One-loop vacuum polarization at $m\alpha^7$ order for the two-center problem

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We present calculations of the one-loop vacuum polarization contribution (Uehling potential) for the two-center problem in the nonrelativistic quantum electrodynamics formalism. The cases of hydrogen molecular ions ($Z_1 = Z_2 = 1$) and antiprotonic helium ($Z_1 = 2$, $Z_2 = -1$) are considered. Numerical results for the vacuum polarization contribution at $m\alpha^7$ order for the fundamental transitions $(v = 0, L = 0) \to (v' = 1, L' = 0)$ in H_2^+ and HD^+ are presented.

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I. INTRODUCTION

In Refs. [1,2] a complete set of $m\alpha^7$-order contributions has been evaluated for the fundamental transitions of the hydrogen molecular ions H_2^+ and HD^+ as well as for two-photon transitions of antiprotonic helium. All calculations at this order were performed in the nonrecoil limit by evaluating the one-electron QED corrections in the two-center approximation. The only exception is the Uehling potential vacuum polarization contribution [3], which was computed with a lower level of accuracy. Following the notations of Eq. (46) in Ref. [4], the Uehling correction at $m\alpha^7$ order for a two-center system can be written as

$$\Delta E_{vp}^{(7)} = \frac{\alpha^5}{\pi}\left[V_{61}\ln(Z\alpha)^{-2} + G_{\rm VP}^{(1)}(R)\right]\langle V_\delta\rangle, \tag{1}$$

where R is the internuclear distance and

$$V_\delta(\mathbf{r}) = \pi\left[Z_1^3\delta(\mathbf{r_1}) + Z_2^3\delta(\mathbf{r_2})\right]. \tag{2}$$

The V_{61} coefficient is known analytically, while the nonlogarithmic term was calculated in [1,2] in the linear combination of atomic orbitals (LCAO) approximation using the hydrogen-atom ground-state value of $G_{\rm VP}^{(1)}$. In this work we present a complete account of the vacuum polarization contribution in the two-Coulomb-center approximation.

We utilize the formalism of nonrelativistic quantum electrodynamics (NRQED); a similar approach has been used in [5] (see Sec. II B of that paper) for pionic hydrogen. We start from the nonrelativistic wave function and then obtain contributions due to the relativistic corrections to the electron wave function and modification of the Coulomb vertex function. This approach is first illustrated by calculating the Uehling potential energy shift for S states of the hydrogen atom in Sec. II.

Section III extends the formalism to the two-center case, and the $G_{\rm VP}^{(1)}(R)$ function is calculated. More precisely, the calculated terms include all higher-order contributions generated by the Uehling potential and leading relativistic corrections. Final results for the fundamental transitions in the H_2^+ and HD^+ ions are presented and discussed in Sec. IV.

We use atomic units throughout.

II. HYDROGEN ATOM

In the NRQED formalism, the zero-order approximation is the nonrelativistic (Schrödinger) wave function Ψ_0 with Pauli spinors, defined by

$$(H_0 - E_0)\Psi_0 = 0, \quad H_0 = \frac{\mathbf{p}^2}{2} + V, \quad V = -\frac{Z}{r}. \tag{3}$$

For higher-order terms the Rayleigh-Schrödinger perturbation theory is used. If one wants to evaluate the one-loop vacuum polarization contribution to the bound electron in the external Coulomb field to the required $m\alpha^7$ order, one needs to evaluate the first-order contribution, which is the Uehling potential $U_{vp}(r)$ [Fig. 1(a)]. The next term is the leading-order relativistic correction to the wave function of the electron [Fig. 1(b)], which produces a second-order contribution with the Breit-Pauli Hamiltonian,

$$H_B = -\frac{p^4}{8} + \frac{1}{8}\Delta V, \tag{4}$$

as the perturbation. The last term is the vertex function modification [Fig. 1(c)]. The only contribution at this order to the vertex with the Coulomb photon interaction is the Darwin term (see Fig. 3 in [6] or Eq. (7) of [7]).

