

Electronic Structure of Fractionally Nuclear Charged Atoms

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Diferentes propriedades da química de quarks são estudadas por cálculos *ab initio* Hartree-Fock em átomos com carga nuclear fracionária. Os estados fundamental e excitado de átomos de sódio com quarks ligados ao núcleo são obtidos usando cálculos de interação de configuração. Este estudo sugere que a transição eletrônica ${}^2P \rightarrow {}^2S$ no sódio pode ser usada como guia para observação de quarks não confinados. A variação da energia de ligação eletrônica com a carga nuclear para a série isoeletrônica de átomos com carga nuclear fracionária $A^{\pm 2/3}$ e $A^{\pm 1/3}$ ($A = H, Li, Na, P$ and Ca) foi analisada. Os cálculos apresentados sugerem, que os quarks não confinados preferem se ligar a núcleos pesados, e que o par quark-antiquark poderia ser estabilizado na presença da matéria atômica.

Different properties of quark chemistry are studied by performing accurate *ab initio* Hartree-Fock calculations on fractionally nuclear charged atoms. Ground and first excited states of sodium atoms with quarks attached to the nucleus are obtained using CI calculations. It is suggested that the sodium ${}^2P \rightarrow {}^2S$ electronic transition can be used as a guide in searching for unconfined quarks. Also, the variation of the binding electronic energy with nuclear charge in the isoelectronic series of fractionally nuclear charged atoms $A^{\pm 2/3}$ and $A^{\pm 1/3}$ ($A = H, Li, Na, P$ and Ca) is analyzed. The present calculations suggest that unconfined colored particles have large appetite for heavy nuclei and that quark-antiquark pairs could be stabilized in presence of the atomic matter.

Keywords: *ab initio* calculations, fractionally nuclear charged atoms, quark chemistry

Introduction

Quantum chromodynamics (QCD) gives a correct phenomenological description of the strong and electroweak interactions, however experimental evidence for quarks is only indirect, being obtained from the properties of hadrons.¹ There are theoretical and experimental evidence that particles having color cannot exist as free entities, but are confined to the interior of hadrons. Although no laboratory experiment has so far liberated a quark from a nucleon, this is not a statement that unconfined quarks do not exist in a stable matter. There may be, e.g., a tiny concentration of primordial quarks that have not found their partners in the expanding Big Bang universe.² Several experiments have been carried out to look for unconfined quark in matter.²⁻⁹ In these search quark experiments, it is important to know the behavior of unconfined quarks in the stable matter, that is, the so-called *quark chemistry*.² By applying quantum mechanics to describe the interaction of a $\pm 1/3e$ or $\pm 2/3e$ electrical charge with the atomic matter,

it is possible to get some useful information on this quark chemistry. In addition, there is the inherent interest to study these exotic systems, which poses new and stimulating questions in computational quantum chemistry.

The hypothesis of unconfined quarks raises the question of where they reside in the real world. A conjecture is that the quark is surrounded by an electron cloud interacting with atoms and molecules or crystals.^{2,9-12} Another possibility is that quarks will absorb baryons from ordinary matter forming quark nucleon complexes.² In this case, atoms with fractionally nuclear charge can be formed.^{2,3,5,11,12} Indeed, it is argued that unconfined quarks must have large nuclear appetite,¹⁰ which may be a reason to consider them as being associated with nuclei. The fractional quark charge in the nucleus of an atom modifies their electronic structure and an appropriated spectroscopic technique should be able to detect this change and assign transitions between quark-atom energy levels. In this paper, the ${}^2P \rightarrow {}^2S$ electronic transition (the D yellow sodium lines) is used as a guide in searching anomalous electronic transitions due to the presence of quarks attached to the nucleus. Total energy calculations of the fractionally nuclear charged H, Li, Na,

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P and Ca atoms indicate that quarks prefer to be bound with nucleus of heavy atoms. The variation of the binding energy with the nuclear charge and some other aspects of the quark chemistry are also discussed in results and discussions section.

Computational Details

Electronic structure calculations of fractionally nuclear charge atoms requires an appropriated choice of wavefunctions in order to take into account the peculiarities of these exotic systems. Here we use the generator coordinate method¹³ to design new basis set for the atomic systems. We maintain the 6-311G set of contracted basis in internal regions and include diffuse¹⁴ and polarization¹⁵ functions in external regions. In sodium case the purpose is to reproduce exactly the first D line (5896 Å). Electronic correlation effects are included by performing configuration interaction (CI) calculations with single, double, triple and quadruple excitations. For calculation of electronic transitions, where we consider differences in total energy, the so-called differential correlation effects are considered. The GAUSSIAN 98 program is used in all calculations.¹⁶

Results and Discussions

Total energies for the systems $\text{Na}^{+2/3}$, $\text{Na}^{+1/3}$, Na , $\text{Na}^{-1/3}$ and $\text{Na}^{-2/3}$ are given in Table 1. The fractional ionic charges in these systems reflect the quark (or antiquark) $\pm 1/3e$ or $\pm 2/3e$ charge added to the sodium nuclei. Each system contains 11 electrons and corresponds to a bound state.

