

the 1s-level for $r_0 = 5, 6, 7$ and 8 atomic units, and Sommerfeld and Welker²⁾ applied the formula (12) to $r_0 = 3$ and 4 atomic units.

Numerical calculation of the sums, occurring in the expressions (12), (13) and (14) can be largely simplified, because it can be shown that they are related to the exponential integral, that has been tabulated⁵⁾. To prove this first of all it can be stated that the sums of equations (12) and (14) are of the general type

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

whereas the sum in (13) is equal to

$$xf_2(x) - f_1(x) + \frac{1}{2}x. \quad (16)$$

The functions $f_m(x)$ can be connected to the general "exponential integral", that will be represented here by the symbol Fi :

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

with the following relation

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

where g_m is a polynomial in x^{-1} :

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

The formula (18) can be derived by developing the exponential under integral sign of (17) and integrating by terms.

The sums $f_m(1)$ are constants; for instance:

$$f_1(1) = 0.59962032, \quad f_2(1) = 0.19066925 \quad \text{and} \quad f_3(1) = 0.04635136 \quad (20)$$

Partial integration leads to a recursion formula for the functions Fi of (17)

$$mFi_{m+1}(x) = Fi_m(x) - e^x x^{-m} + c, \quad (21)$$

so that Fi_m can be expressed with Fi_1 and elementary transcendent functions. Lastly Fi_1 is, apart from an additive constant, equal to the tabulated⁵⁾ exponential integral \overline{Ei} :

$$Fi_1(x) = \overline{Ei}(x) - \overline{Ei}(1) = \overline{Ei}(x) - 1.895168, \quad (22)$$

where

$$\overline{Ei}(x) = \lim_{\epsilon \rightarrow 0} \left(\int_{-\infty}^{-\epsilon} e^t t^{-1} dt + \int_{+\epsilon}^{\infty} e^t t^{-1} dt \right). \quad (23)$$

The formulae (15)-(22) enable a simple calculation of the expressions (12)-(14).