

to provide good estimates of scattering parameters for a variety of scattering systems with a reasonable amount of computational effort. In this connection, the important question which has not yet been answered is the rate of convergence of $\{\lambda\}$ as the number of parameters in $P\Psi_t$ and $Q\Psi_t$ increases. This problem may best be studied by many careful applications of the procedure to different physical

systems, such as e^+H , nd , and pd . For the present approach to be effective, it is important to ascertain whether $P_b\Psi_t$ in (3.2) can be obtained readily when the effect of $Q_b\Psi_t$ is neglected. The rest of the problem may not be so crucial then, since the integrals involved in (3.3) are essentially of the same type as those in (3.2) and, in addition, M_a is bounded in the Q_b subspace.

¹Y. Hahn, Phys. Rev. C **1**, 12 (1970). We refer to this paper for details of the notation. Specifically, we impose the standing wave boundary conditions throughout. The scattering parameter λ depends on the way in which the scattering functions are normalized and is directly related to the reaction matrix.

²J. F. Dirks and Y. Hahn, Phys. Rev. A **2**, 1861 (1970); **3**, 310 (1971); and B. H. Bransden and Z. Jundi, Proc. Phys. Soc. (London) **92**, 880 (1967).

³Y. Hahn, Ann. Phys. (N.Y.) **67**, 389 (1971).

⁴Y. Hahn, Phys. Rev. A **4**, 1881 (1971).

⁵F. E. Harris, Phys. Rev. Letters **19**, 173 (1967);

R. K. Nesbet, Phys. Rev. **179**, 60 (1969).

⁶M. H. Mittleman, Phys. Rev. **152**, 76 (1966); A. Temkin and J. F. Walker, *ibid.* **140**, A1520 (1965).

⁷Y. Hahn and J. F. Dirks, Phys. Rev. A **3**, 1513 (1971).

⁸Y. Hahn, Phys. Rev. **169**, 794 (1968).

⁹Y. Hahn, Ann. Phys. (N.Y.) **58**, 137 (1970).

¹⁰Y. Hahn, Nucl. Phys. **A146**, 62 (1970).

¹¹L. M. Delves and A. C. Phillips, Rev. Mod. Phys. **41**, 497 (1969).

¹²N. Austern, *Direct Nuclear Reaction Theories* (Wiley-Interscience, New York, 1970).

Minima of Generalized Oscillator Strengths for Electron-Impact Excitation of the 6^1P_1 and $6p'^3P_1$ States of Hg

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Differential cross sections for excitation of the 6^1P_1 and $6p'^3P_1$ states of mercury have been measured at angles where minima of the generalized oscillator strengths could be expected. The minima appeared for both channels. Contrary to the results of the first Born approximation, their position depends not only on the momentum transfer but also on the primary energy. The confidence of some authors in the reliability of the Born approximation for inelastic scattering is not justified.

Recent experimental¹ and theoretical² studies of spin polarization and differential cross sections of electrons which have been scattered by Hg atoms showed the following facts: At lower energies (25 and 30 eV) these curves look quite different for elastically and inelastically scattered electrons, whereas with increasing energy a striking resemblance between elastic and inelastic curves becomes noticeable.

There is, however, one exception to the latter statement: At small angles there appears a shoulder in the inelastic cross sections which does not match the features in the elastic cross sections. Its origin can be explained on the basis of the first Born approximation by a minimum of the generalized oscillator strength f .³⁻⁵

For a systematic study of this feature measurements of inelastic differential cross sections for

excitation of the 6^1P_1 and $6p'^3P_1$ states of mercury have been made. These measurements are an extension to smaller angles of our experiments on spin polarization and differential cross sections for inelastic electron scattering. For a description of the apparatus we refer to these experiments, which were published elsewhere.^{1,6}

We must emphasize, however, the point discussed in the above papers^{1,6} that at the smaller angles studied here the errors are somewhat larger than in the range of larger angles. The error of the cross sections for the 6^1P_1 channel is about 5%. It is larger for the $6p'^3P_1$ channel, since, owing to the limited over-all energy resolution of 0.8 eV, neighboring channels (particularly the $6p'^1P_1$ channel) may contribute to the observed intensity. This contribution is at most 15% at the smallest angles observed. Its influence on the shape of the

