Calculating the many-potential vacuum polarization density of the Dirac equation in the finite-basis approximation

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European Research Council
Established by the European Commission

Abstract

In this work, we propose an efficient and accurate computational method to evaluate the many-potential $\alpha\,(Z\alpha)^{n\geq 3}$ vacuum polarization density of hydrogen-like atoms within the finite-basis approximation of the Dirac equation. To prove the performance of our computational method, we choose to work with the one-electron $^{238}_{92}$U atom. In summary, we find that compliance with charge conjugation symmetry is a priori required to obtain physical results that are in line with our knowledge of the analytical problem. We also note that the final numerical results are found to be in excellent agreement with previous formal analytical (and numerical) evaluations that are limited to a few simple nuclear distribution models. Our technique can be efficiently implemented and evaluated in codes that solve the radial Dirac equation in the finite basis set framework and allows the use of arbitrary (radial) nuclear charge distribution. The obtained numerical results of the non-perturbative vacuum polarization density automatically account for the extended nuclear size effect. This method is hence of special importance for atomic Dirac problems whose analytical Green's functions expressions are not at hand or have relatively complicated analytical forms.

Theory

The vacuum polarization (VP) four-current can be written as a

$$J^{\text{VP}}_{\mu}(x) = i\hbar e c \text{Tr}\left[\gamma_\mu S^F_A(x,y)\right]_{y\to x}, \tag{1}$$

where $x = (ct, \boldsymbol{x})$ and $S^F_A(x,y)$ is the Feynman propagator (time-ordered propagator) solving the inhomogenous linear differential equation

$$\left[\gamma^\mu\left(i\hbar\partial_\mu + eA^{\text{ext.}}_\mu(x)\right) - mc\right] S^F_A(x,y) = \delta^4(x-y), \tag{2}$$

in the presence of an external four-potential $A^{\text{ext.}} = (\phi^{\text{ext.}}/c, \boldsymbol{A}^{\text{ext.}})$. In the case where the external potential is time-independent, the VP four-current reads

$$J^{\text{VP}}_{\mu}(\boldsymbol{x}) = \left(c\rho^{\text{VP}}, -\boldsymbol{J}^{\text{VP}}\right) = \frac{ec}{2}\Big[\sum_{E_n>0}\bar{\psi}_n(\boldsymbol{x})\gamma_\mu\psi_n(\boldsymbol{x}) - \sum_{E_n<0}\bar{\psi}_n(\boldsymbol{x})\gamma_\mu\psi_n(\boldsymbol{x})\Big], \tag{3}$$

where $\bar{\psi}_n = \psi^\dagger_n\gamma^0.\psi_n(\boldsymbol{x})$ and E_n form an eigensolution of the time-independent Dirac equation

$$\left[c\boldsymbol{\alpha}\cdot\left[-i\hbar\boldsymbol{\nabla} + e\boldsymbol{A}^{\text{ext.}}(\boldsymbol{x})\right] + \beta mc^2 - e\phi^{\text{ext.}}(\boldsymbol{x})\right]\psi_n(\boldsymbol{x}) = E_n\psi_n(\boldsymbol{x}). \tag{4}$$

In the absence of an external vector potential $\boldsymbol{A}^{\text{ext.}}$ and using $\mathcal{T}$-symmetry, we have shown that the VP three-current must vanish. We shall now focus on the static VP density cloud, represented by

$$\rho^{\text{VP}}(\boldsymbol{x}) = \frac{e}{2}\Big[\sum_{E_n>0}\psi^\dagger_n(\boldsymbol{x})\psi_n(\boldsymbol{x}) - \sum_{E_n<0}\psi^\dagger_n(\boldsymbol{x})\psi_n(\boldsymbol{x})\Big], \tag{5}$$

forming around (and inside) a radial nucleus of normalized charge distribution $\rho^{\text{n}}(\boldsymbol{x})$ that generates a scalar potential

$$-e\phi^{\text{ext.}}(\boldsymbol{x}) = -(Z\alpha)\hbar c\int d^3y\frac{\rho^{\text{n}}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{6}$$

