CALCULATION OF THE DIAMAGNETIC SUSCEPTIBILITY OF HELIUM

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Submitted to JETP editor September 15, 1961

J. Exptl. Theoret. Phys. (U.S.S.R.) **42**, 820 (March, 1962)

It is shown that a more exact computation of the wave function for the helium atom does not remove the discrepancy noted by Bethe and Salpeter[1] between the theoretical and experimental values (based on magnetic data) of $\overline{r^2}$.

IN the discussion of the diamagnetism of helium it is pointed out in the book by Bethe and Salpeter[1] that the average value $\overline{r^2}$ for a single electron in the ground state of helium, which calculated with the aid of a Hartree wave function equals 1.19 atomic units, does not fully agree with the value derived from the latest experimental data for the diamagnetic susceptibility of helium ($\overline{r^2} = 1.220 \pm 0.006$ at. units).

As a test of whether the origin of this discrepancy lies in an inaccuracy of the wave function we calculated $\overline{r^2}$ with functions of the Hylleraas type obtained by Kinoshita[2]:

$$\Psi = e^{-s/2}\sum_{l,m,n} C_{lmn} s^{l-m} u^{m-n} t^n, \qquad s = r_1 + r_2,$$

$$t = r_1 - r_2, \qquad u = r_{12},$$

where C_{lmn} are the variational parameters, r_1 and r_2 the electron coordinates and l, m, n integers chosen in a well defined way. The calculation reduced to the computation of a sixfold sum which was evaluated with the help of a BÉSM-2 computer. With 80 variational parameters in the wave function, the value $\overline{r^2} = 1.1935$ was obtained. It is apparent that there is no significant change in $\overline{r^2}$ in comparison with the Hartree value.

If one assumes the electrons to be noninteracting, relativistic effects contribute a correction $\sim a^2Z^2 \sim 10^{-4}$ to the value of $\overline{r^2}$, which is insufficient to bring about agreement with experiment. (The correction due to nuclear motion is $\sim 5 \times 10^{-4}$.) Analytical Hylleraas type functions are not completely satisfactory,[3,4] (for example, functions with different numbers of parameters have differing asymptotic behavior at infinity). However this appears to affect $\overline{r^2}$ only weakly, since $\overline{r^2}$ changes only by 1×10^{-4} on going from 34 to 80 variational parameters. It seems therefore that the experimental value for the diamagnetic susceptibility of helium needs verification to find the source of the discrepancy between calculation and experiment.

We express our thanks to Ya. A. Smorodinskiĭ for a discussion of this work.

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[2] T. Kinoshita, Phys. Rev. **105**, 1490 (1957); Phys. Rev. **115**, 366 (1959).

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[4] J. H. Bartlett, Phys. Rev. **98**, 1067 (1955).

Translated by D. A. Uhlenbrock
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