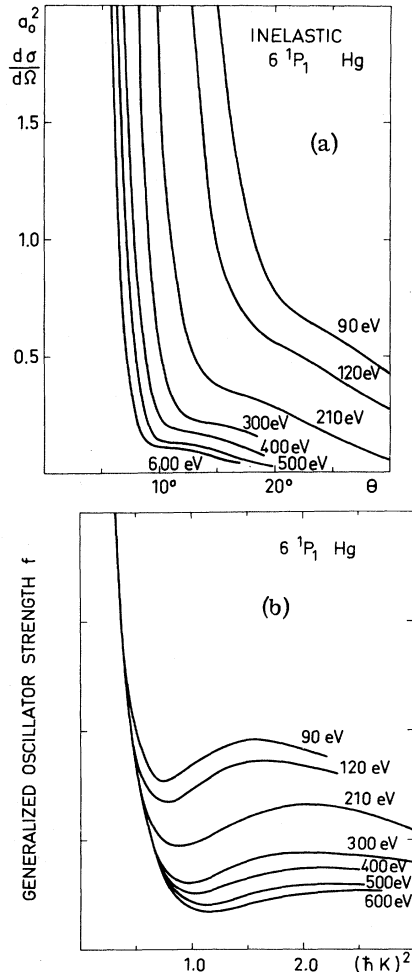


FIG. 1. (a) Differential cross sections for excitation of the 6^1P_1 state of Hg (energy loss 6.7 eV). Curves are fitted at the smallest angles to the data of Skerbele and Lassette (Ref. 5). (b) Generalized oscillator strengths for excitation of the 6^1P_1 state of Hg. At the smallest momentum transfers the curves are fitted to the data of Skerbele and Lassette (Ref. 5). $(\hbar K)^2$ in atomic units.

cross section observed should be much smaller because of the similarity of the cross-section curves. Experiments of the present type are of no value unless they include thorough studies of the influence of plural scattering. By the tests described in Ref. 1 and in the thesis quoted there, we made sure that the measurements were not affected by plural scattering. It was experimentally verified that the results did not change when the target density was reduced.

Figure 1(a) shows differential cross sections for excitation of the 6^1P_1 state of mercury. In the first Born approximation the cross section can be written

$$\frac{d\sigma(K)}{d\Omega} = \frac{2me^4}{(\hbar K)^2} \frac{k_n}{k_0} \frac{1}{W} f(K), \quad (1)$$

where f is the generalized oscillator strength

$$f(K) = \frac{2m}{(\hbar K)^2} W \left| \int \Psi_0 \sum_j e^{i\vec{k} \cdot \vec{r}_j} \Psi_n^* d\vec{r}_1 \dots d\vec{r}_N \right|^2, \quad (2)$$

$\hbar K = \hbar |\vec{K}| = \hbar |\vec{k}_0 - \vec{k}_n|$ being the momentum transfer, W the excitation energy, \vec{r}_j the position vector of the j th electron of the atom, and Ψ_0 and Ψ_n the atomic wave functions in the ground state and the excited state. Figure 1(b) shows the generalized oscillator strengths calculated from the cross sections of Fig. 1(a) by means of Eq. (1). The curves are fitted to the universal curve of Skerbele and Lassette⁵ at our smallest momentum transfers, since there was agreement between their results and ours at the energies 300, 400, and 500 eV which we had in common. Because of the angular resolution of 0.75° the uncertainty of this fit is about 20%.

According to Eq. (2), f is a function of K only, so that one should get a universal curve $f(K^2)$ for all primary energies. Figure 1(b) shows that this is not true, except for the smallest momentum transfers. The first Born approximation on which Eqs. (1) and (2) are based is therefore no longer valid for most of the angular range covered by our measurements. At the higher energies the differences between the curves are small, showing that the deviations from the Born approximation are not serious. With decreasing energy, however, the differences are rapidly increasing.

Figure 2 shows the position of the minimum of f for different primary energies. According to the first Born approximation, the minimum should stay at a fixed value of $(\hbar K)^2$.

The results of Geltman and Hidalgo⁷ on the unreliability of the first Born approximation for non-forward inelastic scattering (though obtained for

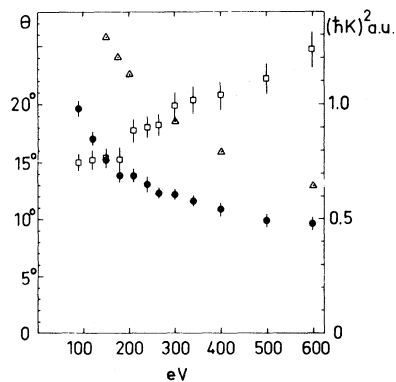


FIG. 2. Position of the minimum of the generalized oscillator strength for excitation of the 6^1P_1 state of Hg at different primary energies: circles, experimental data, θ scale; squares, experimental data, $(\hbar K)^2$ scale; triangles, theoretical data from Bonham (Ref. 9), θ scale. Error bars caused by angular resolution.