Radial Dirac problem

In spherical symmetry, i.e. when the nuclear distribution becomes radial $\rho^{\text{n}}(\boldsymbol{x}) = \rho^{\text{n}}(r)$, the Dirac spinor can be written as

$$\psi_{n,\kappa,m_j}(\boldsymbol{x}) = \frac{1}{r}\begin{bmatrix} P_{n,\kappa}(r)\,\Omega_{\kappa,m_j}(\hat{\boldsymbol{x}}) \\ iQ_{n,\kappa}(r)\,\Omega_{-\kappa,m_j}(\hat{\boldsymbol{x}})\end{bmatrix}, \tag{7}$$

where Ω_{κ,m_j} are the two-component spherical spinors, and the radial functions $P_{n,\kappa}$ and $Q_{n,\kappa}$ form a solution of the radial Dirac (eigenvalue) equation

$$\begin{bmatrix} mc^2 - e\phi^{\text{ext.}}(r) & -c\hbar\left[\frac{d}{dr} - \frac{\kappa}{r}\right] \\ c\hbar\left[\frac{d}{dr} + \frac{\kappa}{r}\right] & -mc^2 - e\phi^{\text{ext.}}(r)\end{bmatrix}\begin{bmatrix} P_{n,\kappa} \\ Q_{n,\kappa}\end{bmatrix} = E_{n,\kappa}\begin{bmatrix} P_{n,\kappa} \\ Q_{n,\kappa}\end{bmatrix}. \tag{8}$$

Using angular summation relations over product of spherical spinors, one can show that the total VP density of Eq.(5) can be written as (see Ref. [1])

$$\rho^{\text{VP}}(\boldsymbol{x}) = \sum_{\kappa=\pm1,\pm2\ldots}\rho^{\text{VP}}_\kappa(\boldsymbol{x}) \tag{9}$$

$$\rho^{\text{VP}}_\kappa(\boldsymbol{x}) = \frac{e\,|\kappa|}{4\pi}\frac{1}{r^2}\sum_n \text{sgn}\left(E_{n,\kappa}\right)\rho_{n,\kappa}(r), \tag{10}$$

where $\rho_{n,\kappa} = P^2_{n,\kappa} + Q^2_{n,\kappa}$ is the radial probability density associated with the n-th solution of the κ problem. The VP densities $\rho^{\text{VP}}_{\pm\kappa}(\boldsymbol{x})$ must be computed in pairs as

$$\rho^{\text{VP}}_{|\kappa|}(\boldsymbol{x}) = \rho^{\text{VP}}_{+\kappa}(\boldsymbol{x}) + \rho^{\text{VP}}_{-\kappa}(\boldsymbol{x}), \tag{11}$$

due to the large cancellation between $\pm\kappa$ contributions. In the free-particle problem ($Z = 0$), the total VP density must vanish due to the total cancellation of these VP densities.

Finite basis approximation

The finite basis set scheme suggests solving the radial eigenvalue problem of Eq.(8) by expanding the radial spinor in a finite set of basis functions. We have considered two main schemes:

1. The kinetic balance (KB) construction, where the radial Dirac wavefunction expands as

$$\begin{bmatrix} P_{n,\kappa} \\ Q_{n,\kappa}\end{bmatrix} \approx \varphi^{\text{KB}}_{n,\kappa} = \sum_{i=1}^{n^+_\kappa} c^+_{n,\kappa,i}\begin{bmatrix}\pi^+_{\kappa,i} \\ 0\end{bmatrix} + \frac{\hbar}{2mc}\sum_{i=1}^{n^-_\kappa} c^-_{n,\kappa,i}\begin{bmatrix} 0 \\ \left[\frac{d}{dr} + \frac{\kappa}{r}\right]\pi^+_{\kappa,i}\end{bmatrix}, \tag{12}$$

