Quantum electrodynamic corrections to the g factor of helium P states

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(Received 27 June 2012; published 10 August 2012)

The Landé g factor describes the response of an atomic energy level to an external perturbation by a uniform and constant magnetic field. In the case of many-electron systems, the leading term is given by the interaction $\mu_B\,(\vec{L}+2\,\vec{S})\cdot\vec{B}$, where $\vec{L}$ and $\vec{S}$ are the orbital and spin angular momentum operators, respectively, summed over all electrons. For helium, a long-standing experimental-theoretical discrepancy for P states motivates a re-evaluation of the higher order terms which follow from relativistic quantum theory and quantum electrodynamics (QED). The tensor structure of relativistic corrections involves scalar, vector, and symmetric and antisymmetric tensor components. We perform a tensorial reduction of these operators in a Cartesian basis, using an approach which allows us to separate the internal atomic from the external degrees of freedom (magnetic field) right from the start of the calculation. The evaluation proceeds in a Cartesian basis of helium eigenstates, using a weighted sum over the magnetic projections. For the relativistic corrections, this leads to a verification of previous results obtained using the Wigner-Eckhart theorem. The same method, applied to the radiative correction (Bethe logarithm term) leads to a spin-dependent correction, which is different for singlet versus triplet P states. Theoretical predictions are given for singlet and triplet $2P$ and triplet $3P$ states and compared to experimental results where available.

DOI: 10.1103/PhysRevA.86.022508 PACS number(s): 31.30.js, 12.20.Ds, 31.15.−p, 06.20.Jr

I. INTRODUCTION AND OVERVIEW

A. Few-electron systems and g factor

The quantum electrodynamic (QED) theory of bound systems describes, among other things, three "fundamental" characteristic effects that involve the spectrum of bound systems, namely, (i) the Lamb shift, which is the energy shift of bound states due to the self-interaction of the electrons and due to tiny corrections to the Coulomb force law at small distances, (ii) the g factor of bound states, which describes the energy shift of a bound state due to the interaction with an external, uniform magnetic field (Zeeman effect), and (iii) the hyperfine splitting, which is given by the interaction of bound electrons with the nuclear magnetic moment. These effects seem to be the three most commonly studied QED effects for bound states, because of prominent high-precision experiments in all three mentioned areas. The leading QED corrections to all three mentioned effects are given by the self-energy of the orbiting particle and by vacuum polarization.

The long-standing discrepancy between theory and experiment for the Zeeman coupling factor g'_L for the 2^3P state of helium [1] has motivated a number of independent theoretical papers [2–5] on the subject. Here, by convention, g'_L is the complete orbital part of the g_J factor for the helium P state, including relativistic and radiative corrections. For hydrogenlike systems, the self-energy corrections to the g_J factor and to the hyperfine splitting can be formulated in a similar framework [6,7], by observing that they can be described as a "dressed" self-energy correction in an additional magnetic field, namely, for the case of the g_J factor, in a uniform external magnetic field, and, for the case of the hyperfine splitting, in the magnetic dipole field of the atomic nucleus.

For more complex atoms and ions, the theory of the g factor is more complicated because in higher order, the electron-electron interaction is intertwined with the coupling to the external magnetic field. In leading order, the total orbital angular momentum $\vec{L}$ and the spin angular momentum $\vec{S}$ couple to the external magnetic field $\vec{B}$ as described by the Hamiltonian matrix element

$$\langle H_M\rangle \approx \langle \mu_B\,(\vec{L}+2\,\vec{S})\cdot\vec{B}\rangle = g_J\,\mu_B\,B\,\mu\,, \tag{1}$$

where g_J is the Landé g factor, and μ_B is the Bohr magneton; that is, $\mu_B=-e/(2m)$ where m is the electron mass and $e=-|e|$ is the electron charge. The orbital angular momentum $\vec{L}$ and the spin angular momentum $\vec{S}$ are summed over all electrons. As long as the separation into terms proportional to $\vec{L}\cdot\vec{B}$ and $\vec{S}\cdot\vec{B}$ remains valid, this gives rise to an orbital $g_L\approx 1$ factor and a spin $g_S\approx 2$ factor, so that

$$g_J = g_L\,\frac{J(J+1)+L(L+1)-S(S+1)}{2J(J+1)} + g_S\,\frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}\,. \tag{2}$$

In leading order, the Landé g factor is thus given by the well-known formula

$$g_J \approx \frac{3J(J+1)-L(L+1)+S(S+1)}{2J(J+1)}\,. \tag{3}$$

In higher order, due to spin-orbit coupling, one cannot separate the magnetic-field interaction any more into terms proportional to $\vec{L}\cdot\vec{B}$ and $\vec{S}\cdot\vec{B}$, and therefore, one cannot uniquely identify the orbital g_L and spin g_S factors any more. For hydrogen, the corresponding mechanism has been discussed in

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Appendix A of Ref. [8]. The separation into g_L and g_S remains valid up to relative order α^3, where α is the fine-structure constant, provided one adds a tiny correction due to a higher order tensor structure, called g_x in Refs. [4,9].

B. Angular-momentum algebra

For P states, as opposed to S states, the angular momentum algebra involved in the calculation of the bound-electron g factor can become rather complicated, and two approaches have been used. In approach (i), used in Refs. [4,9], the authors formulate the entire theory in terms of Wigner $3J$, $6J$, and $9J$ symbols, which enables them to perform all calculations in terms of reduced matrix elements. In turn, these can be written in terms of the radial component of the wave functions as obtained from variational calculations.

In approach (ii), which has been used for hydrogenlike systems [8], one first chooses a specific component of the Hamiltonian "vector" $\mu_B(\vec{L}+2\vec{S})$, multiplying the magnetic field $\vec{B}$, and a specific magnetic projection of the reference state. Natural choices consist in the z component of the Hamiltonian "vector" and the state with magnetic projection $\mu = \frac{1}{2}$ as indicated in Eqs. (15) and (16) of Ref. [8]. Due to the Wigner-Eckhart theorem, one can then formulate all relative corrections to the g factor in terms of ratios, relating the effect calculated with a correction to the magnetic Hamiltonian to the leading-order effect, provided one uses the same state for each matrix element. This disentangles the internal atomic degrees of freedom from the external degrees of freedom (the magnetic field). For the hyperfine splitting, a similar approach is outlined around Eq. (7) of Ref. [7].

