g-factor of H^-

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Nuclear magnetic shielding of a closed-shell atom can be expressed as the coupling of nuclear magnetic moment $\vec{\mu}$ with a homogeneous magnetic field $\vec{B}$ modified by the presence of atomic electrons, which is expressed in terms of the nuclear magnetic shielding constant σ

$$\delta H = -\vec{\mu} \cdot \vec{B}(1 - \sigma). \tag{1}$$

The most accurate theoretical predictions of nuclear magnetic shielding for light atomic and molecular systems can be obtained using NRQED theory [1, 2, 3]. In this theory, the nuclear magnetic shielding constant σ is expanded as a double series in the fine-structure constant α and the electron–nucleus mass ratio m/m_n

$$\sigma = \sigma^{(2,0)} + \sigma^{(2,1)} + \sigma^{(2,2)} + \sigma^{(4,0)} + \sigma^{(4,1)} + \sigma^{(5,0)} + \sigma^{(6,0)} + \ldots \tag{2}$$

where $\sigma^{(n,k)} \propto \alpha^n (m/m_n)^k$ in $\hbar = c = \epsilon_0 = 1$ units.

In this work, we present highly accurate calculations of the nuclear magnetic shielding constant of the ground state of the hydride ion (H^-). We calculate the relativistic $\sigma^{(4,0)}$ and (very often neglected) nuclear recoil $\sigma^{(2,1)}, \sigma^{(2,2)}$ corrections to the shielding constant. The latter are of particular importance in the H^- system because they are more significant than the relativistic effects. Including all these effects allows us to achieve a relative accuracy exceeding 10^{-9} for the nuclear magnetic shielding of the H^- system.

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References

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