sections  $\sigma_e$  implies equality of the total cross sections. Thus for the purposes of this paper it is sufficient that at low energies  $\sigma_e$  in H<sub>2</sub> be very nearly independent of the molecular rotational state. That this is indeed the case stems from the fact that, apart from the small contribution of long-range forces [comparable to the inelastic cross sections in Eq. (20) of I], the zero energy elastic cross section involves only incoming and outgoing s-waves, coupling through the spherical part of the interaction. At zero energy, consequently, the interaction, Eq. (12) of I, can be replaced by its spherical part, which part is readily seen to yield a scattering amplitude independent of J. A more detailed analysis<sup>13</sup> shows that  $\sigma_e$  remains very nearly independent of rotational state at energies less than a few tenths of an electron volt.

In conclusion, we stress: (1) We have not found any experimental comparisons of the total cross sections, and therefore are forced to rely on a theoretical argument. (2) Since our argument is wholly theoretical, and in many respects qualitative, we feel it would be worth while to measure these total cross sections using some suitable and identical procedure, e.g., Varnerin's.<sup>5</sup> (3) The swarm mobility and diffusion measurements<sup>2</sup> which yield  $\lambda'$  also yield a measurement of  $\sigma_t$ , so that the proposed swarm experiments can check, albeit somewhat equivocally<sup>14</sup> our assumption about  $\sigma_t$ .

<sup>13</sup> S. Stein, thesis, University of Pittsburgh, 1955 (unpublished). <sup>14</sup> Since the swarm experiments determine an effective  $\sigma_t$  from complicated averages over the electron distribution, and since the

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## APPENDIX

The examination of the validity of the theory in  $H_2$ parallels I, Sec. IV. Because both Q and the molecular radius  $r_0$  are smaller in H<sub>2</sub> than in N<sub>2</sub>, and because we are here interested in even slower electrons than in the previous paper, the only question requiring detailed examination is the ratio  $A_1/A_2$  of "near-" and "far-" field amplitudes. Using, much as in I, the Wang potential<sup>15</sup> with the nuclei at their equilibrium separation to compute for H<sub>2</sub> the quantity  $f_a(\theta)$ , we obtain for small  $k_a$ 

$$A_1 = 1.8 (k_a a_0)^2 A_2. \tag{1}$$

Estimating  $f_a(\theta)$  from the measured elastic cross section gives nearly the same result, the factor being 2.3 instead of 1.8. At the vibrational threshold, Eq. (1) makes  $A_1/A_2 = 0.07$ ; at 0.075 ev,  $A_1/A_2 = 0.01$ . These numbers indicate that the cross sections of I are valid for  $H_2$  at electron energies below the vibrational threshold, and are surely valid at the very low energies of interest in the proposed low-temperature experiments.

electron energy distribution is affected by inelastic losses, it is possible for the swarm experiments to indicate unequal  $\sigma_t$  even though the total cross sections in these gases actually are the same. Thus, for definitive experiments detailed knowledge of the distribution functions is required, but we may expect that there should be at least qualitative significance to comparing the magnitudes of  $\sigma_{t \text{ eff}}$  in different gases. <sup>15</sup> S. C. Wang, Phys. Rev. **31**, 579 (1928).

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## Generation of Coulomb Wave Functions by Means of Recurrence Relations

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A discussion of the computation of Coulomb wave functions from their recurrence relations is given. Specifically, it is demonstrated that the regular solution  $F_L$  and the irregular solution  $G_L$  may be obtained recursively based on the knowledge of the functions for L=0.

HE present paper is concerned with the computation of the regular and irregular Coulomb wave functions  $F_L$  and  $G_L$ , for L a positive integer, with the aid of the recurrence relations satisfied by these functions. Thus if  $y_L$  stands for either  $F_L(\eta,\rho)$  or  $G_L(\eta,\rho)$  we have

$$L\frac{dy_{L}}{d\rho} = (L^{2} + \eta^{2})^{\frac{1}{2}} y_{L-1} - \left(\frac{L^{2}}{\rho} + \eta\right) y_{L}, \qquad (1)$$

$$(L+1)\frac{dy_L}{d\rho} = \left[\frac{(L+1)^2}{\rho} + \eta\right] y_L - \left[(L+1)^2 + \eta^2\right]^{\frac{1}{2}} y_{L+1}, \quad (2)$$

$$L[(L+1)^{2} + \eta^{2}]^{\frac{1}{2}}y_{L+1} = (2L+1)\left[\eta + \frac{L(L+1)}{\rho}\right]y_{L} - (L+1)[L^{2} + \eta^{2}]^{\frac{1}{2}}y_{L-1}.$$
 (3)

<sup>1</sup> J. L. Powell, Phys. Rev. 72, 626-627 (1947).

