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Extended Abstract

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Topological study of the H3 ++ molecular system: H3 ++ as a cornerstone for building molecules during the Big Bang

Michael Baer

The Hebrew University of Jerusalem, Israel
E-mail: michaelb@fh.huji.ac.il

The present study is devoted to the possibility that tri-atomic molecules were formed during or shortly after the Big Bang. For this purpose we consider the ordinary H3 + and H3 molecular systems and the primitive tri-atomic molecular system, H3 ++, which, as is shown, behaves differently. The study is carried out by comparing the topological features of these systems as they are reflected through their non-adiabatic coupling terms. Although H3 ++ is not known to exist as a molecule, we found that it behaves as such at intermediate internal distances. However, this illusion breaks down as its asymptotic region is reached. Our study indicates that whereas H3 + and H3 dissociate smoothly, the H3 ++ does not seem to do so. Nevertheless, the fact that H3 ++ is capable of living as a molecule on borrowed time enables it to catch an electron and form a molecule via the reaction H3 ++ + e Y H3 + that may dissociate properly: Thus, the two unique features acquired by H3 ++, namely, that it is the most primitive system formed by three protons and one electron and topologically, still remain for an instant a molecule, may make it the sole candidate for becoming the cornerstone for creating the molecules. Corollary – NACTs as Gluons: In order to discuss the buildup of protons Gell-mann and Zweig suggested that Hadrons (e.g. protons) are made out of smaller particles called Quarks. Quarks (usually three of them) are assumed to be hold together by particles - Gluons - that convey the force among them. In the present case, we face a similar problem, viz., building-up a molecular system out of protons and electrons. Indeed the Born-Oppenheimer-Huang (BOH) approach supplies us with the means to build the required magnitudes- the NACTs - as discussed in the above Molec. Phys. Article. Thus, the NACTs stand for the gluon that enforces the nuclei to form the molecule.

The foremost purpose of the numerical treatment is to reveal to what extent this possibility can be justified, at least topologically. The present study revealed the tendency of this molecule to form spiky NACTs to the level of Dirac-δ functions. Mathematically this implies that the molecular system at stake, most likely, loses its electron and breaks-up into three protons before reaching, chemically, its asymptotic 15 region. If indeed that happens, the chemical dissociative process is inhibited and such a The foremost purpose of the numerical treatment is to reveal to what extent the H3 ++ molecular system differs from the H3 and H3 + systems, mainly topologically but eventually also in other ways. The means to carry out this study are the NACTs calculated along closed circular contours formed by the various equilateral cis. From the results presented in Tables V and VI the two systems, H3 and H3 + , respectively, are behaving smoothly all the way from the internal regions of the CS up to the asymptotic ones. Mathematically this implies that the relevant Schrödinger-BOH equations for these systems can be solved along the whole CS for any foresee/anticipative set of asymptotic conditions. The H3 ++ does not seem to behave like that at all. While watching the NACTs produced at CSs surrounding different D3h points the following is revealed: (i) The D3h NACTs are 14 significantly affected while moving from the internal region towards the asymptotic one(ii) Once the asymptotic region is reached we find, that the smoothly behaving NACTs formed in the internal regions are replaced by spiky NACTs to the level of becoming Dirac-δ functions. Thus, summarizing the findings regarding the H3 ++ molecular system, the following can be said: Although along the intermediate regions of CS the behavior of this system as reflected via the contour-dependent NACTs is bearable, we encounter essentially a non-molecular conduct at its asymptotic region In the present article three molecular systems are studied– two of them, H3 and H3 + – are characteristic prototypes for chemical systems and thus both are capable of forming di-atom molecules following scattering exchange processes or also, as in case of H3 + , (36) form either, H2 or H2 + , via dissociation. In contrast, the third molecular system, H3 ++ behaves differently: following the present study it looks like that H3 ++, is not capable of reaching its asymptotic region and therefore once created will not be able to dissociate and form its (just) two constituents. namely (H2 + ,H+). The only way it may dissociate is by absorbing an electron and forming NACTs typical for an ordinary molecule via the reaction H3 ++ + e → H3 + that now may dissociate properly, in the form: 2 3 2 H H H H H + + + ⌈ + → ⌊ + thus yielding ordinary di-atoms or di-atomic ions. At this stage we return to the Introduction in which we mentioned that according to Hawking molecules seemed to appear too early. In the present chapter we try to use the findings revealed earlier in order examine molecule, is not capable to behave chemically. This study was performed with the aim of showing that, eventually, tri-atomic molecules could be formed during at or shortly after the Big Bang. In the present study we referred to the more primitive tri-atomic molecular system, H3 ++, for which we showed that although it satisfies, up to a certain level, topological features as required by the BOH theory it cannot be considered as a normal molecule because its chemical asymptotic region is essentially out of reach. Still its two unique features, namely, being formed by three protons and one electron and behave as a molecule - topologically - on borrowed time makes it a candidate for becoming the cornerstone to form molecules.

Bottom Note: *This work is partly presented at 5th World Congress on Physics July 17-18, 2018, Prague, Czech Republic*