   widely used in molecular calculations and biased towards positive-energy solutions (PES).
2. The dual kinetic balance (DKB) construction, introduced by Shabaev *et al.* in Ref. [2], giving

$$\begin{bmatrix} P_{n,\kappa} \\ Q_{n,\kappa}\end{bmatrix} \approx \varphi^{\text{DKB}}_{n,\kappa} = \sum_{i=1}^{n^+_\kappa} c^+_{n,\kappa,i}\begin{bmatrix}\pi^+_{\kappa,i} \\ \frac{\hbar}{2mc}\left[\frac{d}{dr} + \frac{\kappa}{r}\right]\pi^+_{\kappa,i}\end{bmatrix} + \sum_{i=1}^{n^-_\kappa} c^-_{n,\kappa,i}\begin{bmatrix}\frac{\hbar}{2mc}\left[\frac{d}{dr} - \frac{\kappa}{r}\right]\pi^-_{\kappa,i} \\ \pi^-_{\kappa,i}\end{bmatrix}, \tag{13}$$

   providing a democratic description between positive- and negative-energy solutions.

In the present work, we have employed the large- and small-component Gaussian (basis) functions

$$\pi^+_{\kappa,i}(r) = r^{|\kappa+\frac{1}{2}|+\frac{1}{2}}e^{-\zeta^+_{\kappa,i}r^2} \tag{14}$$

$$\pi^-_{\kappa,i}(r) = r^{|\kappa-\frac{1}{2}|+\frac{1}{2}}e^{-\zeta^-_{\kappa,i}r^2}. \tag{15}$$

These radial functions follow the right behavior of the exact wavefunctions $P_{n,\kappa}$ and $Q_{n,\kappa}$ in the finite nuclear distribution case. We need to carefully select sets of exponents $\{\zeta^\pm_{\kappa,1},\ldots,\zeta^\pm_{\kappa,n^\pm_\kappa}\}$ that effectively cover the relevant radial range. In addition, we have shown that the:

1. RKB construction can be made $\mathcal{C}$-symmetric iff one uses the free-particle Dirac solutions (spherical Bessel functions) as basis functions.
2. DKB construction can be made $\mathcal{C}$-symmetric if one forces large and small functions to obey $\pi^+_{\pm\kappa,i} = \pi^-_{\mp\kappa,i}$, meaning that for Gaussian functions of Eqs.(14 and 15) we must set $\zeta^\pm_{\kappa,i} = \zeta^\mp_{-\kappa,i}$.

Numerical calculations

Our VP density ρ^{VP}_κ of Eq.(10) can be expanded in powers of the external potential (Z) as

$$\rho^{\text{VP}}_\kappa(\boldsymbol{x};Z) = \sum_{n=0}^{\infty}\rho^{\text{VP},n}_\kappa(\boldsymbol{x};Z) \quad \text{where} \quad \rho^{\text{VP},n}_\kappa(\boldsymbol{x};Z) = \frac{\partial^n}{\partial Z^n}\rho^{\text{VP}}_\kappa(\boldsymbol{x};Z)\Big|_{Z=0}\frac{Z^n}{n!}. \tag{16}$$

The bound-electron interaction with this VP density is represented in Fig. (1). Recall from Furry's theorem (Ref. [3]) that fermion loops with an odd number of vertices (even n) must yield a vanishing contribution. Moreover, the VP process that is linear in Z (containing the Uehling process) is logarithmically divergent. We eliminate this divergence by computing the many-potential VP density

$$\rho^{\text{VP},n\geq3}_\kappa(\boldsymbol{x};Z) = \rho^{\text{VP}}_\kappa(\boldsymbol{x};Z) - \rho^{\text{VP},1}_\kappa(\boldsymbol{x};Z) \tag{17}$$

$$\rho^{\text{VP},1}_\kappa(\boldsymbol{x};Z) = \lim_{\delta\to0}\frac{Z}{\delta}\left[\rho^{\text{VP}}_\kappa(\boldsymbol{x};\delta) - \rho^{\text{VP}}_\kappa(\boldsymbol{x};0)\right]. \tag{18}$$

To test our technique, we chose to work with the shell nucleus model, represented by the nuclear distribution $\rho^{\text{n}}(\boldsymbol{x}) = \delta(r-r_{\text{n}})/4\pi r^2_{\text{n}}$ with $r = 5.86$ fm for the hydrogen-like uranium atom ($Z = 92$).