In addition, we have the Wronskian relations

$$F_L'G_L - F_LG_L' = 1, (4)$$

$$F_{L-1}G_L - F_L G_{L-1} = L(L^2 + \eta^2)^{-\frac{1}{2}}.$$
 (5)

The method is entirely similar to that employed for the generation of Bessel functions of integral order.<sup>2</sup> This is to be expected in view of the fact that the functions  $F_L$  and  $G_L$  bear the same relation to each other as the Bessel functions  $J_n$  and  $Y_n$  or the modified Bessel functions  $I_n$  and  $K_n$ ; namely, for  $L \rightarrow \infty$ , that  $F_L$  is a decreasing function of L while  $G_L$  is an increasing function of L. The recurrence relation (3) will be stable when applied in decreasing order to  $F_L$  and in increasing

<sup>&</sup>lt;sup>2</sup> Bessel Functions, Part II (British Association for the Advancement of Science, Cambridge, 1952). The method is credited to J. C. P. Miller.

order to  $G_L$ . By this we mean no error will be propagated if we generate  $F_L(G_L)$  in decreasing (increasing) order. The technique described may be applied for other sets of functions such as the spherical Bessel functions.

To generate the functions  $G_L$  we need only be able to calculate  $G_0$  and  $G_0'$ . The application of (2) will produce  $G_1$  and then (3) may be used to obtain as many values of  $G_L$  as may be desired.

To determine the values of  $F_L$  recursively for given  $\eta$ and  $\rho$  it would appear that  $F_L$  and  $F_{L'}$  (say) would be required as starting values for some L>0. Actually, this is not the case as we shall show. We can start with arbitrary values  $\overline{F}_L$  and  $\overline{F}_{L+1}$  which we consider as the values of the solution of the respective differential equations at the given  $\eta$  and  $\rho$ . Then, given  $\overline{F}_{L+1}$ , there is a one-parameter family of  $\alpha$  and  $\beta$  such that

$$\alpha F_{L+1} + \beta G_{L+1} = \overline{F}_{L+1}. \tag{6}$$

In order to fix  $\alpha$  and  $\beta$  uniquely we require that

$$\alpha F_L + \beta G_L = \bar{F}_L. \tag{7}$$

Then, by virtue of (5) we can solve this system for  $\alpha$  and  $\beta$ . For example, with  $\overline{F}_L = 1$ ,  $\overline{F}_{L+1} = 0$  we get

$$\alpha = G_{L+1} \frac{\{(L+1)^2 + \eta^2\}^{\frac{1}{2}}}{(L+1)}, \quad \beta = -\alpha \frac{F_{L+1}}{G_{L+1}}.$$
 (8)

If we now generate a sequence  $\overline{F}_m \equiv \alpha F_m + \beta G_m$  for  $m = L - 1, L - 2, \dots, 1, 0$  by the use of (3) we have

$$\bar{F}_{m} = \alpha \bigg\{ F_{m} - \frac{F_{L+1}}{G_{L+1}} G_{m} \bigg\}.$$
<sup>(9)</sup>

Since  $F_L \rightarrow 0$  and  $G_L \rightarrow \infty$  as  $L \rightarrow \infty$  we may choose L so large that the second factor in the brackets can be made as small as we please and thus

$$\bar{F}_m \sim \alpha F_m$$
 (10)

where  $\alpha = \alpha(L,\eta,\rho)$  and  $\alpha$  is defined in (8).

It is now clear that if  $\alpha$  is known we can determine  $F_m$ from  $\overline{F}_m$ . However, the knowledge of  $\alpha$  implies the knowledge of  $G_{L+1}$ . On the other hand, if for some integer m where  $0 \le m \le L' \ll L$  we know  $F_m$ , then by virtue of (10) we can determine  $\alpha \sim \overline{F}_m/F_m$  and use this value of  $\alpha$  to calculate  $F_k$  for  $0 \le k \le L' \ll L$  from the corresponding  $\overline{F}_k$ . In particular we can therefore take  $\alpha = \overline{F}_0/F_0$  provided  $F_0 \ne 0$ . In practice, this means that if  $\eta$  and  $\rho$  are near a zero of  $F_0$  we should choose some other value for m, say m = 1.