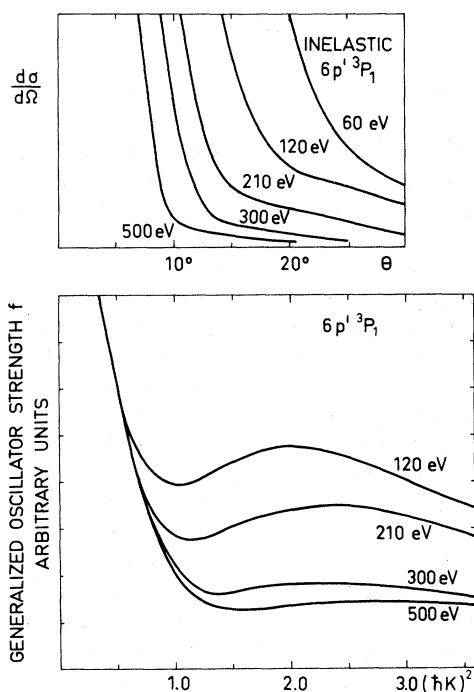


FIG. 3. Like Fig. 1, but for the $6p' \ ^3P_1$ state (energy loss 11.0 eV). Curves fitted to yield energy-independent data for f at the smallest momentum transfers.

hydrogen) are therefore strongly supported by our measurements, whereas Skerbele and Lassettres expectation "that the Born approximation also holds at larger values of the momentum change"⁵ could not be confirmed. It should be mentioned that the discrepancy between our results and the curve of Fig. 2 of Skerbele and Lassettre for $(\hbar K)^2 > 2$ disappeared when Miss Skerbele kindly remeasured her values.⁸

There appears at present to be only a few wave functions available for computing the oscillator strength for the 6^1P_1 state of Hg.⁹ The function of Bates and Damgaard,¹⁰ based on a Coulomb approximation, in the one-electron excitation approximation gives reasonable agreement with the optical oscillator strength but no zeros in the generalized oscillator strength. The radial $6s$ wave function of Hartree and Hartree¹¹ and the radial $6p$ wave function of Mishra,¹² both based on the Hartree approximation, lead to the prediction of several zeros in the first Born cross section in the one-electron excitation approximation but yield values of the optical oscillator strength that differ from experiment by more than a factor of 3. The results of the calculation using the latter wave functions are shown for the first zero in the cross section in Fig. 2. The present work points up the desirability of obtaining accurate theoretical generalized oscillator strengths for heavy atoms.¹³

Similar measurements for the $6p' \ ^3P_1$ channel are shown in Fig. 3. Also for this state, pronounced minima of the generalized oscillator strengths were found. Their position is shifted to somewhat larger momentum transfers compared with the 6^1P_1 channel.

At energies of 60 and 30 eV the minima disappeared in both channels. Because of the great theoretical interest^{4,13} in these results we plan to continue the measurements for some other elements, where minima of the generalized oscillator strengths can be expected, too.

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¹W. Eitel and J. Kessler, Phys. Rev. Letters **24**, 1472 (1970); Z. Physik **241**, 355 (1971).

²D. H. Madison and W. N. Shelton, in *Proceedings of the Seventh International Conference on Electronic and Atomic Collisions*, edited by L. M. Branscumb *et al.* (North-Holland, Amsterdam, 1971), p. 359.

³R. A. Bonham, J. Chem. Phys. **36**, 3260 (1962).

⁴Y.-K. Kim, M. Inokuti, G. E. Chamberlain, and S. R. Mielczarek, Phys. Rev. Letters **21**, 1146 (1968).

⁵A. Skerbele and E. N. Lassettre, J. Chem. Phys. **52**, 2708 (1970).

⁶F. Hanne and J. Kessler, Z. Physik (to be published).

⁷S. Geltman and M. B. Hidalgo, J. Phys. B **4**, 1299 (1971).

⁸A. Skerbele (private communication).

⁹This paragraph is based on a private communication by Professor R. A. Bonham.

¹⁰D. R. Bates and A. Damgaard, Phil. Trans. Roy. Soc. London **A242**, 101 (1969).

¹¹D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A149**, 210 (1935).

¹²B. Mishra, Proc. Cambridge Phil. Soc. **48**, 511 (1952).

¹³Y.-K. Kim and M. Inokuti, in Ref. 2, p. 762.