For helium, it is preferable to formulate the theory in terms of elements of the radial wave functions alone, by expressing the matrix elements in terms of sums over magnetic projections, where the angular and spin degrees of freedom are summed over and evaluated in closed form. The latter sum can naturally be expressed in terms of a "radial" representation of a P state as obtained from a variational calculation in a fully correlated, nonrelativistic basis. Here, we thus choose an approach combining ideas from (i) and (ii). First, the relativistic and radiative corrections are expressed in terms of particular tensor structures, and then, we evaluate these on a weighted sum over the projections m of the total angular momentum of the helium state. This approach combines the advantages of approach (i), namely, the easy applicability to helium, with the advantages of approach (ii), namely, the full disentanglement of the external degrees of freedom (magnetic field) from the internal atomic degrees of freedom right from the start of the calculation.

Our investigation is motivated in part by an interesting theoretical-experimental disagreement between the experimental result reported in Ref. [1] and theory work described in Refs. [2–4] and Sec. V of Ref. [5]. Our calculation is valid up to and including relativistic and radiative correction of relative order α^3 and to second order in the electron-nucleus mass ratio (for the leading nonrelativistic term). We proceed as follows. In Sec. II, the terms in the Hamiltonian which govern the bound-state g factor are analyzed in terms of their tensor structure. The discussion is complemented in Sec. III by an analysis of the spin and the tensor reduction of the particular correction terms. Finally, in Sec. IV, numerical evaluations are described which allow us to obtain a highly accurate theoretical prediction for the g_J factor in helium, for $2P$ and $3P$ states. Conclusions are reserved for Sec. VI. Atomic units with $e = \hbar = 1$ (e denotes the physical electron charge), unit electron mass $m = 1$, $\alpha = 1/c$, and $\epsilon_0 = 1/(4\pi)$ are used throughout the paper.

II. HAMILTONIAN

A. Leading order

A careful treatment of the g factor requires an analysis of the reduced-mass dependence. We denote the electron mass as m and the mass of the nucleus as M. The reduced mass μ and the mass ratio λ are given by

$$\mu = \frac{mM}{m+M}, \quad \lambda = -\frac{\mu}{M}. \tag{4}$$

The interaction with the external magnetic field, in leading order plus the reduced-mass correction, is given by [10,11]

$$H_M = \mu_B \sum_a \left[g_L\,(\vec{r}_a \times \vec{p}_a) + \frac{g_S}{2}\,\vec{\sigma}_a \right] \cdot \vec{B} - \mu_B \frac{m}{M} \sum_{a\neq b} (\vec{r}_a \times \vec{p}_b) \cdot \vec{B}\,. \tag{5}$$

The finite mass of the nucleus yields a correction term (second term) of order $\mathcal{O}(\lambda)$. The sum over a and b in Eq. (5) counts the electrons of the bound system. The well-known spin factor g_S can be expressed in the form (including two-loop corrections)

$$g_S = 2\left(1 + \frac{\alpha}{2\pi} - 0.328\,478\,695\,\frac{\alpha^2}{\pi^2} + \cdots\right). \tag{6}$$

It is equal to the g factor of the free electron including the anomalous magnetic moment. The terms proportional to g_L in Eq. (5) give rise to an orbital factor $g_L = 1 - m/M$. The terms in Eq. (5) contain all terms of relative order $\mathcal{O}(\lambda)$. We note that this scaling of g_L, which has originally been derived in Ref. [10], goes beyond the "trivial scaling" of momenta and distances, which is discussed below.

Namely, in general, the scaling of the momenta and distances with the reduced mass entails the scaling factors (see the Appendix)

$$\vec{p} \to \vec{p}\,(1+\lambda), \quad \vec{r} \to (1+\lambda)^{-1}\,\vec{r}\,. \tag{7}$$

It results in prefactors of the form $(1+\lambda)^n$ with a certain scaling degree n. For the leading terms given in Eq. (5), we have $n = 0$, and the terms commute with the nonrelativistic Hamiltonian of the helium atom [without mass polarization; see Eq. (A2) below]:

$$H_0 = \sum_a \left(\frac{\vec{p}_a^{\,2}}{2\mu} - \frac{Z}{r_a}\right) + \sum_{a>b} \frac{1}{r_{ab}}\,. \tag{8}$$

While the first-order correction to the wave function due to the magnetic interaction vanishes, the mass polarization

term $H_{\rm mp}$

$$H_{\rm mp} = -\frac{\lambda}{\mu} \sum_{a>b} \vec{p}_a \cdot \vec{p}_b \,. \tag{9}$$

generates a nonvanishing perturbation to the wave function. The perturbation can then be evaluated on the leading-order Hamiltonian (5). For the finite-mass effect of order $O(\lambda^2)$, one additional effect is the mass polarization correction to the second term in Eq. (5). The third-order term involving the leading magnetic interaction term in Eq. (5) and two mass polarization insertions also yields a finite-mass correction of second order in λ. Its effect on the g_L prefactor and off-diagonal corrections are discussed in the following.

