Self-energy correction to the bound-electron g factor of P states

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The radiative self-energy correction to the bound-electron g factor of $2P_{1/2}$ and $2P_{3/2}$ states in one-electron ions is evaluated to order $\alpha(Z\alpha)^2$. The contribution of high-energy virtual photons is treated by means of an effective Dirac equation, and the result is verified by an approach based on long-wavelength quantum electrodynamics. The contribution of low-energy virtual photons is calculated both in the velocity and in the length gauge, and gauge invariance is verified explicitly. The results compare favorably to recently available numerical data for hydrogenlike systems with low nuclear charge numbers.

I. INTRODUCTION

When a bound electron interacts with an external, uniform, and time-independent magnetic field (Zeeman effect), the energetic degeneracy of the atomic energy levels with respect to the magnetic projection quantum number is broken, and the different magnetic sublevels split according to the formula

$$\Delta E = g_j \mu_B B \mu, \qquad (1)$$

where g_j is the bound-electron (Landé) g factor, $\mu_B = -e/(2m)$ is the Bohr magneton, and B is the magnetic field which is assumed to be oriented parallel to the quantization axis. Finally, μ is the magnetic projection quantum number of the electron, i.e., the projection of its total angular momentum (divided by $\hbar$) onto the quantization axis.

In leading order, the bound-electron g factor is determined by nonrelativistic quantum theory and is equal to a rational number for all bound states in a hydrogenlike ion. Both relativistic atomic theory as well as quantum electrodynamics (QED) predict deviations from the nonrelativistic result. The relativistic effects follow from Dirac theory and can be expressed in terms of a power series in the parameter $Z\alpha$, where Z is the nuclear charge number and α is the fine-structure constant. The QED effects are caused mainly by the anomalous magnetic moment of the electron, which is turn in caused by the exchange of high-energy virtual photons before and after the interaction with the external magnetic field. Here, by "high-energy" we refer to a virtual photon with an energy of the order of the electron rest mass. A second source for QED effects are exchanges of virtual photons with an energy commensurate with the atomic binding energy scale, which is smaller than the electron rest mass energy by a factor $(Z\alpha)^2$. Here, the electron emits and absorbs a virtual photon before and after the interaction with the external magnetic field, undergoing a virtual transition to a excited atomic state in the middle. For P states, the latter effects lead to a correction to the bound-electron g factor of order $\alpha(Z\alpha)^2$. The complete result for the correction of order $\alpha(Z\alpha)^2$ is obtained after adding the anomalous magnetic moment correction (high-energy part) and the low-energy photon contribution of the same order.

Previous studies of the bound-electron g factor for P states in hydrogenlike systems include Refs. [1–5]. Quite recently, the problem has received renewed interest [6,7]. For few-electron ions, the bound-electron g factor has been investigated in Refs. [6–10]. For the 2^3P states of helium,

there is still an unresolved discrepancy of theoretical and experimental results (see Refs. [10–12]).

The expansion of the quantum electrodynamic radiative correction to the electron g factor, which is an expansion in powers of α for a free electron, is intertwined with an expansion in powers of $Z\alpha$ for a bound electron (this fact has been stressed in Ref. [13]). For an nP_j state in a hydrogenlike system, we can write down the following intertwined expansion in powers of α and $Z\alpha$,

$$\delta g(nP_j) = g_{00} + (Z\alpha)^2 \frac{g_{20}}{n^2} + O(Z\alpha)^4$$
$$+ \frac{\alpha}{\pi}\left\{ b_{00} + (Z\alpha)^2 \frac{b_{20}}{n^2} + O(Z\alpha)^4 \right\}. \qquad (2)$$

The coefficients g_{00} and g_{20} characterize the relativistic effects, whereas b_{00} and b_{20} are obtained from the one-loop radiative correction. The nonrelativistic result for the Landé g factor reads

$$g_{00}(nP_{1/2}) = \tfrac{2}{3}, \qquad g_{00}(nP_{3/2}) = \tfrac{4}{3}. \qquad (3)$$

The relativistic correction follows from Breit theory and the Dirac equation in an external magnetic field [3,14],

$$g_{20}(nP_{1/2}) = -\tfrac{2}{3}, \qquad g_{20}(nP_{3/2}) = -\tfrac{8}{15}. \qquad (4)$$

The leading correction due to the anomalous magnetic reads as (see Refs. [1,3]),

$$b_{00}(nP_{1/2}) = -\tfrac{1}{3}, \qquad b_{00}(nP_{3/2}) = \tfrac{1}{3}. \qquad (5)$$

We are concerned here with the evaluation of the b_{20} coefficient of nP_j states, which is determined exclusively by self-energy type corrections (vacuum polarization does not contribute).

