EFFECT OF NUCLEAR SYMMETRY IN ION-ATOM SCATTERING*

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Everhart and his co-workers first observed interference fringes in symmetric ion-atom charge-exchange scattering as a function of energy at fixed angle,[1] and later as a function of angle at fixed energy.[2] The oscillating pattern represents an interference between even (g) and odd (u) electronic states of the molecule-ion system. These oscillations have been the subject of considerable recent experimental[3] and theoretical[4] study.

We wish to report the observation of a second type of oscillation appearing only in collisions involving identical nuclei. In that case it is impossible to distinguish experimentally between a glancing collision that scatters the incident ion through the angle θ and a knock-on collision with resonant charge exchange that scatters the target as an ion to the detector at the same angle θ. Classically, the two processes involve contributions from very different regions of the impact parameter b, and the observed cross section would be the sum of two terms; quantally, an interference between the two processes is expected, leading to a second type of oscillation in the scattering pattern. In the scattering of $^4He^+$ on ^4He, we have seen secondary oscillations which we attributed to this nuclear symmetry[5,6]; we have now confirmed their identification by parallel experiments using $^4He^+$ on ^3He, in which no trace of the secondary pattern appears.

The oscillations in question were first seen in the course of an experimental study of the elastic differential scattering of He^+ ions from He atoms in the laboratory energy range 20-600 eV and angular range 1-36°.[5] Cross-section data points for the $^4He^+$-^4He system at 300-eV center-of-mass energy (600-eV lab) are given in Fig. 1; these measurements are absolute within an error of ±25% and were not normalized to the theoretical curve. The smooth oscillations observed in the angular range 2-20° result from the interference between the two states, g and u, of the molecular ion. At larger angles a secondary pattern of oscillations is observed superimposed upon the major pattern with a frequency 4 to 5 times that of the major oscillation and an amplitude increasing with angle. In a companion theoretical study[6] a semiclassical calculation of the elastic-scattering pattern using the best available g and u potentials[7] is found to give good agreement with experiments both in respect to the absolute envelopes and the major interference peaks; an example is shown here in the upper solid curve of Fig. 1 (at this energy the experimental upper envelope at large angles declines below the theoretical, probably because of loss of intensity into inelastic channels). The secondary oscillations observed at large angles on the theoretical curve result when nuclear symmetry is properly taken into account. The

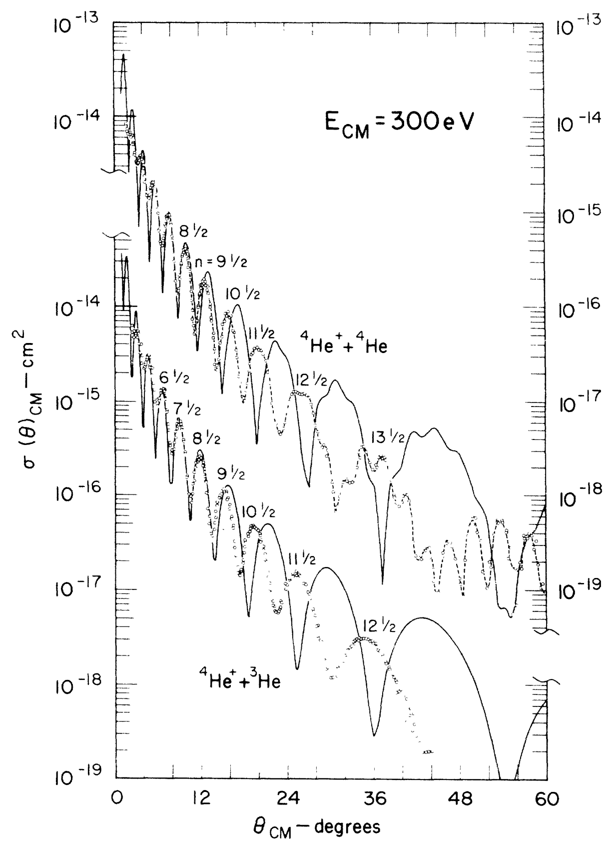

FIG. 1. Experimental (open circles) and theoretical (solid line) differential cross sections for the elastic scattering of $^4He^+$ ions from ^3He and ^4He at 300 eV. All quantities are given in the center-of-mass system. The numerical labeling on the experimental peaks is in accordance with that used by Everhart.[4]

calculated secondary oscillations agree reasonably in both frequency and amplitude with those observed (the amplitude relationship is obscured by the logarithmic scale in Fig. 1; for further details see reference 6). This suggests strongly that the observed oscillations are due to nuclear symmetry.

To confirm this suggestion the scattering experiment has now been repeated using ^{3}He as a target. The nuclear symmetry is then removed and the interference should not appear. The data given in Fig. 1 for the ^{4}He$^+$-^{3}He scattering at 300-eV center-of-mass energy (700-eV lab) show no sign of secondary oscillations. In this case absolute cross sections were not measured, and the data were normalized by comparison with the ^{4}He data as described below.