B. Tensor decomposition of the Zeeman Hamiltonian

Let us now turn to the tensor decomposition of the Zeeman Hamiltonian. The first term in Eq. (5) can be rewritten in the form

$$H_{M0} = \mu_B \, \vec{G}_0 \cdot \vec{B} \,, \tag{10a}$$

$$G_0^i = \sum_a \left(g_L \, v_{0,a}^i + \frac{g_S}{2} \, d_0 \, \sigma_a^i \right), \tag{10b}$$

$$v_{0,a}^i = (\vec{r}_a \times \vec{p}_a)^i \,, \quad d_0 = 1 \,, \tag{10c}$$

where $v_{0,a}^i$ is a vector coefficient and d_0 is a diagonal (scalar) coefficient multiplied only by a spin matrix. Here and in the following, Cartesian coordinates are denoted by superscripts; that is, the x component of $\vec{v}_{0,a}$ is given as $v_{0,a}^x$ (the superscript assumes the values $i = x,y,z$). In general, a superscript i denotes a Cartesian component, whereas the lowercase variable i (no superscript or subscript) is otherwise reserved for the imaginary unit. We have decomposed the tensor structure of Eq. (10) into a vector and a spin part. This approach is now generalized to other corrections δH to the leading Zeeman Hamiltonian H_{M0},

$$\delta H_M = \mu_B \sum_\gamma \vec{G}_\gamma \cdot \vec{B}, \tag{11}$$

where γ counts the correction terms. The operators $\vec{G}_\gamma$ are linearly coupled to the magnetic field $\vec{B}$. We split each element G_γ into a tensor structure of spatial coordinates coupled to the magnetic field $\vec{B}$ as well as spin matrices $\vec{\sigma}_a$. From the spinless terms of the form $\vec{v} \cdot \vec{B}$, we obtain the vector coordinates v^i.

The second-order spatial tensors A^{ij} in terms of the form $A^{ij}\sigma_a^i B^j$ can be tensorially decomposed into a diagonal (scalar) part d, a symmetric tensor part t, and an antisymmetric tensor part r,

$$A^{ij} = \frac{d}{3}\,\delta^{ij} + t^{ij} + r^{ij}, \tag{12a}$$

$$d = A^{kk}, \tag{12b}$$

$$t^{ij} = \frac{A^{ij} + A^{ji}}{2} - \frac{1}{3}\delta^{ij}\,A^{kk}, \tag{12c}$$

$$r^{ij} = \frac{A^{ij} - A^{ji}}{2}, \tag{12d}$$

where the summation convention is used for the Cartesian coordinates as is done throughout the paper.

The orbital angular momentum part in leading order is identified as the vector term $v_{0,a}^i$, and the spin part as related to the scalar operator d_0. For the finite-mass correction in Eq. (5) with G_1^i in tensor form, we have the identification

$$G_1^i = -\frac{m}{M} \sum_{a\neq b} v_{1,ab}^i, \tag{13a}$$

$$v_{1,ab}^i = (\vec{r}_a \times \vec{p}_b)^i, \tag{13b}$$

which is included as the first term ($\gamma = 1$) in δH_M. This grouping is extended to higher order terms and to make contact with the literature. According to Appendix A of Ref. [9] and Eqs. (2)–(4) of Ref. [4], we can split the g_L and g_S factors into leading-order terms, denoted by the same symbols, and corrections δg_L and δg_S, which, when added to g_L and g_S, yield the complete results g_L' and g_S', which include the correction terms. So, for triplet P states,

$$\delta g_L = g_L' - g_L, \quad \delta g_S = g_S' - g_S. \tag{14}$$

This notation has been introduced in the theoretical analysis of the experimental data for helium $2\,^3P$ states [9] based on angular momentum methods [4,12,13]. Compared to Eqs. (22) and (23) of Ref. [4], the prefactors in the expressions $\delta g_L = g_L' - \sqrt{(2L+1)L(L+1)/6}\; g_L$ and $\delta g_S = g_S' - \sqrt{(2S+1)S(S+1)/6}\; g_S$ evaluate to unity for triplet P states; for singlet P states, the first equality in Eq. (14) remains valid while $g_S = 0$. The symmetric tensor parts t^{ij} are related to the g_x factor [9], and the mean values of the antisymmetric part r^{ij} result in a zero correction. Later, these quantities were determined in subsequent theoretical calculations of other authors [4,14]. We follow these conventions in order to be able to compare our final formulas with their results. We here use a Cartesian decomposition of the higher order Zeeman Hamiltonian, as an alternative to angular algebra methods with $3J$, $6J$, and $9J$ symbols [9], and identify the tensor contributions to g_L, g_S, g_x as described in the following.

C. Relativistic corrections

Relativistic corrections have been derived from the Breit Hamiltonian [15–17]. We follow formulas from Eq. (32) of Ref. [5] with six relativistic corrections to the Zeeman effect,

$$\delta H_{\rm rel} = \mu_B\,\alpha^2 \sum_a \left\{ -\frac{\vec{p}_a^{\,2}}{2}[(\vec{r}_a \times \vec{p}_a) + \vec{\sigma}_a] \cdot \vec{B} + Z\,\frac{g_S - 1}{4}\,\frac{(\vec{r}_a \times \vec{\sigma}_a)(\vec{r}_a \times \vec{B})}{r_a^3} - \frac{g_S - 2}{4}(\vec{p}_a \cdot \vec{\sigma}_a)(\vec{p}_a \cdot \vec{B}) \right\}$$

$$+ \mu_B\alpha^2 \sum_{a\neq b} \left\{ -\frac{g_S - 1}{4}\,\frac{(\vec{r}_{ab} \times \vec{\sigma}_a)(\vec{r}_a \times \vec{B})}{r_{ab}^3} - \frac{g_S}{4}\,\frac{(\vec{r}_{ab} \times \vec{\sigma}_b)(\vec{r}_a \times \vec{B})}{r_{ab}^3} + \frac{p_a^i}{2}\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i\, r_{ab}^j}{r_{ab}^3}\right)(\vec{r}_b \times \vec{B})^j \right\}, \tag{15}$$

$$\delta H_{\rm rel} = \mu_B\,\vec{G}_2 \cdot \vec{B} \,.$$

It is straightforward to identify the Cartesian tensor form of the relativistic correction $\vec{G}_2$,

