The Accurate Determination of Nuclear Multipole Moments in Heavy Elements

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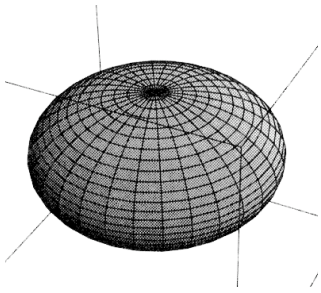
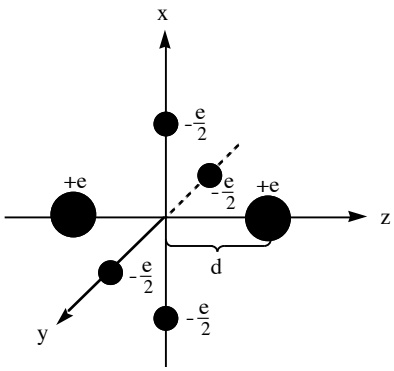


An important property of the atomic nucleus is the nuclear multipole moment. A very common way to get a high accuracy of the nuclear multipole moment (NQM) is the combination of rotational spectroscopy data with accurately calculated values for the electric field gradient tensor (EFG) on a quantum mechanical basis. The main goal is therefore the most accurate determination of the EFG including especially relativistic and electron correlation effects for heavy nuclei. Since a simplification of the four-component Dirac-Fock equation is highly desirable, a transformation to two-component forms like the Douglas-Kroll transformation is standard now in computational quantum physics. Unfortunately the transformation of the EFG or higher moment operators may yield essentially singular operators, this method may not be very useful. Moreover, current density functional theory is incapable to predict accurate EFGs and one relies on conventional wave-function based theory. Instead of transforming the EFG operator one calculates the expectation value of the untransformed operator using the transformed wave functions.



Clearly, this way of calculation must bear an error, which is called the picture change error. This picture change error is not present, of course, if one uses the fully four-component Dirac-Fock-Coulomb formalism, but this is computationally expensive. It is highly desirable then to account for most of the relativistic and correlation effects not including the picture change error which can be achieved by applying an arrangement of distributed charges around the core which cause an artificial NQM (see figure on the left). A variation of the charges varies the NQM and via the coupling through the EFG also the total electronic energy. According to perturbation theory the numerical differentiation of the total energy with respect to the artificially varied NQM immediately yields the EFG and therefore the NQM at the nucleus. The method does not include any picture change error because only integrals of the Coulomb type operators are evaluated which are transformed in the usual way. Higher moments and then importance of QED effects for EFGs are also discussed.