We adopt the following outline for this paper. In Sec. II, we reexamine the contribution of high-energy virtual photons (see also Ref. [3]). Two alternative derivations are presented, which are based on an effective Dirac equation (Sec. II A) and on an effective low-energy long-wavelength quantum electrodynamic theory (Sec. II B) which is obtained from the fully relativistic theory by a combined Foldy-Wouthuysen and Power-Zienau transformation [10]. The low-energy part is also treated in two alternative ways. The velocity-gauge calculation in Sec. III A is contrasted with the length-gauge derivation in Sec. III B. Conclusions are reserved for Sec. IV. Natural units ($\hbar = c = \epsilon_0 = 1$) are used throughout the paper.

II. HIGH-ENERGY PART

A. Effective Dirac equation

In Ref. [3], the contribution to b_{20} due to high-energy virtual photons was obtained on the basis of the two-body Breit Hamiltonian. Here, we perform the calculation using a simple approach, based on an effective Dirac Hamiltonian (see Chap. 7 of Ref. [15]). For an electron interacting with external electric and magnetic fields, this equation reads

$$H_{\rm rad} = \vec{\alpha} \cdot [\vec{p} - {\rm e}F_1(\vec{\nabla}^2)\vec{A}] + \beta m + F_1(\vec{\nabla}^2)V$$
$$+ F_2(\vec{\nabla}^2)\frac{e}{2m}({\rm i}\vec{\gamma} \cdot \vec{E} - \beta\vec{\Sigma} \cdot \vec{B}). \qquad (6)$$

We here take into account the Dirac form factor F_1 and the Pauli form factor F_2. The matrices $\vec{\alpha} = \gamma^0\vec{\gamma}$ and $\beta = \gamma^0$ are the standard Dirac matrices in the Dirac representation [15], m is the electron mass, and $e = -|e|$ is the electron charge. Up to the order relevant for the current calculation, we may approximate both form factors in the limit of vanishing momentum transfer as

$$F_1(\vec{\nabla}^2) \approx F_1(0) = 1, \quad F_2(\vec{\nabla}^2) \approx F_2(0) \approx \kappa \equiv \frac{\alpha}{2\pi}. \qquad (7)$$

The vector potential $\vec{A}$ corresponds to a uniform external magnetic field, i.e., $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$, and the electric field $\vec{E}$ is that of the Coulomb potential ($e\vec{E} = -\vec{\nabla}V$). Finally, $V = -Z\alpha/r$ is the binding potential. So,

$$H_{\rm rad} \approx \vec{\alpha} \cdot \vec{p} + \beta m + V - \frac{e}{2}\vec{\alpha} \cdot (\vec{B} \times \vec{r})$$
$$- \frac{{\rm i}\kappa}{2m}\vec{\gamma} \cdot \vec{\nabla}V - \frac{e}{2m}\kappa\beta\vec{\Sigma} \cdot \vec{B}. \qquad (8)$$

Dirac eigenstates fulfill $(\vec{\alpha} \cdot \vec{p} + \beta m + V)\psi = E_D\psi$, where E_D is the Dirac energy. The first few terms in the perturbative expansion of E_D in a magnetic field read

$$\Delta E = \langle\psi| - \frac{e}{2}\vec{\alpha} \cdot (\vec{B} \times \vec{r})|\psi\rangle - \frac{e}{2m}\kappa\langle\psi|\beta\vec{\Sigma} \cdot \vec{B}|\psi\rangle$$
$$+ \frac{e\kappa}{2m}\langle\psi|({\rm i}\vec{\gamma} \cdot \vec{\nabla}V)\frac{\mathcal{Q}}{2m}[\vec{\alpha} \cdot (\vec{B} \times \vec{r})]|\psi\rangle, \qquad (9)$$

where $\mathcal{Q} = \frac{1}{2}(1 - \gamma^0)$ is a projector onto virtual negative-energy states, and ψ is the relativistic wave function. An evaluation of the first term on the right-hand side of Eq. (9) with Dirac wave functions confirms the results for g_{00} and g_{20} given in Eqs. (3) and (4). The second term on the right-hand side of Eq. (9) yields the result for b_{00} as given in Eq. (5). When the Dirac wave functions are properly expanded in powers of $Z\alpha$, the second and third terms on the right-hand side of Eq. (9) yield the following high-energy contribution $b_{20}^{(H)}$ to the b_{20} coefficient defined in Eq. (2),

$$b_{20}^{(H)}(nP_{1/2}) = -\frac{1}{2}, \quad b_{20}^{(H)}(nP_{3/2}) = \frac{1}{10}. \qquad (10)$$

These results are in agreement with those given in Eq. (5) of Ref. [3].

B. Long-wavelength quantum electrodynamics

It is instructive to compare the fully relativistic approach outlined above to an effective nonrelativistic theory. In Ref. [16], a systematic procedure has been described in order to perform a nonrelativistic expansion of the interaction

Hamiltonian for a light atomic system with slowly varying external electric and magnetic fields. This procedure involves two steps, (i) a Foldy-Wouthuysen transformation of an interaction of the type Eq. (6), suitably generalized for many-electron systems, and (ii) a Power-Zienau transformation to express the vector potentials in terms of physically observable field strengths. The result is an interaction, given in Eq. (30) of Ref. [16], which describes a nonrelativistic expansion of the atom-field interaction in powers of $Z\alpha$ and can be used in order to identify terms which contribute at a specified order.