Table 1. Total energy and ${}^2\text{P} \rightarrow {}^2\text{S}$ transition for sodium and quark-sodium systems

Z	State ${}^2\text{S}$ (a.u.)	State ${}^2\text{P}$ (a.u.)	${}^2\text{P} \rightarrow {}^2\text{S}$ transition (Å)
11.666	-185.7585139	-189.3493139	3453
11.333	-173.2188732	-174.7132732	4411
11.000	-161.1172950	-163.2200950	5896
10.666	-149.4535019	-150.9479019	8297
10.333	-138.2260326	-139.2148326	12539

CI calculations of the ${}^2\text{P} \rightarrow {}^2\text{S}$ electronic transition yield a wavelength of 5896 Å, which reproduces exactly the first sodium D line and is 6 Å away from the second yellow line, *i.e.*, an error about 0.1% (as relativistic effects such as spin-orbit coupling are not included in the calculations, only one transition energy is obtained). The accurate wavelengths calculated here can be a guide in search-for-quarks spectroscopic experiments. For example, the D line of the $\text{Na}^{+1/3}$ system lies in the violet region (4411 Å) and the

observance of this line would be indication of a $+1/3$ -quark attached to the nucleus.

Table 1 shows that the wavelength increases by decreasing the nuclear charge, indicating that the energy levels of the same principal quantum number (3s, 3p, 3d) approach each other for the negative $\text{Na}^{-1/3}$ and $\text{Na}^{-2/3}$ systems. Table 1 also shows that the variation of total energy is larger for the positive quark as compared to the corresponding negative quark. This is consistent with the fact that the total binding energy varies as $E = -kZ^\alpha$ (Z is the total nuclear charge, not just the number of protons) with $\alpha \geq 2$ (for Hydrogen $\alpha = 2$). Considering electronic binding energy for atoms from $Z = 1$ to 20, including $Z \pm 1/3$ and $Z \pm 2/3$ nuclei, we obtain $\alpha = 2.39$ (Figure 1).

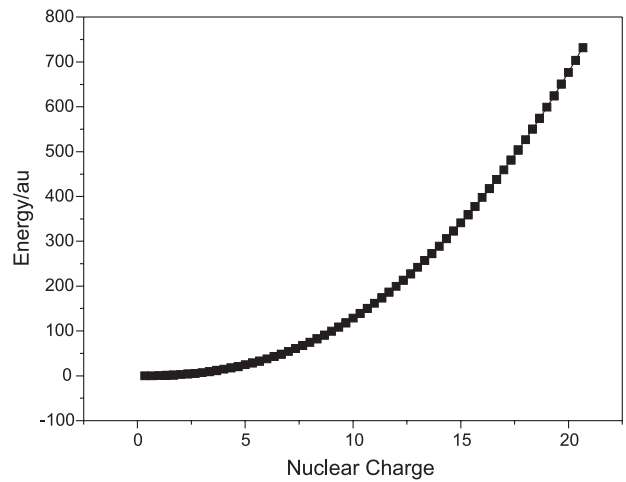


Figure 1. Electronic binding energy versus nuclear charge.

There are other consequences of the nonlinear dependence of the binding energy with the nuclear charge. In QCD, the vacuum state can be described as the lowest energy condensate state of gluons and quark-antiquark pairs. A primary creation process occurs when a quark-antiquark pair is produced by a gluon:



As the pair separates and becomes energetically favorable, another pair is created. This process goes until the hadron limit, where quarks are confined. When the mean separation between these particles exceeds the hadron limit, quarks are free. In this circumstance, if atomic matter is present we can consider formation of quark atoms according the equation:



where A is a neutral atom, Aq and A \bar{q} are fractionally nuclear

charged atoms with opposite ion charge. Considering the Z^a dependence, the reaction for the Aq and $A\bar{q}$ formation (equation 2) will be an exothermic process. Here we are neglecting the color interaction, which overwhelms all the energies considered here. However, our purpose is to analyze only the atom-quark electronic interaction and consequences of the Z non-linear dependence of binding energy. Table 2 shows the amount of energy liberated (ΔE) when the quark-antiquark pair interacts with H, Li, Na, P and Ca atoms.

Table 2. Energy released in equation 2 for different atoms

System	ΔE (eV) u, \bar{u}	ΔE (eV) d, \bar{d}
H	-12.09	-3.02
Li	-25.90	-6.56
Na	-47.65	-11.91
P	-54.51	-13.63
Ca	-66.07	-14.23

We can observe that ΔE increases from Hydrogen to Calcium. Then, more energy is released as the nuclear charge is increased, indicating that quarks prefer to bound with nuclei of heavy atoms, in agreement with predictions of De Rújula *et al.*¹⁰ Another consequence of the negative signal of ΔE is that atomic matter stabilizes the quark-antiquark pair in relation to the condensate gluon state, which favors the hadron formation process.

Conclusions

The electronic structure of fractionally nuclear charged atoms is investigated using CI calculations. Even though more sophisticated calculation could affect the present numerical results and interpretations, our calculated ${}^2P \rightarrow {}^2S$ electronic transition for quark-sodium atoms illustrates how usual methods of quantum chemistry can be useful in searching for unconfined quarks. In addition, the electronic energy calculations of fractionally nuclear charged atoms produce new information on the interaction of quarks with the atomic matter, not generally considered by researchers in this area. Our results suggest the possibility that unconfined quarks have preference for heavy nuclei and that quark-antiquark pairs could be stabilized in the interaction with the atomic matter.

Acknowledgments

The authors would like to acknowledge Professor Ricardo Ferreira for his incentive to continue our research

on exotic systems. The financial support is from CNPq and CAPES Brazilian agencies.

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Received: September 2, 2007

Published on the web: February 27, 2008