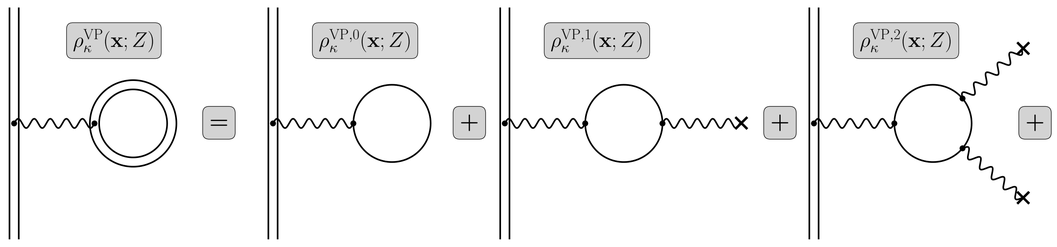
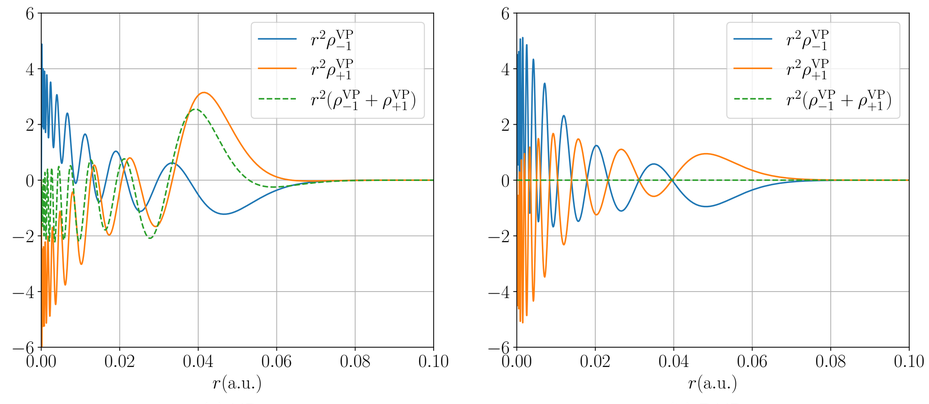


Figure 1. Bound-state VP density expanded in powers of Z.

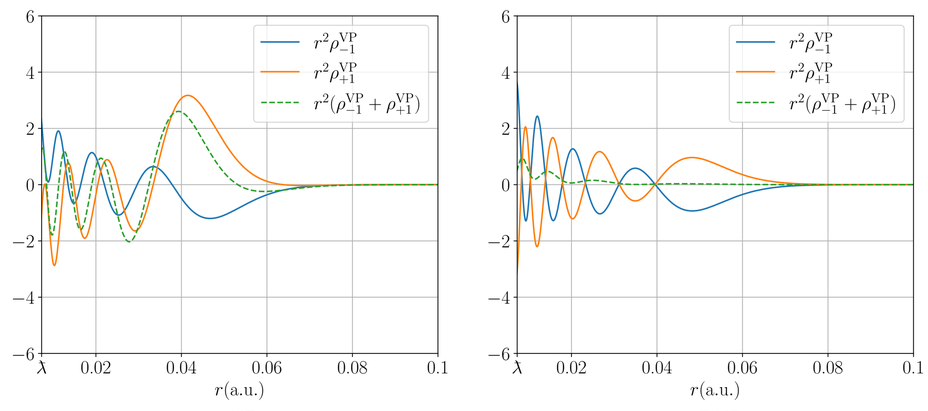
We first run two free-particle calculations ($Z = 0$) with a set of 10 Gaussian exponents within both KB and DKB constructions, and present the obtained results in Figs. (2a) and (2b), respectively. Notice that the KB construction yields non-vanishing free VP densities due to $\mathcal{C}$-symmetry violation.



