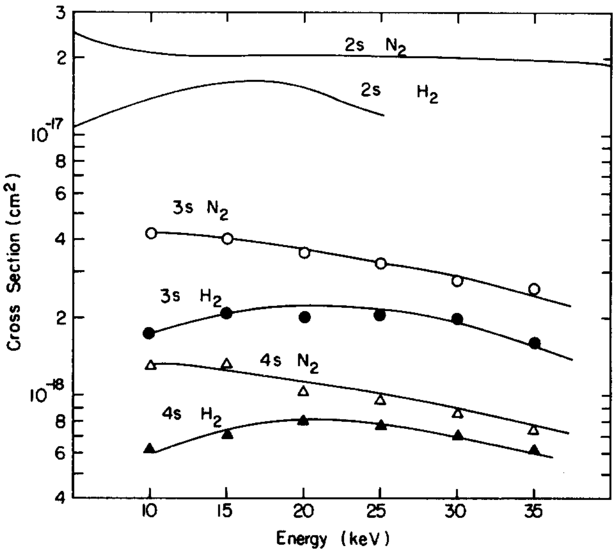

FIG. 1. Cross sections for exciting ground-state hydrogen atoms to the ns states by ground-state H-atom impact on N_2 and H_2. Cross sections for producing $H(2s)$ by impact on N_2 and H_2 are taken from Refs. 4 and 5, respectively. Cross sections for producing $H(3s)$ are taken from Ref. 1 while the $H(4s)$ cross sections are from this work.

of an 8-cm long collision chamber. The radiation from atoms excited in the collision chamber was entirely $4s \rightarrow 2p$ radiation at these distances since the H_β intensity decayed exponentially with distance according to the theoretical $4s$ radiative lifetime. The intensity per beam particle was proportional to the pressure in the collision chamber. The relative measurements were put on an absolute basis by determining the ratio of the H_β intensity per beam particle produced by a 25-keV atom beam to the intensity per beam particle produced by a 25-keV proton beam while holding the collision chamber pressure constant. This ratio was then multiplied by the absolute cross section for producing $H(4s)$ by 25-keV proton impact.[2]

The results are shown in Fig. 1. Reproducibility is estimated to be about $\pm 25\%$. Confidence in each individual $4s$ cross section is limited by a large optical background. Under the conditions of most data runs, the background represented about 60% of the total H_β signal for impact on H_2 while it ranged from 40% to 80% for impact on N_2 at 10 and 35 keV, respectively. The size of the background was determined by recording the signal when the collision chamber was evacuated and the observation chamber was filled to a pressure which had previously recorded for a data run. (Differential pumping maintained a pressure difference of 100 to 1 across the collision-chamber apertures.) This background was subtracted from the gross signal obtained during the data run.

A large part of the background appeared to be fairly independent of the pressure in the observation chamber and was due to radiation from surviving atoms that had originally been excited in the neutralizer. (A spatial scan of the radiation on the entrance side of the collision chamber verifies this statement.) These atoms had to survive a flight path of 17 cm through an electric field of a few hundred volts per centimeter which is strong enough to totally Stark mix the $n=4$ states. This part of the background is subject to quenching reactions[3] like $H^*+T \rightarrow H^+ + e + T$. Thus, the background that we subtract off may overestimate the true background during the data run. The part of the background that is proportional to the observation chamber pressure is due to fast-atom reactions with the background gas in the observation chamber and should be adequately taken care of in the subtraction process. Within experimental uncertainty no serious error is apparent since a poor treatment of the background would result in a $4s$ spatial decay curve which would be inconsistent with the theoretical $4s$ lifetime.

Also plotted in Fig. 1 are the $3s$ measurements from Ref. 1 along with the $2s$ measurements for $H(1s)$ impact on N_2 and H_2, taken from Hughes and Choe[4] and from Birely and McNeal,[5] respectively. The ratio of $3s$ excitation to $4s$ excitation is strikingly similar for impact on H_2 and N_2. The ratio is three for all energies (an n^{-4} dependence). In this energy range excitation to ns states appears to go $\sim n^{-4.5}$ for these two gases.

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† Present address: Oklahoma Medical School, Oklahoma City, Okla. 73106.