In atomic units the Uehling potential is expressed as

$$U_{vp}(r) = -\frac{2}{3}\frac{Z\alpha}{\pi r}\int_1^\infty dt\, e^{-\frac{2r}{\alpha}t}\left(\frac{1}{t^2} + \frac{1}{2t^4}\right)(t^2-1)^{1/2}. \tag{5}$$

Evaluation of the first-order correction with the nonrelativistic wave functions of the hydrogen S states is straightforward and results in the following expression:

$$\Delta E_{vp}^a = \langle nl|U_{vp}|nl\rangle = \frac{\alpha(Z\alpha)^4}{\pi n^3}\left[-\frac{4}{15} + \frac{5\pi}{48}(Z\alpha) - \frac{2}{7}\left(1 + \frac{1}{5n^2}\right)(Z\alpha)^2 + \frac{\pi}{768}\left(49 + \frac{35}{n^2}\right)(Z\alpha)^3 + \cdots\right]. \tag{6}$$

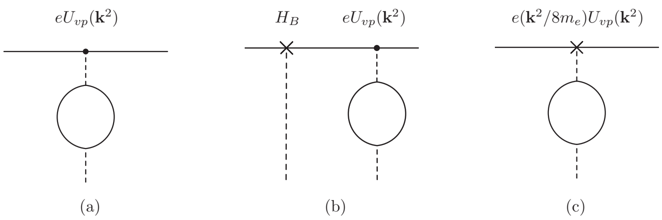

FIG. 1. Feynman diagrams for the one-loop vacuum polarization NRQED contributions.

The second-order term, determined by the diagram in Fig. 1(b), has the form

$$\Delta E^b_{vp} = 2\langle (H_B - \langle H_B\rangle)(E_0 - H)^{-1}(U_{vp} - \langle U_{vp}\rangle)\rangle \quad (7)$$

and may be evaluated using $\Psi_B = (E_0 - H)^{-1}(H_B - \langle H_B\rangle)\Psi_0$. An analytical expression of Ψ_B can be found, e.g., in [7]. For the S states, one gets

$$\Delta E^b_{vp} = \frac{\alpha(Z\alpha)^4}{\pi n^3}\left\{-\frac{3\pi}{16}(Z\alpha) - \frac{2}{15}\left[\ln(Z\alpha)^{-2} - 2\left(\psi(n+1) - \psi(1) - \ln n + \ln 2 - \frac{107}{60} - \frac{2}{n} + \frac{5}{2n^2}\right)\right](Z\alpha)^2 \right.$$
$$\left. + \frac{5\pi}{96}\left[\ln(Z\alpha)^{-2} - 2\left(\psi(n+1) - \psi(1) - \ln n - \ln 2 - \frac{43}{60} - \frac{2}{n} + \frac{3}{n^2}\right)\right](Z\alpha)^3 + \cdots\right\}, \quad (8)$$

where ψ is the logarithmic derivative of the Euler gamma function $\Gamma(z)$.

As discussed above, the NRQED effective Hamiltonian at $m\alpha(Z\alpha)^6$ order contains just one contribution determined by the diagram in Fig. 1(c):

$$H^{(7)}_{vp} = \tfrac{1}{8}\Delta U_{vp}. \quad (9)$$

Using

$$\Delta\left(\frac{e^{-\Lambda r}}{r}\right) = -4\pi\delta(\mathbf{r}) + \Lambda^2\,\frac{e^{-\Lambda r}}{r},$$

one gets

$$H^{(7)}_{vp} = -\frac{1}{12}\frac{Z\alpha}{\pi}\int_1^\infty dt\left[-4\pi\delta(\mathbf{r}) + \frac{4t^2}{\alpha^2}\frac{e^{-\frac{2r}{\alpha}t}}{r}\right]\left(\frac{1}{t^2} + \frac{1}{2t^4}\right)(t^2-1)^{1/2}. \quad (10)$$