If we are interested in evaluating the corrections to the g factor up to order $\alpha(Z\alpha)^2$, i.e., all corrections listed in Eq. (2), the relevant effective interactions for a one-electron system are

$$H_{\rm mag} = H_M + \sum_{i=1}^{3} H_i, \quad H_M = \mu_B(\vec{L} + \vec{\sigma}) \cdot \vec{B}, \qquad (11a)$$

$$H_1 = -\frac{\mu_B}{2m^2}\vec{p}^2(\vec{L} + \vec{\sigma}) \cdot \vec{B}, \qquad (11b)$$

$$H_2 = \frac{\mu_B(1 + 2\kappa)}{4m}\frac{Z\alpha}{r^3}(\vec{r} \times \vec{\sigma}) \cdot (\vec{r} \times \vec{B}), \qquad (11c)$$

$$H_3 = -\frac{\mu_B\kappa}{2m^2}(\vec{p} \cdot \vec{\sigma})(\vec{p} \cdot \vec{B}), \qquad (11d)$$

where $\mu_B = -e/(2m)$ is the Bohr magneton. We denote the Schrödinger-Pauli two-component wave function by ϕ in order to distinguish it from the fully relativistic wave function ψ. Specifically, ϕ reads as $\phi(\vec{r}) = R(r)\chi_\kappa^\mu(\hat{r})$ in the coordinate representation, where $R(r)$ is the nonrelativistic radial component of the wave function and $\chi_\kappa^\mu(\hat{r})$ is the standard two-component spin-angular function [17]. An evaluation of the perturbation

$$\Delta E = \langle\phi|H_{\rm mag}|\phi\rangle \qquad (12)$$

confirms the results of Eqs. (3), (4), (5), and (10) for the high-energy part. No second-order effects need to be considered in this formalism up to the order in the $Z\alpha$-expansion relevant for the current study.

III. LOW-ENERGY PART

A. Velocity gauge

The most economical approach to the calculation of the low-energy contribution of order $\alpha(Z\alpha)^2$ to the g factor of P states consists in a calculation of the orbital g_ℓ factor, with a conversion of the orbital g_ℓ factor to the Landé g_j factor in a second step of the calculation. In the order $\alpha(Z\alpha)^2$, one may indeed convert the spin-independent correction to the orbital g_ℓ factor to a spin-dependent correction to the g_j factors of the $2P_{1/2}$ and $2P_{3/2}$ states, as described in Appendix A. However, a more systematic approach to the problem, which is also applicable to higher-order (in $Z\alpha$) corrections, is based on a perturbation of the nonrelativistic self-energy of the bound electron by the magnetic interaction Hamiltonian (11). This is the approach outlined below.

We thus investigate the perturbation of the nonrelativistic bound-electron self-energy [18] due to the magnetic interaction Hamiltonian

$$H_M = -\frac{e}{2m}(\vec{L} + \vec{\sigma}) \cdot \vec{B} \qquad (13)$$

given in Eq. (11a). In the velocity gauge, the interaction of the electron with the vector potential $\vec{A}$ of the quantized electromagnetic field is given by the term $-\vec{p} \cdot \vec{A}/m$, where $\vec{p}$ is the electron momentum. In an external magnetic field, it is the physical momentum $\vec{p} - \frac{e}{2}(\vec{B} \times \vec{r})$, not the canonical momentum $\vec{p}$, which couples to the quantized electromagnetic field. This amount to a correction $\delta\vec{J}$ to the electron's transition current given by

$$\delta J^i = -\frac{e}{2m}(\vec{B} \times \vec{r})^i = -\frac{e}{2m}\epsilon^{ijk}B^j r^k. \qquad (14)$$

Because of the symmetry of the problem (Wigner-Eckhart theorem), we may fix the axis of the B field to be along the quantization axis (z axis) and the projection of the reference state to be $\mu = \frac{1}{2}$. This procedure allows one to simplify the angular algebra. It is inspired by the separation of nuclear and electronic tensors that are responsible for the hyperfine interaction. Such a separation has been used in Eq. (1) of Ref. [19] and in Eqs. (10) and (11) of Ref. [20]. In the case of the g factor, the magnetic field of the nucleus is replaced by the external, homogeneous magnetic field of the Zeeman effect.