$$G_2^i = \mu_B\,\alpha^2 \sum_a \left\{ -\frac{1}{2}\left(v_{2,a}^i + d_{2,a}\,\sigma_a^i\right) + \frac{Z\,(g_S-1)}{4}\left(\frac{2}{3}\,d_{3,a}\,\sigma_a^i - t_{3,a}^{ij}\,\sigma_a^j\right) - \frac{g_S-2}{2}\left(\frac{d_{2,a}\,\sigma_a^i}{3} + t_{4,a}^{ij}\,\sigma_a^j\right)\right\}$$
$$+\mu_B\,\alpha^2 \sum_{a\neq b} \left\{ -\frac{g_S-1}{4}\left(\frac{2}{3}\,d_{5,ab}\,\sigma_a^i - t_{5,ab}^{ij}\,\sigma_a^j + r_{5,ab}^{ij}\,\sigma_a^j\right) - \frac{g_S}{4}\left(\frac{2}{3}\,d_{5,ab}\,\sigma_b^i - t_{5,ab}^{ij}\,\sigma_b^j + r_{5,ab}^{ij}\,\sigma_b^j\right)\right.$$
$$\left. -\frac{1}{2}\left(v_{61,ab}^i - v_{62,ab}^i\right)\right\}. \tag{16}$$

Indeed, the tensor components from the first four terms in Eq. (16a) read as follows:

$$d_{2,a} = \vec{p}_a^{\,2}, \tag{17a}$$
$$v_{2,a}^i = \vec{p}_a^{\,2}\,(\vec{r}_a \times \vec{p}_a)^i, \tag{17b}$$
$$d_{3,a} = \frac{1}{r_a}, \tag{17c}$$
$$t_{3,a}^{ij} = \frac{1}{r_a^3}\left(r_a^i r_a^j - \frac{1}{3}\,\delta^{ij}\,r_a^2\right), \tag{17d}$$
$$t_{4,a}^{ij} = p_a^i\,p_a^j - \frac{1}{3}\,\delta^{ij}\,\vec{p}_a^{\,2}. \tag{17e}$$

Furthermore, we have the following terms from the fifth corrections in Eq. (16a):

$$d_{5,ab} = \frac{\vec{r}_a\cdot\vec{r}_{ab}}{r_{ab}^3}, \tag{17f}$$
$$t_{5,ab}^{ij} = \frac{1}{r_{ab}^3}\left(\frac{r_a^i r_{ab}^j + r_a^j r_{ab}^i}{2} - \frac{\vec{r}_a\cdot\vec{r}_{ab}}{3}\,\delta^{ij}\right), \tag{17g}$$
$$r_{5,ab}^{ij} = \frac{1}{2r_{ab}^3}\left(r_a^i r_b^j - r_a^j r_b^i\right). \tag{17h}$$

Finally, the sixth term in Eq. (16a) yields a remaining vector structure,

$$v_{61,ab}^i = \frac{(\vec{r}_a\times\vec{p}_b)^i}{r_{ab}}, \tag{17i}$$
$$v_{62,ab}^i = \frac{(\vec{r}_a\times\vec{r}_b)^i\,(\vec{r}_{ab}\cdot\vec{p}_b)}{r_{ab}^3}. \tag{17j}$$

We proceed to a final numerical evaluation of these corrections later.

D. Self-energy correction

We follow Ref. [5] and base the calculation of the low-energy part of the self-energy proceeds on a nonrelativistic Hamiltonian in the presence of an electromagnetic field in the length gauge,

$$H = H_0 + H_{M0} + H_\gamma - e\,\vec{r}_1\cdot\vec{E} - e\,\vec{r}_2\cdot\vec{E}, \tag{18}$$

where H_0 is the unperturbed Hamiltonian of the atom, H_γ is the Hamiltonian of the photon field, H_{M0} is the leading-order magnetic interaction given in Eq. (10), and the two dipole interaction operators describe the interaction of the bound electrons with the quantized electromagnetic field. The self-energy has the form

$$\delta E = -\frac{2\,\alpha}{3\,\pi}\int_0^\epsilon \mathrm{d}\omega\,\omega^3\,\langle\phi|(\vec{r}_1+\vec{r}_2)$$
$$\times\,\frac{1}{H_0+H_M-E_0+\omega}(\vec{r}_1+\vec{r}_2)|\phi\rangle. \tag{19}$$

It is understood that δE is to be expanded in first order in the magnetic field $\vec{B}$. Then, replacing the coordinates by electron momenta and using commutation relations, it is easy to rederive Eq. (38) of Ref. [5], additionally assuming that the state ϕ has definite m_L and m_S quantum numbers (projections of the orbital and spin angular momenta onto the quantization axis). We might just as well assume that the reference state has a defined value of the magnetic quantum number m_J of the total angular momentum,

$$\delta E = -2\,\mu_B\,\frac{\alpha}{\pi}\{\mathrm{i}\,\epsilon_{irs}\langle m_J|(\vec{p}_1+\vec{p}_2)^r$$
$$\times\,\ln|2(H_0-E)|\,(\vec{p}_1+\vec{p}_2)^s\,|m_J\rangle\}B^i. \tag{20}$$

Adjusting the self-energy correction to our convention, we obtain the tensor structure

$$\delta E = -2\,\mu_B\,\frac{\alpha}{\pi}\langle m_J|\vec{G}_3\cdot\vec{B}|m_J\rangle, \tag{21}$$

where $G_3^i \equiv v_7^i$ is given by the expression in curly brackets in Eq. (20). Thus, the self-energy correction has a simple vector structure and contributes to the orbital momentum L part.