Taking the expectation values of this effective Hamiltonian, one immediately gets for S states

$$\Delta E^c_{vp} = \frac{1}{8}\langle nl|(\Delta U_{vp})|nl\rangle = \frac{\alpha(Z\alpha)^4}{\pi n^3}\left[\frac{3\pi}{16}(Z\alpha) - \frac{1}{3}\left(1 + \frac{1}{5n^2}\right)(Z\alpha)^2 + \frac{5\pi}{576}\left(7 + \frac{5}{n^2}\right)(Z\alpha)^3 + \cdots\right]. \quad (11)$$

The NRQED contribution, which is determined by the three terms of Fig. 1, should be exact up to $m\alpha(Z\alpha)^7$ order. The sum of these three contributions for S states gives the final result

$$\Delta E_U = \frac{\alpha(Z\alpha)^4}{\pi n^3}\left\{-\frac{4}{15} + \frac{5\pi}{48}(Z\alpha) - \frac{2}{15}(Z\alpha)^2\ln(Z\alpha)^{-2} + \frac{4}{15}(Z\alpha)^2\left[\psi(n+1) - \psi(1) - \ln\left(\frac{n}{2}\right) - \frac{431}{105} - \frac{2}{n} + \frac{57}{28n^2}\right] + \cdots\right.$$
$$- \frac{2}{15}\left[\ln(Z\alpha)^{-2} - 2\left(\psi(n+1) - \psi(1) - \ln n + \ln 2 - \frac{431}{105} - \frac{2}{n} + \frac{57}{28n^2}\right)\right](Z\alpha)^2$$
$$\left. + \frac{5\pi}{96}\left[\ln(Z\alpha)^{-2} - 2\left(\psi(n+1) - \psi(1) - \ln n - \ln 2 - \frac{153}{80} - \frac{2}{n} + \frac{103}{48n^2}\right)\right](Z\alpha)^3 + \cdots\right\}. \quad (12)$$

The first three lines are in complete agreement with the combined result of [8,9]. The last line extends the general expression of ΔE_U by one further order in $Z\alpha$; for the $1s$ state it coincides with the analytical result of [10].

III. TWO-CENTER PROBLEM

Now, we are ready to study two-center systems. The nonrelativistic Hamiltonian of an electron is then

$$H_0 = \frac{p^2}{2} + V, \quad V = -\frac{Z_1}{r_1} - \frac{Z_2}{r_2}. \quad (13)$$

The energy and wave function of the ground ($1s\sigma$) state will be denoted by E_0 and ψ_0, respectively. The Uehling potential is a sum of interactions with both nuclei:

$$U_{vp}(\mathbf{r}) = U_{vp}(r_1) + U_{vp}(r_2). \quad (14)$$

We now want to calculate the contributions corresponding to Figs. 1(a), 1(b), and 1(c) in the same way as in the previous section for the hydrogen atom.

The first of these diagrams contains the leading-order contributions [of orders $\alpha(Z\alpha)^4$ and $\alpha(Z\alpha)^5$], which were already included in earlier calculations [11]. We are thus interested in higher-order [$\alpha(Z\alpha)^6$ and above] terms, which can be obtained by the following subtraction:

$$\Delta E_a^{(7+)} = \langle\psi_0|U_{vp}|\psi_0\rangle - \Delta E_{vp}^{(5)} - \Delta E_{vp}^{(6)}$$
$$= \langle\psi_0|U_{vp}|\psi_0\rangle + \frac{4\alpha^3}{15}\langle Z_1\delta(\mathbf{r_1}) + Z_2\delta(\mathbf{r_2})\rangle$$
$$- \frac{5\alpha^4}{48}\pi\left\langle Z_1^2\delta(\mathbf{r_1}) + Z_2^2\delta(\mathbf{r_2})\right\rangle. \quad (15)$$