We divide out a prefactor $-e/(2m)$ from both the magnetic Hamiltonian H_M and from the current δJ^i and obtain the perturbative Hamiltonian $h_{M,0}$ and the scaled current δj_0^i. In the spherical basis, this procedure leads to the operators

$$h_{M,0} = L_0 + \sigma_0, \quad \delta j_0^i = \epsilon^{i3k}r^k, \qquad (15)$$

which are aligned along the quantization axis of the external magnetic field. The index zero of the operators, in the spherical basis, denotes the z component in the Cartesian basis (see Ref. [17]). The following shorthand notation for the atomic states with magnetic projection $\mu = \frac{1}{2}$ proves useful:

$$\left| j\tfrac{1}{2} \right\rangle \equiv \left| nP_j\left(\mu = \tfrac{1}{2}\right) \right\rangle, \quad \langle h_{M,0} \rangle \equiv \left\langle j\tfrac{1}{2} \middle| h_{M,0} \middle| j\tfrac{1}{2} \right\rangle. \quad (16)$$

Finally, we can proceed to the calculation of the perturbed self-energy. The nonrelativistic (Schrödinger) Hamiltonian of the atom is

$$H_{NR} = \frac{\vec{p}^2}{2m} + V, \qquad (17)$$

and the nonrelativistic self-energy reads

$$\delta E = -\frac{2\alpha}{3\pi m^2}\int_0^{m\epsilon} d\omega\, \omega \left\langle j\tfrac{1}{2} \middle| \vec{p}\,\frac{1}{H_{NR} - E_{NR} + \omega}\,\vec{p} \middle| j\tfrac{1}{2} \right\rangle. \qquad (18)$$

The wave-function correction to the self-energy reads

$$\delta E_\psi = -\frac{4\alpha}{3\pi m^2}\int_0^{m\epsilon} d\omega\, \omega \left\langle j\tfrac{1}{2} \middle| \vec{p}\,\frac{1}{H_{NR} - E_{NR} + \omega} \right.$$
$$\left. \times\, \vec{p}\left(\frac{1}{E_{NR} - H_{NR}}\right)' h_{M,0} \middle| j\tfrac{1}{2} \right\rangle. \qquad (19)$$

Here, $[1/(E_{NR} - H_{NR})]'$ is the reduced Green function, with the reference state being excluded from the sum over virtual states. The contribution of virtual nP_j states (with j being equal to that of the reference state and $n \geq 2$) vanishes because of the orthogonality of the nonrelativistic radial wave

functions. The interaction $h_{M,0}$ couples $2P_{1/2}$ and $2P_{3/2}$ states, but the contribution of virtual states with different j as compared to the reference state vanishes after angular algebra [17] because the self-energy interaction operator $\{\vec{p}[1/(H_{NR} - E_{NR} + \omega)]\vec{p}\}$ is diagonal in the total angular momentum. Virtual states with different orbital angular momentum than the reference state are not coupled at all to the reference state by the action of the perturbative Hamiltonian $h_{M,0}$. Because all contributions vanish individually, we can thus conclude that $\delta E_\psi = 0$.

Hence, we have to evaluate first-order corrections to the Hamiltonian and to the energy corresponding to the replacements $H_{NR} \to H_{NR} + h_{M,0}$ and $E_{NR} \to E_{NR} + \langle h_{M,0} \rangle$ in Eq. (18). Furthermore, we have a correction to the current corresponding to $\vec{p}/m \to \vec{p}/m + \delta\vec{j}_0$. The energy correction reads as

$$\delta E_E = -\frac{2\alpha}{3\pi m^2}\langle h_{M,0} \rangle \int_0^{m\epsilon} d\omega\, \omega$$
$$\times \left\langle j\tfrac{1}{2} \middle| \vec{p}\left(\frac{1}{H_{NR} - E_{NR} + \omega}\right)^2 \vec{p} \middle| j\tfrac{1}{2} \right\rangle, \qquad (20)$$

where $m\epsilon$ is an upper cutoff for the photon energy [18] (the scale-separation parameter ϵ is dimensionless). It corresponds to the following g factor correction:

$$\delta g_E(nP_j) = g_{00}(nP_j)\frac{\delta E_E}{\langle h_{M,0} \rangle}. \qquad (21)$$

A numerical evaluation of this correction according to established techniques [21] yields

$$\delta g_E(2P_{1/2}) = \frac{2\alpha}{3\pi}(Z\alpha)^2\left[-\frac{1}{6}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) - 0.12831\right], \qquad (22a)$$

$$\delta g_E(2P_{3/2}) = \frac{4\alpha}{3\pi}(Z\alpha)^2\left[-\frac{1}{6}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) - 0.12831\right]. \qquad (22b)$$

For the correction to the Hamiltonian, we get

$$\delta E_H = \frac{2\alpha}{3\pi m^2}\int_0^{m\epsilon} d\omega\, \omega$$
$$\times \left\langle j\tfrac{1}{2} \middle| \vec{p}\left(\frac{1}{H_{NR} - E_{NR} + \omega}\right)^2 h_{M,0}\vec{p} \middle| j\tfrac{1}{2} \right\rangle, \qquad (23)$$

where we have used the relation $[H_{NR}, h_{M,0}] = 0$. This translates into the following correction for the g factor:

$$\delta g_H(nP_j) = g_{00}(nP_j)\frac{\delta E_H}{\langle h_{M,0} \rangle}. \qquad (24)$$