III. EVALUATION OF THE *g* FACTOR

In first-order perturbation theory, one requires only the diagonal matrix elements in the total angular momentum $\vec{J}$. Insofar as first-order theory is concerned, one may replace $H_{M0}+\delta H_M$ by its restriction to the $(2J+1)$-dimensional subspace spanned by the orthonormal vectors for $m_J = -J, -J+1,\ldots,J$. Then, the magnetic Hamiltonian linear in the $\vec{B}$ field can be rewritten as follows, in terms of the g_J factor and $\vec{J}$,

$$H_{M0}+\delta H_M = \mu_B\sum_{\gamma=0}^{3}\vec{G}_\gamma\cdot\vec{B} = \mu_B\,g_J\,\vec{J}\cdot\vec{B}. \tag{22}$$

In order to calculate the g_J factor, it is helpful to write it as an average over all magnetic projections. Using the shorthand notation $|m_J\rangle$ for the state with quantum numbers $|L,S,J,m_J\rangle$,

an important relation is

$$\langle m_J|\vec{G}\cdot\vec{B}|m_J\rangle = \langle m_J|\frac{\vec{G}\cdot\vec{J}\,\vec{J}\cdot\vec{B}}{\vec{J}^2}|m_J\rangle = m_J\, g_J\, B,$$
$$g_J = \frac{\langle m_J|\vec{G}\cdot\vec{J}|m_J\rangle}{J(J+1)}. \tag{23}$$

This relation holds for any m_J, and $\vec{G}$ may stand for any of the $\vec{G}_\gamma$ or for the sum $\vec{G} = \sum_{\gamma=0}^{3}\vec{G}_\gamma$. Summing over m_J and dividing by the number of states $2J+1$, the g_J factor can be determined as follows:

$$g_J = \frac{1}{J(J+1)(2J+1)}\sum_{i=0}\sum_{m_J=-J}^{J}\langle m_J|\vec{G}_i\cdot\vec{J}\,|m_J\rangle. \tag{24}$$

This expression involves a sum over the angular momentum projections and is manifestly independent of m_J.

A. Reduction of spin degrees and J

The $\vec{G}_\gamma$ with $\gamma = 0,1,2,3$ have been defined in Secs. II B–II D. According to Eq. (12), the terms can be decomposed into diagonal d terms and symmetric as well as antisymmetric t and r terms. Using Eq. (24), one can express the g-factor contribution of a term of the form $\vec{G}\cdot\vec{J}$ in terms of the multiplicative factor $J(J+1)(2J+1)$, a correction to the g_J factor, and radial matrix elements. For a contribution to $\vec{G}_\gamma\cdot\vec{J}$ of the form $d\,\vec{\sigma}\cdot\vec{J}$, one can deduce for P states the formula

$$\sum_{m_J=-J}^{J}\langle m_J|\,d\,\vec{\sigma}\cdot\vec{J}\,|m_J\rangle = A_{JS}\,J(J+1)\,(2J+1)\sum_a\langle\psi^k|d|\psi^k\rangle, \tag{25a}$$

$$A_{21} = A_{11} = \frac{1}{2},\quad A_{10} = 0. \tag{25b}$$

The Cartesian basis $|\psi^k\rangle$ of P states is normalized to $\langle\psi^k|\psi^l\rangle = \frac{1}{3}\,\delta_{kl}$ [see Eq. (31)]. The basis of the $|\psi^k\rangle$ states contains states without an explicit spin wave function, where the coordinate part is symmetrized or antisymmetrized, according to Eq. (31) below. For a vector $\vec{v}$ coupled to $\vec{J}$ in Eq. (24), we use the following reduction scheme:

$$\sum_{m_J=-J}^{J}\langle m_J|\vec{v}\cdot\vec{J}|m_J\rangle = B_{JS}\,J(J+1)\,(2J+1)\,\mathrm{i}\,\epsilon_{ijk}\langle\psi^i|v^j|\psi^k\rangle, \tag{26a}$$

$$B_{21} = B_{11} = -\frac{1}{4},\quad B_{10} = -\frac{1}{2}. \tag{26b}$$

For a symmetric, traceless (quadrupole) tensor, we can project onto the Cartesian basis for P states as follows:

$$\sum_{m_J=-J}^{J}\langle\, m_J|\,t^{ij}\,\sigma^i\,J^j|m_J\rangle = C_{JS}\,J(J+1)\,(2J+1)\sum_a\langle\psi^j|t^{jk}|\psi^k\rangle, \tag{27a}$$

$$C_{21} = -\frac{1}{10},\quad C_{11} = \frac{1}{2},\quad C_{10} = 0. \tag{27b}$$

Finally, for a antisymmetric tensor r^{ij} coupled to $\sigma_a^i\,J^j$, the total contribution to the g_J factor vanishes for all states under investigation here.

For excited helium P states, the leading-order expression (2) evaluates to

$$g_J(n^3P_{J=0,1,2}) = \tfrac{3}{2},\quad g_J(n^1P_1) = 1, \tag{28}$$

where n is the principal quantum number of the excited state, and the result for n^3P_0 is not of physical interest because the magnetic projection for the state with $J=0$ always is $\mu = 0$. The correction δg_J to the Landé g factor can be expressed in terms of δg_L, δg_S, and g_x [see Eq. (14)], and prefactors A_{JS}, B_{JS}, and C_{JS},

$$\delta g_J = A_{JS}\,\delta g_S - 2\,B_{JS}\,\delta g_L + \tfrac{1}{3}\,C_{JS}\,\delta g_x, \tag{29}$$

where the A_{JS}, B_{JS}, and C_{JS} coefficients are given in Eqs. (25)–(27), respectively. It is probably useful to note that our scheme is easily generalized to other low orbital momentum states, for example, D states, which have submanifolds with $S=0$ and $S=1$, and $J = 1,2,3$.

IV. NUMERICAL EVALUATION

The nonrelativistic wave function of the P state ψ and its energy E_0 are determined for a Schrödinger equation with a nonrelativistic Hamiltonian Eq. (8),

$$H_0\,\psi = E_0\,\psi, \tag{30}$$

based on the Rayleigh-Ritz variational principle. We use a basis set of explicitly exponentially correlated functions (following Refs. [18,19])

$$\psi^k = \sum_{m=1}^{N} w_m\big[r_1^k e^{-a_k r_1 - b_k r_2 - c_k r_{12}} \mp (r_1 \leftrightarrow r_2)\big], \tag{31}$$

which for the singlet (triplet) states is symmetric (antisymmetric) under an exchange of spatial coordinates, as required by the Pauli exclusion principle. We re-emphasize that the superscript k denotes the Cartesian coordinate; that is, the wave function with an orientation along the x axis would be denoted as ψ^x and involve the x coordinates r_1^x and (in the exchange term) r_2^x. The parameters (a,b,c) for the ith function are randomly generated from an optimized box $(A_1,A_2)\times(B_1,B_2)\times(C_1,C_2)$ under the additional constraints $a_k + b_k > \varepsilon$ as well as $b_k + c_k > \varepsilon$ and $c_k + a_k > \varepsilon$, where $\varepsilon = \sqrt{2\,(E_0^+ - E_0)}$ with E_0^+ being the lowest singlet (triplet) P state energy for He^+.

