Orbital swelling, breathing, fusion, fission and re-ordering in atoms under penetrable confinement

Valeriy K. Dolmatov

Department of Physics and Earth Science, University of North Alabama, One Harrison Plaza, Florence, Alabama 35632, The United States of America
vkdolmatov@una.edu

The structure and spectra of atoms, spatially confined by various types of confinements whose sizes are commensurable with an atomic size, have seized minds of theorists starting since early days [1,2] to now (see review papers [3-6] and references therein). To date, numerous aspects of the structure and spectra of atoms under various kinds of confinements - impenetrable, open boundaries, spheroidal, conoidal, Deby-like, C_{60}-like, *etc*. - have been attacked from different angles by many research teams [3-6]. This is because a confined atom concept provides insights into various aspects of interdisciplinary significance, such as, e.g., atoms under high pressure, quantum dots, atoms in a plasma environment, *etc*.

The present contribution focuses on the author's recent study of the structure of atoms under a repulsive spherical potential of an inner radius r_0, finite thickness Δ and height U_0. There, a variety of spectacular effects have been theoretically uncovered in the structure of thus confined atoms with increasing pressure (decreasing r_0). They are reviewed below.

It is the ultimate aim of this conference contribution to demonstrate that, as the radius r_0 of the confining potential is progressively decreasing, the structure of confined atom starts developing such spectacular effects as orbital swelling (one or more of the atomic orbitals suddenly swell(s) rather than keep(s) shrinking in size, when r_0 falls below a certain critical value), orbital breathing (alternate drastic expansions and contractions of one or more of the atomic orbitals with decreasing r_0), orbital fusion (both the energies and radial functions of two certain orbitals become equal through some range of r_0 values), orbital fission (the two fused together orbitals separate once again in a different range of r_0 values), as well as orbital re-ordering (the order of orbitals in the atom changes with varying r_0). The above reviewed effects will be illustrated by calculated data performed for confined atoms with semifilled subshells, namely, H(1s), Li($1s^2 2s^1$), N($2s^2 2p^3$), P($3s^2 3p^3$) and Cr($3d^5 4s^1$).

It is argued in this contribution that such effects as *orbital fusion* and *fission* are characteristic effects of specifically atoms with semifilled subshells. As for the rest of the discussed effects, the author sees no reason preventing them for emerging in arbitrary structured atoms as well.

This work was supported by the RUI NSF grant No.PHY-0969386. A partial travel support provided by the UNA CAS grant award No.42914 is gratefully acknowledged.

References:
[1] A. Michels, J. de Boer and A. Bijl, Physica **4**, 981 (1937).
[2] A. Sommerfeld and H. Welker, Ann. Phys. **32**, 56 (1938).
[3] W. Jaskólski, Phys. Rep. **271**, 1 (1996).
[4] V. K. Dolmatov, A.S. Baltenkov, J.-P. Connerade and S.T. Manson, Radiat. Phys. Chem. **70**, 417 (2004).
[5] J. R. Sabin, E. Brändas and S. A. Cruz (ed), Advances in Quantum Chemistry: *Theory of Confined Quantum Systems*: Part 1 vol. **57** (New York: Academic) p.p. 1-334 (2009).
[6] J. R. Sabin, E. Brändas and S. A. Cruz (ed), Advances in Quantum Chemistry: *Theory of Confined Quantum Systems*: Part 2 vol. **58** (New York: Academic) p.p.1-297 (2009).