A numerical evaluation leads to the following results:

$$\delta g_H(2P_{1/2}) = \frac{2\alpha}{3\pi}(Z\alpha)^2\left[\frac{1}{6}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) + 0.25134\right], \qquad (25a)$$

$$\delta g_H(2P_{3/2}) = \frac{4\alpha}{3\pi}(Z\alpha)^2\left[\frac{1}{6}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) + 0.15907\right]. \qquad (25b)$$

The correction to the current is given by

$$\delta E_C = -\frac{4\alpha}{3\pi m^2} \int_0^{m\epsilon} d\omega \, \omega$$
$$\times \left\langle j\frac{1}{2} \left| p^i \frac{1}{H_{\text{NR}} - E_{\text{NR}} + \omega} \delta j_0^i \right| j\frac{1}{2} \right\rangle, \quad (26)$$

where we take into account the multiplicity factor due to the current acting on both sides of the propagator. The corresponding correction to the g factor is

$$\delta g_C(nP_j) = g_{00}(nP_j)\frac{\delta E_j}{\langle h_{M,0}\rangle}. \quad (27)$$

We obtain the following numerical results:

$$\delta g_C(2P_{1/2}) = \frac{2\alpha}{3\pi}(Z\alpha)^2 \, 0.24607, \quad (28a)$$

$$\delta g_C(2P_{3/2}) = \frac{4\alpha}{3\pi}(Z\alpha)^2 \, 0.06151. \quad (28b)$$

Summing all low-energy corrections, the spurious logarithmic terms cancel, and we obtain

$$b_{20}^{(L)}(2P_{1/2}) = 0.98428, \quad (29a)$$

$$b_{20}^{(L)}(2P_{3/2}) = 0.49216, \quad (29b)$$

as the spin-dependent low-energy contribution to the bound-electron g factor. The result for $2P_{3/2}$ is equal to half the correction for $2P_{1/2}$ (this fact is independently proven also Appendix A). We denote the low-energy contribution to the b_{20} coefficient defined in Eq. (2) by $b_{20}^{(L)}$.

B. Length gauge

In the length gauge, the interaction with the quantized electromagnetic field is given by the dipole interaction $-e\vec{x} \cdot \vec{E}$, where $\vec{E}$ is the electric-field operator [22]. The gauge-invariant [22] nonrelativistic self-energy in the length-gauge reads

$$\delta E = -\frac{2\alpha}{3\pi} \int_0^{m\epsilon} d\omega \, \omega^3 \left\langle j\frac{1}{2} \left| \vec{x} \frac{1}{H_{\text{NR}} - E_{\text{NR}} + \omega} \vec{x} \right| j\frac{1}{2} \right\rangle. \quad (30)$$

In the length gauge, the contribution of the wave-function correction vanishes because of the same reasons as for the velocity gauge. Also, there is no correction to the transition current, because the canonical momentum does not enter the interaction Hamiltonian in the length gauge. We only have corrections to the Hamiltonian and to the energy. We start with the energy perturbation,

$$\delta E_{\mathcal{E}} = -\frac{2\alpha}{3\pi}\langle h_{M,0}\rangle \int_0^{m\epsilon} d\omega \, \omega^3$$
$$\times \left\langle j\frac{1}{2} \left| \vec{x} \left(\frac{1}{H_{\text{NR}} - E_{\text{NR}} + \omega}\right)^2 \vec{x} \right| j\frac{1}{2} \right\rangle. \quad (31)$$

The subscript $\mathcal{E}$ instead of E serves to differentiate the length-gauge as opposed to the velocity-gauge form of the correction. Indeed, the numerical results for the corresponding correction to the bound-electron g factor are different from those given

in Eq. (22) and read

$$\delta g_{\mathcal{E}}(2P_{1/2}) = \frac{2\alpha}{3\pi}(Z\alpha)^2 \left[-\frac{1}{2}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) - 0.88488\right], \quad (32a)$$

$$\delta g_{\mathcal{E}}(2P_{3/2}) = \frac{4\alpha}{3\pi}(Z\alpha)^2 \left[-\frac{1}{2}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) - 0.88488\right]. \quad (32b)$$

For the correction to the Hamiltonian, we get

$$\delta E_{\mathcal{H}} = \frac{2\alpha}{3\pi} \int_0^{m\epsilon} d\omega \, \omega^3$$
$$\times \left\langle j\frac{1}{2} \left| \vec{x} \left(\frac{1}{H_{\text{NR}} - E_{\text{NR}} + \omega}\right)^2 h_{M,0}\vec{x} \right| j\frac{1}{2} \right\rangle. \quad (33)$$

A numerical evaluations leads to

$$\delta g_{\mathcal{H}}(2P_{1/2}) = \frac{2\alpha}{3\pi}(Z\alpha)^2 \left[\frac{1}{2}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) + 1.25399\right], \quad (34a)$$

$$\delta g_{\mathcal{H}}(2P_{3/2}) = \frac{4\alpha}{3\pi}(Z\alpha)^2 \left[\frac{1}{2}\ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) + 0.97716\right]. \quad (34b)$$

Adding the length-gauge corrections, the logarithmic terms cancel, and it is straightforward to numerically verify the gauge-invariance relation

$$\delta g_E + \delta g_H + \delta g_C = \delta g_{\mathcal{E}} + \delta g_{\mathcal{H}} \quad (35)$$

and thus, the numerical results already given in Eq. (29).