As shown in Sec. II, Figs. 1(b) and 1(c) both contain $\alpha(Z\alpha)^5$-order terms, which cancel each other. Writing ΔE_b in terms of the first-order perturbation wave function ψ_B associated with the Breit-Pauli Hamiltonian,

$$\Delta E_b = 2\langle\psi_B|U_{vp}|\psi_0\rangle, \quad (16)$$

with

$$(E_0 - H_0)\psi_B = (H_B - \langle H_B\rangle)\psi_0, \quad (17)$$

one can see that the $\alpha(Z\alpha)^5$-order term in ΔE_b comes from the leading $1/r$ singularity of ψ_B. In order to get the contribution of order $\alpha(Z\alpha)^6$ and above, it is convenient to subtract this singularity and use the wave function $\tilde{\psi}_B$ defined by

$$\psi_B = \tilde{\psi}_B + (U_1 - \langle U_1\rangle)\psi_0, \quad U_1 = -\frac{V}{4}, \quad (18)$$

which satisfies the following relation [7,12]:

$$(E_0 - H_0)\tilde{\psi}_B = (H'_B - \langle H'_B\rangle)\psi_0,$$
$$H'_B = -(E_0 - H_0)U_1 - U_1(E_0 - H_0) + H_B. \quad (19)$$

One thus obtains

$$\Delta E_b^{(7+)} = 2\langle\tilde{\psi}_B|U_{vp}|\psi_0\rangle + \tfrac{1}{2}\langle V\rangle\langle\psi_0|U_{vp}|\psi_0\rangle. \quad (20)$$

Finally, the subtracted term is added to the contribution ΔE_c, which is thus redefined as

$$\Delta E_c^{(7+)} = \tfrac{1}{8}\langle\psi_0|\Delta U_{vp}|\psi_0\rangle - \tfrac{1}{2}\langle\psi_0|VU_{vp}|\psi_0\rangle. \quad (21)$$

Integration by parts and the use of the Schrödinger equation $\Delta\psi_0 = 2(V - E_0)\psi_0$ provide the following relationship, in which the $\alpha(Z\alpha)^5$-order term has been explicitly canceled out:

$$\Delta E_c^{(7+)} = \frac{1}{4}\langle\psi_0|\mathbf{p}U_{vp}\mathbf{p}|\psi_0\rangle - \frac{E_0}{2}\langle\psi_0|U_{vp}|\psi_0\rangle. \quad (22)$$

The final result is

$$\Delta E_U^{(7+)} = \Delta E_a^{(7+)} + \Delta E_b^{(7+)} + \Delta E_c^{(7+)} \quad (23)$$

and may be put in the form [see Ref. [4], Eq. (46)]

$$\Delta E_U^{(7+)} = \frac{\alpha^5}{\pi}\left[V_{61}\ln(\alpha^{-2}) + G_{\rm VP}^{(1)}(R)\right]\langle V_\delta\rangle, \quad (24)$$

with $V_{61} = -2/15$. The logarithmic term comes from the logarithmic singularity in $\tilde{\psi}_B$ and should thus be subtracted from $\Delta E_b^{(7)}$:

$$G_{\rm VP}^{(1)}(R) = \pi\Delta E_a^{(7+)}/\langle V_\delta\rangle + \left[\pi\Delta E_b^{(7+)}/\langle V_\delta\rangle - V_{61}\ln(\alpha^{-2})\right]$$
$$+ \pi\Delta E_c^{(7+)}/\langle V_\delta\rangle. \quad (25)$$

Since the initial NRQED approximation is valid up to and including $m\alpha^8$ order, the result of Eq. (25) should be accurate to $O(\alpha^2)$.

IV. RESULTS AND CONCLUSION

We calculated all operator mean values appearing in Eqs. (16), (20), and (22) for the ground ($1s\sigma$) electronic state of the two-center problem for both $Z_1 = Z_2 = 1$ for application to $H_2{}^+$ and HD^+ and $Z_1 = 2$, $Z_2 = -1$ for application to antiprotonic helium. The numerical approach has been described previously (see, e.g., [13]). The following expansion for the σ electronic wave function is used:

$$\Psi_0(\mathbf{r}) = \sum_{i=1}^{\infty} C_i e^{-\alpha_i r_1 - \beta_i r_2}. \quad (26)$$

For $Z_1 = Z_2$ the variational wave function should be symmetrized,

$$\Psi_0(\mathbf{r_1},\mathbf{r_2}) = \sum_{i=1}^{\infty} C_i\left(e^{-\alpha_i r_1 - \beta_i r_2} \pm e^{-\beta_i r_1 - \alpha_i r_2}\right), \quad (27)$$

where (+) is used to get a *gerade* electronic state and (−) is for an *ungerade* state. Parameters α_i and β_i are generated in a quasirandom manner.