In order to obtain a more accurate representation of the wave function, we use two boxes that model the short-range and medium-range asymptotics of the helium wave functions. In this basis, the matrix element of the nonrelativistic Hamiltonian H_0 can be represented as a linear combination of the integrals

$$\Gamma(a,b,c,n_1,n_2,n_{12}) = \int \mathrm{d}^3r_1\,\mathrm{d}^3r_2\,r_1^{n_1-1}r_2^{n_2-1}r_{12}^{n_{12}-1}\,\mathrm{e}^{-ar_1-br_2-cr_{12}}, \tag{32}$$

with non-negative n_1, n_2, and n_{12}. Methods for their computation are well known [20]. The linear coefficients d_m in Eq. (31) are obtained from a solution of a generalized

TABLE I. Mean values of the tensor structures entering Eqs. (25)–(27), for $2\,^1P$, $2\,^3P$, and $3\,^3P$ states. In view of $A_{10} = C_{10} = 0$, only the phenomenologically relevant results are indicated for singlet P states.

Operator	$2\,^1P$	$2\,^3P$	$3\,^3P$
$\mathrm{i}\,\epsilon_{ijk}\langle\psi^i\|v^j_{0,a}\|\psi^k\rangle$	−2.0	−2.0	−2.0
$\mathrm{i}\,\epsilon_{ijk}\langle\delta\psi^i_{mp}\|v^j_{0,a}\|\delta\psi^k_{mp}\rangle$	−0.805 549 556(6)	−1.096 171 714(2)	−1.366 172(4)
$\mathrm{i}\,\epsilon_{ijk}\langle\delta\psi^i_{mp}\|\delta\psi^i_{mp}\rangle$	0.402 774 778(8)	0.548 085 857 1(4)	0.683 086 2(2)
$\mathrm{i}\,\epsilon_{ijk}\langle\psi^i\|v^j_{1,ab}\|\psi^k\rangle$	−0.131 044 018 6(5)	0.256 875 920 7(3)	0.069 756 861(4)
$\mathrm{i}\,\epsilon_{ijk}\langle\psi^i\|v^j_{1,a}\|\delta\psi^k_{mp}\rangle$	−1.131 383 6(3)	−1.204 232 1(4)	−1.025 36(6)
$\langle\psi^k\|d_{2,a}\|\psi^k\rangle$	$A_{10} = 0$	4.110 292 724 2	4.116 162 168 5
$\mathrm{i}\,\epsilon_{ijk}\langle\psi^i\|v^j_{2,a}\|\psi^k\rangle$	−0.483 020 291 31	−0.216 764 422 66	−0.259 969 064 25
$\langle\psi^k\|d_{3,a}\|\psi^k\rangle$	$A_{10} = 0$	2.109 944 701 6	2.116 045 575 2
$\langle\psi^j\|t^{jk}_{3,a}\|\psi^k\rangle$	$C_{10} = 0$	0.072 236 399(2)	0.080 111 516 9(4)
$\langle\psi^j\|t^{jk}_{4,ab}\|\psi^k\rangle$	$C_{10} = 0$	0.077 581 379(2)	0.084 694 997 4(3)
$\langle\psi^k\|d_{5,a}\|\psi^k\rangle$	$A_{10} = 0$	0.109 596 679 06	0.115 928 981 92
$\langle\psi^j\|t^{jk}_{5,ab}\|\psi^k\rangle$	$C_{10} = 0$	0.066 891 418 855(5)	0.075 528 036 275(1)
$\mathrm{i}\,\epsilon_{ijk}\langle i\|v^j_{61,ab}\|\psi^k\rangle$	−0.077 009 223 65(3)	−0.024 049 685(6)	0.030 684 751 1(4)
$\mathrm{i}\,\epsilon_{ijk}\langle\psi^i\|v^j_{62,ab}\|\psi^k\rangle$	0.029 866 744 798(1)	0.008 854 469 40(2)	−0.001 716 909 955(6)
$\mathrm{i}\,\epsilon_{ijk}\langle\psi^i\|v^j_{7,ab}\|\psi^k_{mp}\rangle$	0.195 754(2)	0.264 705(2)	0.088 415(4)

eigenvalue problem. The numerical accuracy of the results is estimated from the apparent numerical convergence of the matrix elements as the size of the basis is increased. For the calculation of ψ^k, we use an expansion with a moderate number up to $2\,N = 900$ basis functions (we use a prefactor 2 in order to clarify the distribution of the basis functions onto two variational boxes, as described in Ref. [19]). The numerical accuracy of the following nonrelativistic reference values,

$$E_0(2\,^1P) = -2.123\,843\,086\,498\,101\,3(3), \tag{33a}$$
$$E_0(2\,^3P) = -2.133\,164\,190\,779\,283\,1(2), \tag{33b}$$
$$E_0(3\,^3P) = -2.058\,081\,084\,274\,275(1), \tag{33c}$$

is fully sufficient for our calculations. All entries in Eq. (33) are consistent with the values given in Table III of Ref. [21]. For $2\,^3P$, our result also is in agreement with the entry in Eq. (20) of Ref. [22].