Let us finally discuss the analytic proof of the gauge invariance. Using the commutator relation

$$\frac{p^i}{m} = i[H_{\text{NR}} - E_{\text{NR}} + \omega, x^i], \quad (36)$$

and with the help of a somewhat lengthy calculation, it is possible to show analytically that the velocity-gauge and the length-gauge forms of the low-energy contributions are equal. The calculation follows ideas outlined in detail in Ref. [23] where the more complicated case of a relativistic correction to a transition matrix element was considered. Here, we are interested mainly in the numerical value of the correction, for which the gauge invariance provides a highly nontrivial check. Note that the matrix elements governing the transitions of the reference to the virtual states are completely different in the length and in the velocity gauges, and the final results are obtained after summing over the discrete and continuous parts of the spectrum of virtual states.

IV. CONCLUSIONS

In our approach to the calculation of the bound-electron g factor of P states, the contribution due to high-energy virtual photons can be obtained using two alternative approaches, based either on an effective Dirac equation or on a low-energy effective Hamiltonian. The contribution due to low-energy photons is treated as a perturbation of the bound-electron self-energy [18] due to the interaction with the external uniform magnetic field. Corrections to the Hamiltonian, to the bound-state energy and (in the velocity gauge) to the

transition current have to be considered. The final results for the low-energy parts in the velocity- and length-gauges agree although the individual contributions differ (including the coefficients of spurious logarithmic terms).

Adding the high-energy contribution to the g factor correction given in Eq. (10) and the low-energy effect given in Eq. (29), we obtain the following results for the self-energy correction of order $\alpha(Z\alpha)^2$ to the bound-electron g factor of $2P$ states ($b_{20} = b_{20}^{(H)} + b_{20}^{(L)}$):

$$b_{20}(2P_{1/2}) = 0.48429, \tag{37a}$$

$$b_{20}(2P_{3/2}) = 0.59214, \tag{37b}$$

where the b_{20} coefficient has been defined in Eq. (2). Both above results compare favorably with recently obtained numerical data for low-Z hydrogenlike ions [24] (see also Appendix B). An obvious generalization of the formalism outlined here to the $3P$ and $4P$ states yields the results

$$b_{20}(3P_{1/2}) = 0.40500, \tag{37c}$$

$$b_{20}(3P_{3/2}) = 0.55250, \tag{37d}$$

$$b_{20}(4P_{1/2}) = 0.31331, \tag{37e}$$

$$b_{20}(4P_{3/2}) = 0.50665. \tag{37f}$$

The two main results of the current investigation can be summarized as follows. First, in Sec. III we formulate a generalizable procedure for the calculation of low-energy corrections to the Landé g_j factors in one-electron ions, applicable to P states and states with higher angular momenta. This procedure is based on choosing a specific reference axis for the external magnetic field. In the future, it might be applied to include higher-order terms from the Hamiltonian (11) which couple the orbital and spin degrees of freedom. Second, we resolve the discrepancy reported in Ref. [24] regarding the low-Z limit of the $\alpha(Z\alpha)^2$ correction to the g_j factor with previous results reported in Ref. [5] for this correction [see Eq. (37) and Appendix B]. In Appendix A, it is shown that the discrepancy to the results of Ref. [5] can be traced to the final evaluation of the logarithmic sums over virtual states, while the angular momentum algebra is in agreement. That is a further reason why the cross-check of our calculation in the length and velocity gauges appeared to be useful.

Regarding the experimental usefulness of the obtained results, we can say that recent proposals [25] concerning measurements of the bound-electron g factor of low-Z hydrogenlike ions are based on double-resonance schemes that also involve transitions to $2P$ states in the presence of the strong magnetic fields of Penning traps. In order to fine-tune the double-resonance setup, the results obtained here might be useful. Also, the results reported here serve as a general verification for the analytic formalism used in the theoretical treatment of α^3 corrections to the g factor of 2^3P states in helium, for which an interesting discrepancy of experimental and theoretical results persists (see Ref. [12] and Sec. V of Ref. [16]).

We conclude with the following remark. Our calculation concerns the g factor of P states, and we confirm that in the order $\alpha(Z\alpha)^2$, low-energy virtual photons yield an important contribution. From the treatment in Sec. III, we can understand physically why there is no such low-energy effect

of order $\alpha(Z\alpha)^2$ for S states. Namely, a Schrödinger-Pauli $S_{1/2}$ state happens to be an eigenstate of the Hamiltonian $h_{M,0}$. We have $h_{M,0}|nS_{1/2}(\mu = \pm\frac{1}{2})\rangle = \pm|nS_{1/2}(\mu = \pm\frac{1}{2})\rangle$. This property holds because an S state carries no orbital angular momentum, and therefore is an eigenstate of the third component of the spin operator σ_0, and b_{20} therefore vanishes for S states [26]. For P states and states with higher orbital angular momenta, the situation is different: these states are not eigenstate of $h_{M,0}$ irrespective of their angular momentum projection, even though $h_{M,0}$ commutes with the nonrelativistic Hamiltonian H_{NR}. Therefore, there is a residual effect of order $\alpha(Z\alpha)^2$ due to low-energy virtual photons for states with nonvanishing angular momenta.

