangles) and those of Junker and Browne (Ref. 9) (solid circles) are also presented.

ments,[6] however, is probably fortuitous.

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Uncertainty Principle for Ensembles

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Uncertainty principles for the average fluctuations of momentum and position per particle in an ensemble are derived. For bosons, these results are similar to the usual uncertainty principle, with slight corrections for the correlated motion of the particles. For fermions, a large correction for the Pauli exclusion principle is necessary, which causes $\langle p^2\rangle\langle r^2\rangle$ to be proportional to the two-thirds power of the number of particles in the ensemble.

Consider the following operator for N indistinguishable particles in one dimension:

$$H=\sum_i\left(-\frac{\hbar^2\partial^2}{\partial X_i^2}+\mu^2(X_i-X_0)^2\right)$$
$$+N^{-1}(\alpha^2-\mu^2)\sum_{i<j}(X_i-X_j)^2\ . \qquad (1)$$

This is a generalization of the operator recently considered by Lévy-Leblond[1] who treated the case, $\mu=0$. The normal coordinates for this harmonic oscillator potential are obvious from symmetry or from the classical analog. The lowest eigenvalue of H for μ and α real positive numbers is

$$E_0=[\mu+(N-1)\alpha]\hbar\ , \qquad (2)$$