Efficient evaluation of the non-linear vacuum polarization density in the finite basis Dirac problem

Maen Salman and Trond Saue

Laboratoire de Chimie et Physique Quantique, UMR 5626 CNRS Université Toulouse III-Paul Sabatier, 118 Route de Narbonne, F-31062 Toulouse, France

In this work, we propose an efficient and accurate method to compute $\alpha (Z\alpha)^{n\geq 3}$ vacuum polarization density of hydrogen-like atoms, within the finite basis approximation of the Dirac equation. In order to prove the functionality of our computational method, we choose to work with the one-electron uranium atom. In summary, we find that the compliance to charge conjugation symmetry is necessary to obtain physical results that are in line with our knowledge of the analytical (exact) problem, as indicated in [1], in addition to Grant and Quiney in [2]. We also note that the final results are found to be in excellent agreement with previous formal analytical (and numerical) evaluations, done by Soff, Mohr and Plünien in [3, 4], as shown in figure (1). Our technique can be easily and efficiently implemented in codes that solve the radial Dirac equation in the finite basis set framework and could be employed for atomic problems with arbitrary (radial) nuclear charge distribution. The obtained numerical results of the non-linear vacuum polarization density are, therefore, automatically accounting for the extended nuclear size effect. This method is hence of special importance for atomic problems with nuclear distributions whose analytical expressions of their associated Dirac Green's functions are not in hand or have relatively complicated analytical forms.



Figure 1: Non-linear VP density of a shell nucleus with Z = 92 and $r_{nuc.} = 5.86$ fm.

^[1] Maen Salman, Doctoral dissertation at Université Paul Sabatier-Toulouse III (2022).

^[2] Ian Grant and Harry Quiney, Atoms 10(4) (2022) 155.

^[3] Gerhard Soff and Peter Mohr, Phys. Rev. A 38 (1988) 5066-5075.

^[4] Peter Mohr, Günter Plunien, and Gerhard Soff, Phys. Rep. 293(5-6) (1998) 227-369.