APPENDIX A: REMARKS ON THE LOW-ENERGY PART

First of all, let us remark that our results reported in Sec. III can be expressed as logarithmic sums over the spectrum of atomic hydrogen. After performing the angular algebra [17], we can write the total low-energy correction $\delta g^{(L)}(nP_j) = \delta g_{\mathcal{E}}(nP_j) + \delta g_{\mathcal{H}}(nP_j)$ as follows:

$$\delta g^{(L)}(nP_{1/2}) = \frac{8\alpha}{9\pi} \sum_m (E_{mS} - E_{nP})^2 \langle mS||\vec{r}||nP\rangle^2$$
$$\times \ln\left(\frac{2|E_{mS}-E_{nP}|}{(Z\alpha)^2 m}\right) - \frac{8\alpha}{9\pi} \sum_m (E_{mD} - E_{nP})^2$$
$$\times \langle nP||\vec{r}||nD\rangle^2 \ln\left(\frac{2|E_{mD} - E_{nP}|}{(Z\alpha)^2 m}\right) \tag{A1}$$

and

$$\delta g^{(L)}(nP_{3/2}) = \frac{4\alpha}{9\pi} \sum_m (E_{mS} - E_{nP})^2 \langle mS||\vec{r}||nP\rangle^2$$
$$\times \ln\left(\frac{2|E_{mS}-E_{nP}|}{(Z\alpha)^2 m}\right) - \frac{4\alpha}{9\pi} \sum_m (E_{mD}-E_{nP})^2$$
$$\times \langle nP||\vec{r}||nD\rangle^2 \ln\left(\frac{2|E_{mD} - E_{nP}|}{(Z\alpha)^2 m}\right). \tag{A2}$$

Here, $\langle mS||\vec{r}||nP\rangle$ and $\langle mD||\vec{r}||nP\rangle$ are reduced matrix elements in the notation of Ref. [27]. Because $(E_{mS} - E_{nP}) \propto (Z\alpha)^2$ and $\langle mS||\vec{r}||nP\rangle \propto (Z\alpha)^{-1}$, the above corrections to the g factor are manifestly of order $\alpha(Z\alpha)^2$. The sums over m extend over both the discrete as well as the continuous part of the hydrogen spectrum and can conveniently be evaluated using basis-set techniques [28].

Because it may not be completely evident from the presentation in Ref. [5], we reemphasize here that the authors of the cited article evaluate a correction δg_ℓ to the orbital g factor according to the definition

$$H_{\mathrm{eff}} = g_s \mu_B \vec{S} \cdot \vec{B} + g_\ell \, \mu_B \vec{L} \cdot \vec{B} \tag{A3}$$

for the effective interaction of a bound electron with an external magnetic field ($\vec{S} = \frac{1}{2}\vec{\sigma}$ measures the electron spin, and we have $g_S \approx 2$, $g_\ell \approx 1$). Here, an interesting analogy to the description hyperfine splitting can be drawn, because the interaction with the nuclear magnetic field can also be separated into distinct components, namely the orbital, spin-dipole, and Fermi contact terms given, e.g., in Eqs. (24)–(33) of Ref. [29].

Returning to the discussion of the g factor, we see that as a combination of g_s and g_ℓ, the Landé g factor is obtained as

$$
\begin{aligned}
g_j &= g_\ell \frac{j(j+1) + \ell(\ell+1) - s(s+1)}{2j(j+1)} \\
&\quad + g_s \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)} \\
&\approx \frac{3j(j+1) - \ell(\ell+1) + s(s+1)}{2j(j+1)}.
\end{aligned}
\tag{A4}
$$

In our notation, the analytic result given in Eq. (14) of Ref. [5] for the correction to the orbital g factor reads

$$
\begin{aligned}
\delta g_\ell(nP) &= \frac{\alpha}{3\pi} \sum_m (E_{mS} - E_{nP})^2 \langle mS||\vec{r}||nP\rangle^2 \\
&\quad \times \ln\left(\frac{2|E_{mS} - E_{nP}|}{(Z\alpha)^2 m}\right) - \frac{\alpha}{3\pi} \sum_m (E_{mD} - E_{nP})^2 \\
&\quad \times \langle nP||\vec{r}||nD\rangle^2 \ln\left(\frac{2|E_{mD} - E_{nP}|}{(Z\alpha)^2 m}\right).
\end{aligned}
\tag{A5}
$$

The prefactors multiplying g_ℓ in Eq. (A4) read $\frac{4}{3}$ for $P_{1/2}$ and $\frac{2}{3}$ for $P_{3/2}$ states, and therefore the analytic formula obtained in Eq. (14) of Ref. [5] is in agreement with our approach for both $P_{1/2}$ and $P_{3/2}$ states, after the correction to g_ℓ is converted into the corresponding modification of g_j. However, their numerical result $\delta g_\ell = -0.24\alpha^3$ disagrees with our result both in sign and in magnitude. Indeed, expressed in terms of our $b_{20}^{(L)}$ coefficient, the results indicated in Ref. [5] would imply that $b_{20}^{(L)}(2P_{1/2}) = -4.02$ and $b_{20}^{(L)}(2P_{3/2}) = -8.04$.