The matrix elements of the Uehling potential in such an exponential basis set are not known in analytical form, in contrast to the case of the three-body problem [14]. We thus resorted to numerical integration for all the terms involving

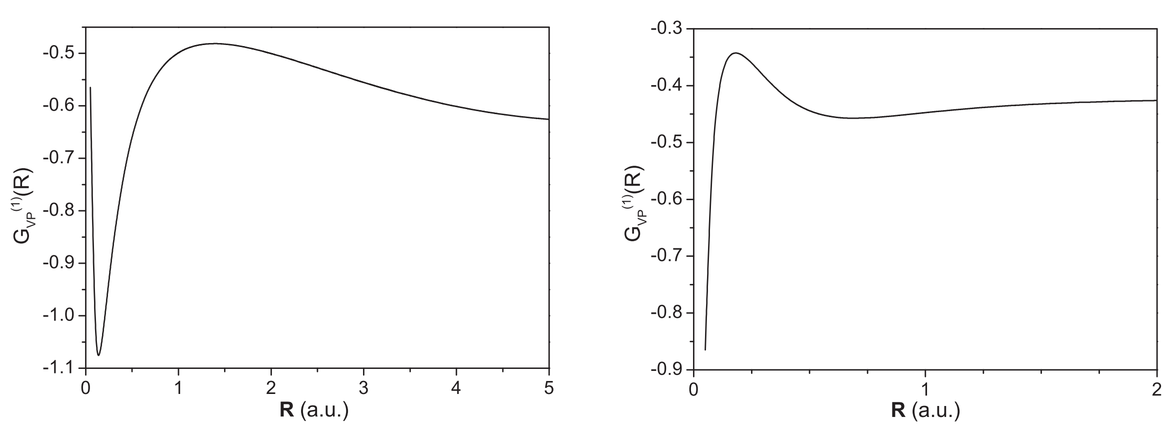

FIG. 2. Effective potentials $G_{\rm VP}^{(1)}(R)$ for (left) the hydrogen molecular ions, $Z_1 = Z_2 = 1$, and (right) antiprotonic helium, $Z_1 = 2$, $Z_2 = -1$.

TABLE I. Results of numerical calculations of the $G^{(1)}_{\rm VP}$ contribution for the ground states of $H_2{}^+$ and HD^+ and the fundamental transitions $(v=0,L=0)\to(v'=1,L'=0)$. A comparison with previous estimates made in [1] within the LCAO approximation is presented.

	$H_2{}^+$		HD^+	
	This work	LCAO [1]	This work	LCAO [1]
Ground state (kHz)	− 28.35	− 34.73	− 28.38	− 34.93
Transition (kHz)	0.42	0.94	0.37	0.82

U_{vp}. To that end we used the approximate form of the Uehling potential presented in [15], which is accurate to at least nine digits.

Results are shown in Fig. 2. As can be seen, the values of $G^{(1)}_{\rm VP}(R)$ at $R\to 0$ tend to infinity and do not obey the continuity relationship that could be expected, $G^{(1)}_{\rm VP}(R)\to G^{(1)}_{\rm VP}(\mathrm{H}_Z(1S))$, where $\mathrm{H}_Z(1S)$ denotes the $1S$ state of a hydrogenic atom with nuclear charge $Z=Z_1+Z_2$. The reason for such behavior is that the coefficients of the $Z\alpha$ expansion have no physical meaning, and only the sum over all orders matters. Only the complete Uehling potential contribution, indeed, is a continuous function of R at the united atom limit. The same observation is also valid for the one-loop self-energy contribution [13] and for higher-order diagrams.