In those situations where the  $G_L$  are also desired the procedure may be modified in the following manner. From  $G_0$  and  $G_0'$  we generate the sequence  $G_m$  in increasing order, the sequence  $\bar{F}_m$  being generated from  $\bar{F}_L$ ,  $\bar{F}_{L+1}$  in decreasing order as above. However, instead of computing  $\alpha$  from  $\bar{F}_0 \sim \alpha F_0$  we can now use

$$F_0G_1 - F_1G_0 = \alpha^{-1}(\bar{F}_0G_1 - \bar{F}_1G_0) = (1 + \eta^2)^{-\frac{1}{2}},$$

which follows from (5) for L=1.

As an illustration of the method let us take  $\eta = 5$ ,  $\rho = 5$  starting with  $\overline{F}_{31} = 0$ ,  $\overline{F}_{30} = 0.1$ . Generating the values of  $\overline{F}_m$  carrying ten figures, we get

$\bar{F}_{20} = 13854 \ 08764,$	$F_{20} = 0.0^{13}1883 \ 426_8,$
$\bar{F}_{11} = 35942\ 29977. \times 10^7$	$F_{11} = 0.0^{6}4886\ 261_{1},$
$\bar{F}_{10} = 17217 50614. \times 10^8$ ,	$F_{10} = 0.0523406746_8$
• • •	
$\bar{F}_1 = 16379 \ 10103 \times 10^{12},$	$F_1 = 0.02226\ 695_7,$
$\bar{F}_0 = 20355\ 68006. \times 10^{12}$	$F_0 = 0.02767 \ 301_2$ .

To eight significant figures the value of  $F_0 = 0.02767\ 3012$ , from which we find  $\alpha^{-1} = 1.3594737 \times 10^{-23}$ . An independent calculation shows that the values of  $F_L$  indicated above are correct to approximately eight significant figures. Starting now with  $G_0 = 18.1933$  and  $G_1$ = 21.7261 and generating the successive values of  $G_L$ , we get ultimately  $G_{19} = 79310\ 46945 \times 10^2$ ,  $G_{20}$  $= 62908\ 14544 \times 10^3$ . Checking the results with the Wronskian relation (5) shows the values of  $G_{19}$  and  $G_{20}$ to be correct to approximately six significant figures. Similar calculations were made for  $\eta = 10$ ,  $\rho = 1$  and  $\eta = 1$ ,  $\rho = 10$  with comparable success.

A suggested procedure for carrying out the aforementioned technique is as follows. Suppose the values of  $F_m$  and  $G_m$  are desired for  $0 \le m \le L'$ . Then choose two values of L (say, L and L+5) with  $L \gg \rho$  and  $L \gg L'$ . Generate the sequences F and G for both values of L and compare. If the results do not agree for  $0 \le m \le L'$  then start with L+10 and compare the results with those for L+5.

The derivatives  $F_L'$  and  $G_L'$  can be generated from (1) and (2) to provide a check once the desired  $F_L$  and  $G_L$  have been obtained. An additional check is obtained from (4).

The values of  $F_m$  may also be derived in the following manner. Once the values of  $\overline{F}_m$  have been generated, it remains only to determine the normalizing factor  $\alpha$ . This may be done with the aid of the relations<sup>3</sup>:

$$\rho \cos\rho = \left(\frac{e^{2\pi\eta} - 1}{2\pi\eta}\right)^{\frac{1}{2}} \sum_{L=0}^{\infty} (2L+1) \cos\delta_L(\eta) \cdot F_L(n,\rho), \quad (11)$$
$$\rho \sin\rho = \left(\frac{e^{2\pi\eta} - 1}{2\pi\eta}\right)^{\frac{1}{2}} \sum_{L=0}^{\infty} (2L+1) \sin\delta_L(\eta) \cdot F_L(\eta,\rho), \quad (12)$$

where

$$\delta_L(\eta) = \frac{L\pi}{2} + \sum_{k=1}^L \arctan(\eta/L).$$

 $\delta_0 = 0$ ,

Since this procedure will yield the values of  $F_0$  and  $F_1$ , only  $G_0$  need be computed independently.  $G_1$  will be found from (5) with L=1, and (3) may then be employed to generate as many additional values of  $G_L$  as may be desired.

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<sup>&</sup>lt;sup>3</sup> The authors are indebted to their colleague, Dr. P. Henrici, for having provided them with these relations.