The nuclear symmetry effect is a consequence of the general requirement that the total wave function be symmetric under exchange of the nuclei if they are identical bosons, and antisymmetric if they are fermions. From this follows the rule that is well known in connection with the permitted rotational states of symmetric diatomic molecules: With identical ^{4}He nuclei, g states are limited to even values of l and u states to odd. It follows that the g and u scattering amplitudes have certain symmetries in the center-of-mass scattering angle θ:

$$f_g(\theta) = f_g(\pi-\theta) \ (l \text{ even}),$$
$$f_u(\theta) = -f_u(\pi-\theta) \ (l \text{ odd}). \tag{1}$$

This statement is precisely identical in physical consequences with the argument that the incident ion scattered without charge exchange into the detector at θ cannot be distinguished in any way from a target atom recoiling at the same angle θ after suffering charge exchange. As Massey and Smith noted,[8] the scattering amplitude can then be written

$$f(\theta) = \tfrac{1}{2}[f_g(\theta) + f_u(\theta) + f_g(\pi-\theta) - f_u(\pi-\theta)]. \tag{2}$$

The component scattering amplitudes can be taken as

$$f_j(\theta) = \sigma_j^{1/2}(\theta) \exp[iA_j(\theta)/\hbar], \tag{3}$$

and at the energies of interest to us it is an excellent approximation to calculate $\sigma_j(E, \theta)$ and $A_j(E, \theta)$ classically—A_j is then the classical action computed for the classical trajectory of the nuclei under the influence of the potential $V_j(r)$ ($j = g$ or u), and σ_j is the corresponding differential scattering cross section.

From (2) the observed cross section can be split up as

$$\sigma(\theta) = |f(\theta)|^2 = \sigma_d(\theta) + \sigma_e(\pi-\theta) + S(\theta, \pi-\theta), \tag{4}$$

where σ_d represents the direct scattering, σ_e the charge-exchange recoil, and S the cross terms:

$$\sigma_d(\theta) = \tfrac{1}{4}|f_g(\theta) + f_u(\theta)|^2,$$
$$\sigma_e(\pi-\theta) = \tfrac{1}{4}|f_g(\pi-\theta) - f_u(\pi-\theta)|^2,$$
$$S = \tfrac{1}{4}\sum_{jk}\alpha_{jk}[f_j(\theta)f_k^*(\pi-\theta) + f_j^*(\theta)f_k(\pi-\theta)],$$
$$\alpha_{gg} = \alpha_{uu} = \alpha_{ug} = -\alpha_{gu} = 1. \tag{5}$$

For small and moderate angles we are sure to have the $f(\theta)$'s much larger than the $f(\pi-\theta)$'s. Consequently, $\sigma_e(\pi-\theta)$ is usually negligible compared with $\sigma_d(\theta)$, and $S(\theta, \pi-\theta)$ has an intermediate magnitude, becoming significant as σ_d declines. The term S is responsible for the subsidiary oscillations observed. In the asymmetric collision, ^{4}He$^+$ + ^{3}He, the symmetry requirement (1) does not exist and the interference term S vanishes.

An approximate scaling law, valid in the limit of large E and L, indicates the proper quantities to be compared when the masses, energies, or angles are varied:

$$\tau = E\theta \to \tau(b), \tag{6a}$$
$$a_i(E, \theta) = (2E/\mu)^{1/2}A_i(E, \theta) \to a_i(\tau), \tag{6b}$$
$$s_i(E, \theta) = E^{-1}\sigma_i(E, \theta)\sin\theta \to s_i(\tau). \tag{6c}$$

Each of these functions approaches a function of the impact parameter b alone in the limit. In consequence, we expect the magnitudes of the envelopes of the curves to be comparable at the same center-of-mass energy and angle, but the locations of the maxima, which depend on the A's, will vary with the mass. The more accurate theory and the experiments confirm this behavior, and so it was used as a basis for normalizing the ^{4}He$^+$-^{3}He data. From the absolutely calibrated ^{4}He$^+$-^{4}He data a reduced curve of the principal maxima was obtained by plotting $s(\tau)$ versus τ. The ^{4}He$^+$-^{3}He scattering data were normalized by comparison with this reduced curve.

The primary maxima appear when the quantity

$$|A_u(E,\theta)-A_g(E,\theta)|/h=n-\tfrac{1}{2} \tag{7}$$

is an integer (we use a slightly inconvenient definition for n in order to conform to the notation of Everhart et al.[2,3]). The shift of the peaks due to the mass effect in (6b) is shown in Fig. 1. This would be true of the secondary peaks as well: If there were a secondary interference in the $^4He^+$-^3He case, its peaks would appear at new locations, but their magnitude would be such that the secondary structure should be visible in the same angular region where it is seen for $^4He^+$-^4He. No sign of the secondary interference is seen in the isotopically asymmetric scattering in the energy range 90 to 300 eV (c.m.) and the angular range 1 to 80° (c.m.).

The cleaner character of the scattering spectrum without nuclear symmetry makes possible a more complete analysis of the features it does contain. For heavier systems in which the potentials are unknown, such as $Ar^+ + Ar$, asymmetric data would give more reliable raw material for the inversion techniques that can be used to extract the potential empirically. Also, in the absence of the secondary structure, other anomalies in the envelopes should be more readily detectable—such anomalies at certain regions of $E\theta$ can already be seen in the $^4He^+$-^3He data; they may be connected with crossings of potential-energy curves and specific inelastic processes. In another direction, a careful combination of the symmetric and asymmetric data should help in the analysis of the information that is potentially available in the secondary oscillations—depending as they do on $f_j(\pi-\theta)$, they reflect the potentials at smaller values of r than the $f_j(\theta)$ alone, so it may be possible to use such data to explore a region of the ion-atom interaction that otherwise is accessible only at much higher energies.

An interesting question raised by the abandonment of nuclear symmetry is the effect on the electronic quantum numbers g and u of the displacement of the molecular center of mass from the center of charge. This introduces a small coupling between the g and u states which might have some effect on the comparison between the symmetric and the asymmetric data. However, this coupling depends on the velocity of the nuclear motion and resembles the other correction terms in the Born-Oppenheimer expansion, becoming negligible at low energies.

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