Using the wave functions ψ^k, we are able to obtain all necessary mean values defined by the tensor components d, v^i, and t^{ij}. In order to perform the calculation, the set of integrals of the form given in Eq. (33a) needs to be extended by additional classes including one or two of the indices n_1, n_2, and n_{12} being equal to -1. The analytic formulas for the master integrals and related recurrence schemes are well known, as given in Ref. [23]. Numerical values for the states with definite orbital momentum and spin-angular symmetries $2\,^1P$, $2\,^3P$, and 3^3P are presented in Table I. Because the coefficients A_{10} and C_{10} vanish, we do not provide values for the d and t^{ij} elements for singlet P states. Values without an error estimation are cut to eleven digits; all of these are believed to be numerically significant.

In order to determine the finite-mass effect of order $O(\lambda^2)$, we first calculate the mass polarization correction to the wave function, scaling the λ parameter out of the perturbation,

$$\lambda\,|\delta\psi^k_{mp}\rangle = -\lambda\,\frac{1}{(E_0 - H_0)'}\,\frac{\vec{p}_1\cdot\vec{p}_2}{\mu}\,|\psi^k\rangle. \tag{34}$$

The expression $|\delta\psi^k_{mp}\rangle$ is relevant for the entries in the third column of Table I. The operator $\vec{p}_1\cdot\vec{p}_2$ in Eq. (9) changes neither the orbital angular momentum nor the spin symmetry when acting on ψ^k in Eq. (34). Thus, it can be expressed using a basis consisting only of the ψ^k defined in Eq. (31). Variational parameters for $\delta\psi_{mp}$ are generated in analogy to those for the wave function ψ, but the size of the basis is chosen to be larger ($2N_{mp} = 3N$). With these results in hand, it is straightforward to calculate the mass polarization correction for a given operator. The only effect is the second-order correction to the $v^i_{1,ab}$ in Eq. (13). Together with part of the third-order correction to $v^i_{0,a}$, we obtain

$$\begin{aligned}\langle\psi^i|G^j_1|\psi^k\rangle &= -\frac{m}{M}\sum_{a\neq b}\left[\langle\,\psi^i|v^j_{1,ab}|\psi^k\rangle + 2\,\lambda\,\langle\psi^i|v^j_{1,ab}|\,\delta\,\psi^k_{mp}\rangle\right]\\ &\quad + \lambda^2\sum_a\langle\delta\psi^i_{mp}|v^j_{0,a}|\delta\psi^k_{mp}\rangle,\end{aligned} \tag{35}$$

where the formula is expressed in compact form by writing the coefficient of the first term as m/M, not μ/M. The other terms in the third-order perturbation of $v^i_{0,a}$ result in the shifted g_L coefficient in the leading term in Eq. (5),

$$\begin{aligned}g_L &= 1 - \frac{m}{M} - \lambda^2\,\langle\delta\psi^i_{mp}|\delta\psi^i_{mp}\rangle\\ &= 0.999\,862\,916\,942\,649(5)(55),\end{aligned} \tag{36}$$

where the first uncertainty estimate refers to the numerical uncertainty of the particular contribution (finite-mass correction to g_L), and the second uncertainty comes from the CODATA electron-α mass ratio $m/M = 1.370\,933\,555\,78(55)\times 10^{-4}$ employed in the calculation.

TABLE II. δg_J contributions to the singlet $2\,{}^1P_1$ state where $\delta g_S = \delta g_x = 0$. The fine-structure constant is $\alpha = 1/137.035\,999\,074(44)$, and the electron-$\alpha$ mass ratio is $m/M = 1.370\,933\,555\,78(55) \times 10^{-4}$ (see Ref. [32]). Theoretical uncertainties come from our estimate of higher order effects in the order α^4 (first parentheses) and finite-mass relativistic correction of order $\alpha^2\lambda$ (second).

$2\,{}^1P_1$	$\delta g_L \times 10^6$
Finite mass [Eq. (35)]	− 8.968 94
Relativistic [Eq. (15)]	− 7.853 19
Self-energy [Eq. (21)]	0.024 22
Total	− 16.798(9)(7)
Theory: Ref. [3]	− 15.771
Theory: Ref. [4]	− 16.810 165. . .[a]

[a]There is no uncertainty estimate given in Ref. [4].

The most numerically intensive part of the g factor calculations in Eq. (24) is the vector component of the self-energy correction (21), which can be reduced [5] to the expression

$$\mathrm{i}\epsilon_{ijk}\langle\psi^i|v_7^j|\psi^k\rangle = (\delta^{ir}\delta^{ks} - \delta^{is}\delta^{kr})\,\langle\psi^i|(\vec{p}_1+\vec{p}_2)^r \times \ln|2(H_0-E)|\,(\vec{p}_1+\vec{p}_2)^s|\psi^k\rangle, \quad (37)$$

which differs from the ordinary Bethe logarithm in the absence of a linear term $H_0 - E$ multiplying the logarithm. Matrix elements involving the logarithm of the Hamiltonian necessitate the use of the methods usually employed for Bethe logarithm calculations for excited states in helium, where, due to conceivable numerical challenges, for a long time asymptotic formulas [24–27] in $1/n$ and $1/Z$ were the preferred method of calculation. Direct and accurate calculations of logarithmic sums over the helium spectrum have become possible only quite recently [28–30]. Here, we closely follow to the integral representation of the Bethe logarithm [31], which for the expression in Eq. (37) has a particular compact form,

$$\mathrm{i}\,\epsilon_{ijk}\langle\psi^i|v_7^j|\psi^k\rangle = \int_0^1 \mathrm{d}t\,\frac{f(t)}{t^3}\,, \quad (38a)$$

$$f(t) = (\delta^{ir}\delta^{ks} - \delta^{is}\delta^{kr})\langle\psi^i|(\vec{p}_1+\vec{p}_2)^r \times \frac{1}{H_0 - E_0 + \omega}\,(\vec{p}_1+\vec{p}_2)^s\,|\psi^k\rangle, \quad (38b)$$

$$t = \frac{1}{\sqrt{1+2\,\omega}}. \quad (38c)$$

We perform an integration over 100 equally spaced and optimized t points, following ideas outlined in Ref. [31]. The well-defined limit of the integrand, $\lim_{t\to 0} f(t)/t^3 = 0$, facilitates the numerical evaluation.

