Ionization mechanisms of captive atoms struck by light matter

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Light interacting with hydrogen atoms enclosed in hollow cages composed of carbon atoms - referred to as fullerene material - produces ionisation. This phenomenon, which has been the subject of intense theoretical scrutiny, is particularly interesting because the light rays can have dramatic effects in inducing small external energy potentials. Specifically, they alter the structural and dynamic properties of the atoms confined within the fullerene molecule. Ana Frapiccini from the CONICET research centre at the Universidad Nacional del Sur, in Bahía Blanca, Argentina, and colleagues have just published a study in *EPJ D* explaining the theory behind the ionisation. Applications of this process include drug delivery, quantum computation, photovoltaics and hydrogen storage.

In this study, the authors have developed a methodology to solve the Schrödinger equation describing the behaviour, over time, of an atom interacting with an external light pulse. This yields a theoretical description of how external light rays affect the energy levels of the hydrogen atoms trapped inside the fullerenes. By solving the equation, the authors have successfully transformed the problem into a much simpler equation, which accounts for the scattering effect of light on the captive atoms.

Thus, they turned their attempt to arrive at a theoretical understanding of ionisation into a study of a simpler semi-empirical model of the energy potentials - which are local, spherically symmetric, and considered to be constant.

Frapiccini and colleagues thus reveal in this study key aspects of the ionisation process on atoms trapped inside a fullerene molecule. The authors then test their theory using an application based on studying the influence of the confinement of a hydrogen atom in fullerene cages of two different sizes; namely C36 and C60. They conclude that the fullerene cage acts as a captor for the electron, which is ionised inside the cage, when subjected to a laser pulse of the same intensity as the difference between the lower energy levels.

More information: Ana Laura Frapiccini et al, Generalized Sturmians in the time-dependent frame: effect of a fullerene confining potential, *The European Physical Journal D* (2017). DOI: 10.1140/epjd/e2017-70686-8

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