

Lower Limit for the Ground State of the Helium Atom

In a recent paper¹ I have derived an expression for a lower limit of the lowest energy level of a Schrödinger equation. In order to show how practical this expression was, it was evaluated for the case of helium with a hydrogen-like function. This turned out to involve an integral which I was not then able to evaluate, and what was thought to be a safe approximation of $(7/16)a^2$ was given. Through Mr. E. B. Wilson, Jr., however, I have obtained the exact value, which is $(2/3)a^2$. The result is that the lower limit is pushed so far down ($9.4 Rh$, experimental value $5.809 Rh$) that this simple example is of no value. This does not vitiate the expression theoretically inasmuch as it approaches the true value from the bottom as rapidly as the upper limit does from the top, but practically its usefulness is strongly impaired since more exact functions, such as those given by Hylleraas,² are required in order to get a reasonably close lower limit; and for these functions the computations are much more involved. So far, the computations have been carried out only for the worst function of a group given by Hylleraas.

¹ D. H. Weinstein, Phys. Rev. **40**, 797 (1932).

² E. A. Hylleraas, Zeits. f. Physik **54**, 347 (1929).

I have found an expression for a lower limit which is an improvement over the one originally given. We have in the same notation as before,

$$I_2 - I_1^2 = \sum_{n=0}^{\infty} (w_n - I_1)^2 a_n^2 \\ = (w_0 - I_1)^2 + \sum_{n=1}^{\infty} (w_n - w_0) \\ (w_n + w_0 - 2I_1) a_n^2.$$

If now $I_1 \leq (w_1 + w_0)/2$, Eq. (1a) will contain positive terms only. Hence, $I_2 - I_1^2 \geq (w_0 - I_1)^2$. Now since $I_1 \geq w_0$, $I_1 - (I_2 - I_1^2)^{1/2} \leq w_0$. This new lower limit is virtually an absolute lower limit since the restriction (2) is nearly always satisfied, and a theoretical discussion of it can be easily made.

It is also worth noting that $I_2 \geq I_1^2$ in general, as is obvious from Eq. (1).

If we use a hydrogen-like function we get $I_1 - (I_2 - I_1^2)^{1/2} = -7.6 Rh$, while the upper limit is $-5.5 Rh$. If we use the Hylleraas function $\xi = (1 + c_1 \rho^2) \exp(c_2 s)$ we obtain $-6.8 Rh$ for the lower limit and $-5.75 Rh$ for the upper limit. It is seen that, as expected, improving the function also improves the lower limit, which, however, does not approach the experimental value so rapidly as the upper limit.

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