

DOT AND C. A. TEN SELDAM

7 and 8 atomic units, and Sommer applied the formula (12) to $r_0 = 3$ and 4

the sums, occurring in the expressions (12), simplified, because it can be shown that they are equal to the general "exponential integral", that has been tabulated ⁵⁾. To be stated that the sums of equations (12) and

$$= \sum_{\tau=1}^{\infty} \frac{x^{\tau}}{\tau(\tau+m)!}, \quad (15)$$

equal to

$$f_2(x) - f_1(x) + \frac{1}{2}x. \quad (16)$$

connected to the general "exponential integral" here by the symbol Fi :

$$f_m(x) = \int_1^x e^x x^{-m} dx, \quad (17)$$

$$f_m(x) = (m!)^{-1} \cdot \ln x + f_m(1) - g_m(1), \quad (18)$$

$$= \sum_{\tau=1}^m \frac{1}{\tau(m-\tau)! x^{\tau}}. \quad (19)$$

derived by developing the exponential under integrating by terms.

nts; for instance:

$$= 0.19066925 \text{ and } f_3(1) = 0.04635136 \quad (20)$$

to a recursion formula for the functions Fi

$$f(x) = Fi_m(x) - e^x x^{-m} + e, \quad (21)$$

ssed with Fi_1 and elementary transcendent part from an additive constant, equal to the integral \overline{Ei} :

$$-\overline{Ei}(1) = \overline{Ei}(x) - 1.895168. \quad (22)$$

$$\int_{-\infty}^{-\epsilon} e^t t^{-1} dt + \int_{+\epsilon}^{\infty} e^t t^{-1} dt. \quad (23)$$

enable a simple calculation of the expressions

In the region of large x it is sometimes convenient, in view of the slow convergence of the series (12)–(14) and the occurrence of nearly equal terms of opposite sign in (18) to use the known semi-convergent asymptotic expansions of the exponential integral.

Table 1 contains the results of the calculations. In figures 1 and 2 the energy E is plotted as function of the radius r_0 of the sphere in which the hydrogen atom lives. The dotted lines represent the asymptotic approximations of this paragraph.

TABLE I

r_0	E 1s level	E 2s level	E 2p level
∞	$-1/2$	$-1/8$	$-1/8$
20		-0.12499	-0.12500
15		-0.12451	-0.12477
10		-0.1162	-0.1194
9		-0.1118	-0.1169
8	-0.49997 ¹⁾	-0.1055	-0.1124
7	-0.49986 ¹⁾	-0.0974	-0.1058
6	-0.49927 ¹⁾		
5	-0.49655 ¹⁾		
4	-0.4852 ²⁾		
3	-0.4475 ²⁾		

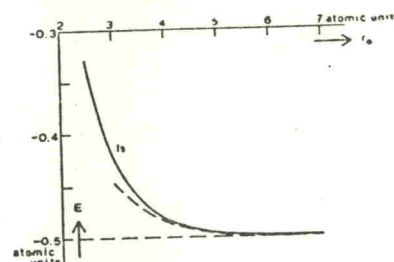


Fig. 1. Detail of the (E, r_0) -curve for the 1s level. The dotted line indicates the asymptote found by the method of Michels, De Boer and Bijl. The line $E = -0.5$ is also an asymptote.

The exact curves that will be calculated in next section are indicated by the symbols 1s, 2s and 2p. The deviations of the asymptotes calculated here from the real curve show where the approximative method is valid, when a certain accuracy is chosen. For the 2s and 2p levels the approximation is only applicable down to a value of r_0 , much larger than that for the 1s level.