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Transition Matrix for Single Phonon Inelastic Surface Scattering

J. R. MANSON
Department of Physics and Astronomy, Clemson University, Clemson, South Carolina 29631

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Recently, a number of improvements to the theory of surface scattering of atoms and molecules have been published.[1,2] The principal advantage of the new theory over previous work[3–5] is its complete unitarity (the number of particles is always conserved) and the straightforward manner in which the many-body effects of the lattice can be included. The purpose of this letter is to extend the work of II with special regard to the contributions due to bound state interactions in single-phonon inelastic scattering.

The starting point is the transition rate,

$$W_{fi}=(2\pi/\hbar)\mid T_{fi}\mid^2\delta(E_f-E_i), \qquad (1)$$

from which the reflection coefficients can be readily obtained.[2] The indices i and f stand for the sets of quantum numbers describing the initial and final states, respectively, of the entire system; T_{fi} is the transition matrix.

The distinguishing feature of surface scattering is the fact that all incident particles are strongly scattered. For this reason it is convenient to treat the total interaction V of the incoming particle with the lattice as a sum of two parts; a "large" part U and the remainder v. If U is chosen to be the average of V over the surface and over thermal vibrations, then it will contribute only to specular scattering, and all diffraction and inelastic effects will be contained in v. Using the two-potential scattering formalism of Gell-Mann and Goldberger[6] the transition matrix in Eq. (1) can be written as

$$T_{fi}=(i/2N_i)\delta_{fs}+t_{fi}, \qquad (2)$$

where the δ function signifies that the first term, which arises from the potential U, contributes only to the specular beam, and N_l is π times the density of states for perpendicular particle motion ($N_l=m/2\hbar^2k_{zl}$) with m the mass of the particle and k_{zl} its wave vector component perpendicular to the surface.

The reduced transition matrix element t_{fi} obeys the integral equation

$$t_{fi}=v_{fs}+\sum_l v_{fl}[1/(E_i-E_l+i\epsilon)]t_{li}, \qquad (3)$$

where the v_{nm} are matrix elements of v taken between eigenstates of the "large" potential U, and the energy denominator is handled by the usual prescription

$$1/(E_i-E_l+i\epsilon)=[P/(E_i-E_l)]-i\pi\delta(E_i-E_l). \qquad (4)$$

It is shown in I and II that if one ignores the principal part contribution of the continuum states in the sum in Eq. (3), the integral equation reduces to a set of linear algebraic equations which can be solved exactly in the cases of elastic and single-phonon scattering. However, we would like to point out that this is a somewhat overly restrictive approximation. If the transition matrix for elastic scattering is known, then Eq. (3) can be solved for single-phonon inelastic scattering without neglecting the principal part contributions. As a simple example, consider the interaction of a particle with a smooth surface such that the only elastic scattering is into the specular beam. With only a single channel for elastic scattering, the transition matrix of Eq. (3) for single phonon inelastic scattering is readily shown to be

$$t_{pi}=v_{ps}/[1+i\phi N_s\sum_l\mid V_{sl}\mid^2/(E_i-E_l+i\epsilon)], \qquad (5)$$

where the summation is restricted to those bound and continuum states which differ from the initial state by a single phonon. This unitary transition matrix differs from the distorted wave Born approximation only by the extra term in the denominator containing the sum over intermediate states. This additional term can be split into an integral over continuum states and a sum over the discrete bound states and each of these can be further divided into a principal part contribution and a δ function or pole contribution according to the prescription given in Eq. (4). The effect of the approximation used in II would be to neglect the principal part contribution arising from the intermediate continuum states.

The result contained in Eq. (5) has a great deal of significance for situations in which the particle can scatter resonantly into a bound state (i.e., situations in which the particle can scatter into the bound state while still conserving energy). The δ-function contribution in the denominator, $\pi N_s\sum_l\mid V_{sl}\mid^2\delta(E_i-E_l)$, is clearly positive definite and is equal to one-fourth of the total number of particles inelastically scattered into both the continuum and bound states in the Born approximation. Thus as long as the contributions from the principal part terms are small (which is usually the case[7]) the effect of resonant scattering into the bound states via a single-phonon process can only reduce the reflection coefficient below that of the distorted wave Born approximation.

It is now apparent that the contributions of the discrete bound states in inelastic scattering can be handled in a very logical manner. The extension of these results to situations in which diffraction can occur follows directly from the treatment given in II if one retains the principal part contribution to the integrals over intermediate single-phonon states. The process is straightforward, although somewhat lengthy, but the interpretation of the results is quite similar to that given in the simple example above.

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