On the deformability of atoms†

T. Naito,[*1,*2] S. Endo,[*3,*4] K. Hagino,[*5] and Y. Tanimura[*3,*6]

Atoms and atomic nuclei share common features as quantum many-body systems of interacting fermions. In atoms, the inter-particle interaction is the repulsive Coulomb interaction, and there exists the spherical external Coulomb potential due to the nucleus. In contrast, in atomic nuclei, the inter-particle interaction is the attractive nuclear force, with no external potential. Despite the differences in the fundamental interactions, many similar properties have been observed in both systems, such as the shell structure and the associated magic numbers.

One of the most important properties of atomic nuclei is collective nuclear deformation. It was discussed that this collective deformation originates from the strong attractive interaction between protons and neutrons.[1,2] A natural question then arises: Can atoms be deformed collectively as in atomic nuclei? Calculations of the atomic structure have been frequently conducted by assuming spherical symmetry, and the non-sphericity has been addressed only in a few studies. Thus, it is widely believed that atoms are rather spherical, in stark contrast to deformed atomic nuclei. What is the physical origin of this difference? To what extent can electron density distributions in atoms be deformed collectively?

To answer these questions, we calculate electron density distributions of atoms and their deformation parameters without assuming spherical symmetry. By estimating the change in the energy induced by the deformation, in nuclear systems, we find that the spin-up and spin-down particles tend to be deformed in the same manner due to the attractive inter-particle nuclear interaction. In contrast, in atomic systems, we find that the spin-up and spin-down particles prefer to be deformed in the opposite manner, cancelling each other and resulting in a small deformation as a whole owing to the repulsive inter-particle Coulomb interaction. Thus, the difference between atoms and atomic nuclei in their deformability primarily originates from the different natures of the inter-particle interactions.

Figure 1 shows the deformation parameters β for atoms from Li to Kr calculated using the unrestricted Hartree-Fock method with the 6-31+G basis.[3] All the noble-gas atoms are spherical ($\beta = 0$). For the other atoms, the electronic configuration of their cores is the same as that of the noble-gas atoms. Hence, as long as the core density is not deformed owing to non-trivial many-body effects, the deformation of the atom is expected to result only from the valence electrons. The valence electrons of the s-block atoms only occupy an s orbital, and the many-body effects between the valence electrons and spherically symmetric core necessarily result in a spherical electron density distribution. This is also true for the half-closed-shell atoms.

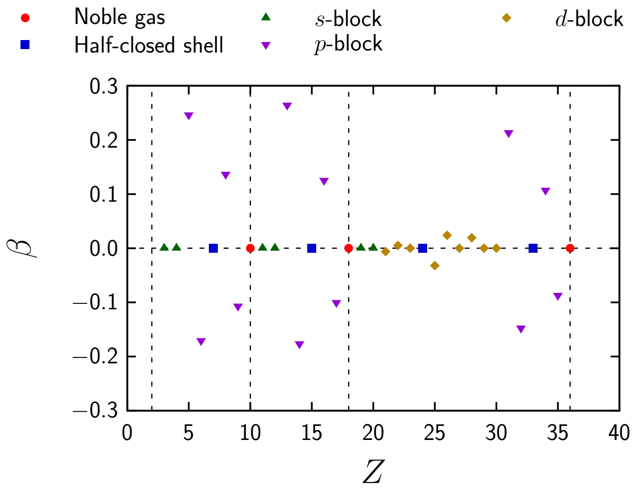

Fig. 1. Deformation parameters β calculated using the unrestricted Hartree-Fock method with the 6-31+G basis.

For the other open-shell atoms, the deformation parameters β are generally non-zero. The deformation parameters for the atoms with the same group exhibit similar tendencies, *i.e.*, $|\beta| \simeq 0.1$–0.3 for the p-block atoms and $|\beta| \lesssim 0.01$ for the d-block atoms. This indicates that the nature of the few valence open-shell electrons contributes significantly to determining β of the whole atom. This deformation originates from single-particle valence orbitals and thus it is misleading to regard it as collective deformation. For example, the deformation of the p-block atoms can be understood as the valence p orbitals that primarily contribute to the deformation. Indeed, $|\beta| \simeq 0.1$–0.3 of the p-block atoms are similar values in order of magnitude to that of a single p orbital, although $|\beta| \simeq 0.3$ might appear a large collective deformation in nuclear physics sense. We conclude in this paper that the p-block atoms can be regarded as an almost inert core plus valence p-electrons, while many-body effects between the core and the valence electrons are relevant in the d-block atoms. In the d-block atoms, the core electrons tend to collectively cancel the deformation of the valence d orbitals.

References

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*1 Department of Physics, University of Tokyo
*2 RIKEN Nishina Center
*3 Department of Physics, Tohoku University
*4 Frontier Research Institute for Interdisciplinary Science, Tohoku University
*5 Department of Physics, Kyoto University
*6 Graduate Program on Physics for the Universe, Tohoku University