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DIPARTIMENTO DI SCIENZE MATEMATICHE E INFORMATICHE, SCIENZE FISICHE E SCIENZE DELLA TERRA
Dottorato di Ricerca in Fisica

Appunti di Fisica '25

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Sala seminari, CNR-IPCF

Accurate determination of helium atom and hydrogen molecule properties using explicitly correlated functions

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Due to the limitations imposed by approximations in computational chemistry methods, theoretical results are typically obtained with significantly lower accuracy than precise spectroscopic experiments. Here, I refer to chemical accuracy, which generally corresponds to approximately 1 kcal·mol^{-1}. However, light atomic and molecular systems can be studied at an entirely different level of precision. Thanks to advancements in theoretical methods based on nonrelativistic quantum electrodynamics (NRQED) and computational approaches using explicitly correlated basis functions, theoretical predictions can now achieve an accuracy of approximately 1 MHz (9.5×10^{-8} kcal·mol^{-1}).

I will present recent progress in calculations concerning the hydrogen molecule and helium atom. We determined the leading order of the shielding constant for H_2, HD, and HT, enabling the precise determination of the deuteron and triton magnetic moments. For helium-3, we computed the QED correction to the shielding constant, reaching an accuracy that opens the possibility of establishing a new standard for absolute magnetometry. Additionally, I will discuss hydrogen molecule energy levels, where applying the QED correction to the HD dissociation energy led to a significant deviation of over 3σ from experimental values—a prediction that was later confirmed by a new experiment published four years later.