TABLE I. Higher-order remainder functions $i_{1/2}(Z\alpha)$ and $i_{3/2}(Z\alpha)$ for the self-energy correction to the g factor of $2P_{1/2}$ and $2P_{3/2}$ states, respectively, as obtained recently in Ref. [24]. The value of α employed in the calculation is $\alpha^{-1} = 137.036$, and the numerical uncertainty of the all-order (in $Z\alpha$) calculation due to the finite number of integration points in the numerical calculation is indicated in brackets.

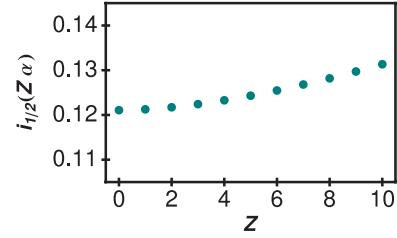| Z	$g_{1/2}(Z\alpha)$	$g_{3/2}(Z\alpha)$
1	0.121258(21)	0.148104(21)
2	0.121715(22)	0.148294(24)
3	0.122414(19)	0.148567(24)
4	0.123280(14)	0.148851(22)
5	0.124305(10)	0.149338(18)
6	0.125473(7)	0.149816(14)
7	0.126803(5)	0.150350(11)
8	0.128186(4)	0.150933(7)
9	0.129711(2)	0.151561(4)
10	0.131336(2)	0.152231(4)

FIG. 1. (Color online) The higher-order remainder function $i_{1/2}(Z\alpha)$ is shown as a function of Z. Numerical values for $i_{1/2}(Z\alpha)$ are given in Table I. The point at $Z = 0$ is given by the coefficient $\frac{1}{4}b_{20}(2P_{1/2})$ and is approached smoothly.

Finally, let us note that the calculation of the orbital correction to the g_j factor is only applicable to order $\alpha(Z\alpha)^2$, not $\alpha(Z\alpha)^4$, because the higher-order terms in the magnetic interaction (II) couple the orbital and spin degrees of freedom. The formalism outlined in Sec. III generalizes easily to the calculation of higher-order corrections that couple spin and orbital angular momentum, which might be needed in the future, whereas the separation into spin and orbital g factors only holds up to order $\alpha(Z\alpha)^2$.

APPENDIX B: COMPARISON TO NUMERICAL DATA

We parametrize the one-loop self-energy correction $\delta^{(1)}g$ to the g factor of P states as

$$
\delta^{(1)}g(2P_j) = \frac{\alpha}{\pi}\{b_{00} + (Z\alpha)^2 i_j(Z\alpha)\},
\tag{B1}
$$

where $i_j(Z\alpha)$ is the nonperturbative (in $Z\alpha$) remainder function. The remainder functions $i_{1/2}(Z\alpha)$ and $i_{3/2}(Z\alpha)$ for $2P_{1/2}$ and $2P_{3/2}$, respectively, have recently been evaluated in Ref. [24]. Numerical values of $i_j(Z\alpha)$ for $Z = 1, \ldots, 10$ are given in Table I. Note that these data imply a spin-dependence of the higher-order correction term b_{20} beyond the spin-dependence of the high-energy part given by Eq. (10). The limit as $Z\alpha \to 0$ of the remainder function $i_j(Z\alpha)$ is

$$
\lim_{Z\alpha \to 0} i_j(Z\alpha) = \tfrac{1}{4}b_{20}(2P_j).
\tag{B2}
$$

As shown in Figs. 1 and 2, this limit is being consistently approached by the numerical data.
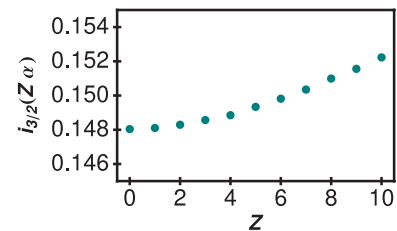

FIG. 2. (Color online) Same as Fig. 1, but for the $2P_{3/2}$ state. The higher-order remainder function $i_{3/2}(Z\alpha)$ is plotted as a function of Z, with numerical values for $i_{3/2}(Z\alpha)$ given in Table I. The point at $Z = 0$ is $\lim_{Z\alpha \to 0} i_{3/2}(Z\alpha) = \tfrac{1}{4}b_{20}(2P_{3/2})$. The limit is approached smoothly.

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