(a) KB (b) DKB

Figure 2. Free VP density $\rho^{\text{VP}}_{|\kappa|=1}(\boldsymbol{x})$ with 10G.

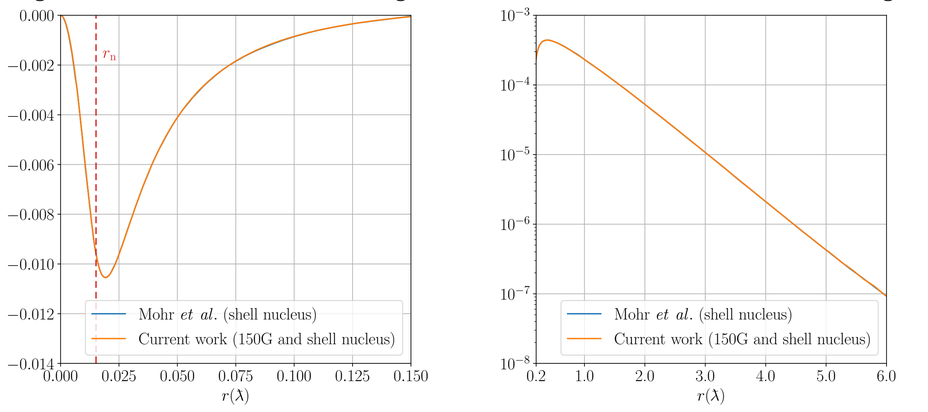
We then run the same calculations on the single-electron uranium atom $Z = 92$, and present the corresponding results of the total VP density of Eq.(11) in Figs. (3a) and (3b). These results show a decaying VP density at relatively large distances with DKB, compared to KB.



(a) KB (b) DKB

Figure 3. Atomic VP density $\rho^{\text{VP}}_{|\kappa|=1}(\boldsymbol{x})$ with 10G.

We finally compute the many-potential VP density $\rho^{\text{VP},n\geq3}_\kappa$ of Eq.(17), for the uranium atom of shell nuclear distribution (hollow sphere), and compare our results to the ones obtained by Mohr *et al.* in Ref. [4] in Figs. (4a) and (4b). An excellent agreement is observed at both small and large distances.



(a) At short distances (b) At large distances

Figure 4. Many-potential VP density $\rho^{\text{VP},n\geq3}_{|\kappa|=1}(\boldsymbol{x})$ with 150G within DKB.

Conclusions

- The DKB construction of finite basis sets allows the compliance to $\mathcal{C}$-symmetry and yields VP density results that are 1) in line with Furry's theorem (for $Z = 0$) and 2) decaying at large distances (for $Z \neq 0$). Both of these essential characteristics are missing in the KB construction.
- One can account for the $n = 3$ VP process using the effective potential (V_{13}) derived by Blomqvist (1972) (limited to point nuclei) or compute the many-potential VP density ($n \geq 3$), following Soff and Mohr (1988) or Gyulassy (1974). These latter proposals are 1) limited to a few nuclear models (sphere and ball) whose radial Green's functions are at hand, and 2) require numerical integrations.
- The proposed procedure allows accurate and efficient computation of the many-potential VP density, within the finite basis set framework, without the need for numerical integrations and in the presence of **arbitrary nuclear distributions**. This procedure is therefore of particular importance for nuclear model problems whose radial Green's function is not at hand, and can be straightforwardly implemented in relativistic molecular calculations to account for the missing physics.

References

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