Egil Hylleraas — A Pioneer of Computational Quantum Mechanics

Trygve Helgaker

Hylleraas Centre for Quantum Molecular Sciences, University of Oslo, Norway
trygve.helgaker@kjemi.uio.no

The Norwegian physicist Egil A. Hylleraas (1898–1965) helped usher in the era of scientific computing by carrying out accurate calculations on the helium atom, thereby confirming the validity of quantum mechanics for more than one particle [1], by predicting the stability of the hydrogen anion, later detected in the Sun's atmosphere [2], and by performing the first calculation of the cohesive energy of a molecular crystal, LiH [3]. Many of the methods and techniques introduced by Hylleraas in the 1920s and 1930s are still important today. In particular, his treatment of electron correlation forms the basis for modern explicitly-correlated electronic-structure methods and F12 techniques. Hylleraas also performed many quantum-mechanical studies of small molecules and presented, for example, the first calculations of nuclear magnetic shielding constants of a molecule in 1950 [4].

Egil Hylleraas was the founding father of quantum chemistry in Norway. Indeed, in a public lecture on the chemical bond given in 1933, he stated (translated from the Norwegian) [5]: 'In closing my presentation, I hope to have convinced the audience of the far-reaching opportunities that now exist for establishing a theoretical chemistry, a quantum chemistry, on the same footing as the physical quantum theory.'

In this talk, an overview is given of the life and career of Egil Hylleraas, with emphasis on his scientific contributions and their relevance for modern theoretical chemistry.

References

1. E. A. Hylleraas, *Z. Phys.* **54** (1929), 347
2. E. A. Hylleraas, *Z. Phys.* **65** (1930), 209
3. E. A. Hylleraas, *Z. Phys.* **63** (1930), 771
4. E. A. Hylleraas and S. Skavlem, Phys. Rev. **79** (1950), 117
5. E. A. Hylleraas, Chr. Michelsens Institutt for Videnskap og Åndsfrihet: Beretninger **3**, (Bergen 1933).