On the contrary, continuity is observed at the other limit, $R\to\infty$. We checked this by direct numerical evaluation of expressions (16), (20), and (22) with $1S$ hydrogenic wave functions. The values of $G^{(1)}_{\rm VP}(R)$ at large R converge towards $G^{(1)}_{\rm VP}(\mathrm{H}_{Z=1}(1S))=-0.618\,45$ in the hydrogen molecular ion case and towards $G^{(1)}_{\rm VP}(\mathrm{H}_{Z=2}(1S))=-0.421\,94$ in the antiprotonic helium case.

The last step is numerical integration of the vacuum polarization "effective" potentials of Fig. 2 over vibrational or heavy-particle degrees of freedom to get the energy corrections for individual states. Numerical results for the ground states of $H_2{}^+$ and HD^+ and for the fundamental transitions $(v=0,L=0)\to(v'=1,L'=0)$ are collected in Table I. Comparison with the LCAO approximation demonstrates that in the case of individual states it may give a reasonable estimate. However, for the transition frequency, due to the slope of the effective potential at the equilibrium position at $R=2.0$, the difference in contributions from the two states becomes substantially sensitive, and the LCAO estimate gives only an order of magnitude. This tendency is less marked in the case of antiprotonic helium; for example, for the two-photon $(33,32)\to(31,30)$ transition in $^4\mathrm{He}\,\bar{p}$ we obtain a shift of 121 kHz, while the LCAO estimate is 98 kHz. That may be explained as follows: the dominating contribution comes from the $1S$ state wave function of hydrogenlike helium ($Z=2$), and the contribution from the antiproton is negligible. However, it is worth noting that for the antiprotonic helium, nonadiabatic effects become essential at this level, and complete three-body calculations are needed to get improved accuracy.

In conclusion, we have calculated the Uehling corrections at orders $m\alpha^7$ and $m\alpha^8$ for the two-center problem. Together with improved numerical calculations of the relativistic Bethe logarithm [13], these results will allow for further improvement of the theoretical accuracy of transition frequencies in $H_2{}^+$, HD^+, and antiprotonic helium.

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[1] V. I. Korobov, L. Hilico, and J.-Ph. Karr, Phys. Rev. A **89**, 032511 (2014).
[2] V. I. Korobov, L. Hilico, and J.-Ph. Karr, Phys. Rev. Lett. **112**, 103003 (2014).
[3] E. A. Uehling, Phys. Rev. **48**, 55 (1935).
[4] P. J. Mohr, B. N. Taylor, and D. B. Newell, Rev. Mod. Phys. **84**, 1527 (2012).
[5] S. Schlesser, E.-O. Le Bigot, P. Indelicato, and K. Pachucki, Phys. Rev. C **84**, 015211 (2011).
[6] T. Kinoshita and M. Nio, Phys. Rev. D **53**, 4909 (1996).
[7] V. I. Korobov, L. Hilico, and J.-Ph. Karr, Phys. Rev. A **79**, 012501 (2009).
[8] P. J. Mohr, Phys. Rev. Lett. **34**, 1050 (1975); Phys. Rev. A **26**, 2338 (1982).
[9] V. G. Ivanov and S. G. Karshenboim, Yad. Phys. **60**, 333 (1997) [Phys. At. Nuclei **60**, 270 (1997)].
[10] S. G. Karshenboim, J. Exp. Theor. Phys. **89**, 850 (1999).
[11] V. I. Korobov, Phys. Rev. A **74**, 052506 (2006).
[12] V. I. Korobov and T. Tsogbayar, J. Phys. B **40**, 2661 (2007).
[13] V. I. Korobov, L. Hilico, and J.-Ph. Karr, Phys. Rev. A **87**, 062506 (2013).
[14] J.-Ph. Karr and L. Hilico, Phys. Rev. A **87**, 012506 (2013).
[15] L. W. Fullerton and G. A. Rinker, Jr., Phys. Rev. A **13**, 1283 (1976).