V. RESULTS

The numerical data for the individual operators allows us to obtain theoretical analysis of the L, S, and the x part of the Landé g factor, as defined in Refs. [4,9] and discussed above. We express our results in terms of δg_J, which is obtained as the difference of the total prediction and the leading term [see Eq. (14)]. For the numerical evaluation, we use Eq. (24). We express the correction δg_J to the Landé g factor in terms of δg_L, δg_S, and δg_x, and prefactors A_{JS}, B_{JS}, and C_{JS}, as given in Eqs. (25)–(27), and (29).

We keep the conventions of Refs. [4,9] and compare our results to the experimental and theoretical literature. In Tables II and III, we provide data split into a finite-mass part related to Eq. (13) including the second-order mass polarization correction Eq. (35), the relativistic correction Eq. (16a), and the self-energy correction given in Eq. (21). The first conceivable source of uncertainty for these contributions is purely numerical, due to the finite numerical accuracy of the components in Table I. However, in most cases, the

TABLE III. δg_J contributions to triplet P states. Again, the theoretical uncertainty of the final theoretical prediction comes from the estimate of higher order effects in the order α^4 and finite-mass relativistic correction of order $\alpha^2\,\lambda$ (first and second parentheses, respectively).

$2\,{}^3P_J$	$\delta g_L \times 10^6$	$\delta g_S \times 10^6$	$\delta g_x \times 10^6$
Finite mass [Eq. (35)]	17.620 32	0.0	0.0
Relativistic [Eq. (16a)]	− 6.912 92	− 80.429 3	− 5.385 487
Self-energy [Eq. (21)]	0.032 74	0.0	0.0
Total	10.740(2)(2)	− 80.43(2)(4)	− 5.385 5(13)(2)
Theory: Ref. [4]	10.719 291 . . .[a]	− 80.436 904 . . .[a]	− 5.391 808 . . .[a]
Theory: Ref. [2]	10.6(4)	− 80.46(1)	− 3.5(1.5)
Theory: Ref. [3]	8.838	− 80.401	− 5.344
Theory: Ref. [5]	10.752 033 . . .		
Experiment: Ref. [1]	4.9(1.9)		
Experiment: Ref. [9]	3.8(9.0)	− 76.0(2.4)	4.0(25.0)
$3\,{}^3P_J$	$\delta g_L \times 10^6$	$\delta g_S \times 10^6$	$\delta g_x \times 10^6$
Finite mass [Eq. (35)]	4.788 03	0.0	0.0
Relativistic [Eq. (16a)]	− 3.029 57	− 75.083 9	− 2.648 665
Self-energy [Eq. (21)]	0.010 94	0.0	0.0
Total	1.769(9)(2)	− 75.08(2)(4)	− 2.648 7(7)(3)
Theory: Ref. [4]	1.772 223 . . .[a]	− 75.096 557 . . .[a]	− 2.650 192 . . .[a]
Theory: Ref. [33]	− 0.17(2.8)	− 75.13(3.27)	− 2.75(10.02)

[a]There is no uncertainty estimate given in Ref. [4].

numerical uncertainty is negligible as compared to the omitted higher-order effects.

We are able to report that our results confirm the numerical data reported previously in Ref. [4] at the level of relativistic operators without finite-mass corrections. Here, we attempt to go beyond the leading relativistic effects. The self-energy correction to the P state g factor consists of two parts, one of which involves a Bethe-logarithm-type term (logarithmic sum over virtual excited states) and is ultraviolet finite, in contrast to the Bethe logarithm contribution to the S state Lamb shift, which is known to be uv divergent [34,35]. The second contribution due to the self-energy is a high-energy contribution, which is manifest in the anomalous magnetic effects of the free electron, which are included into the relativistic Zeeman Hamiltonian given in Eq. (15). These contributions are ir finite. We obtain very good agreement with a numerical result reported in Ref. [5] for the-self energy correction δg_L for $2\,^3P$. Combining relativistic and radiative effects, we should mention the presence of an additional third term with a prefactor $g_S - 2$ in Eq. (15). In Ref. [4], this term had not been taken into account, apparently, but its numerical magnitude does not shift the final result significantly. Our self-energy correction, which we add to the relativistic result of Ref. [4], includes the relativistic anomalous magnetic moment effects of the electron and the spin dependence of the Bethe logarithm term. We also include $O(\lambda^2)$ corrections to the leading order, resulting in the finite-mass correction in Eq. (35). Such correction gives -0.8×10^{-8}, -1.0×10^{-8}, and -1.3×10^{-8} to the δg_L of $2\,^1P$, $2\,^3P$, and $3\,^3P$ respectively, having the order of the self-energy correction.

There are two significant sources of theoretical uncertainty for the final results, which are given by finite-mass corrections to the relativistic effects and by higher order QED contributions. In the results reported in Ref. [4], the mass scaling and mass polarization corrections to the relativistic effects have been included; these results are of relative order $O(\alpha^2\,\lambda)$ with respect to the leading g-factor term. However, there are additional finite-mass relativistic effects of the same order, which can be deduced from Eq. (40) in Ref. [11] and which should be included in a systematic treatment. Here, we do not perform a complete calculation of the terms of order $O(\alpha^2\,\lambda)$, and so we do not include the relativistic reduced-mass correction at all in our final results. We use some partial results we have obtained in the order $\mathcal{O}(\alpha^2\,\lambda)$ in order to estimate the size of the relativistic-recoil correction.

These include the scaling and the mass polarization corrections for the L part in $2\,^1P_1$ (4.4×10^{-9}), as well as for the x part (1.6×10^{-9}) and the S part (2.5×10^{-8}). In $2\,^3P_J$, we have 1.1×10^{-10} for the x part, 9.2×10^{-10} for the L part, and 2.5×10^{-8} for the S part. Finally, for the x part in $3\,^3P_J$, we have a result of 1.7×10^{-10}. These results guide our estimates of the theoretical uncertainty indicated in Tables II and III, where we multiply the partial results with a conservative weight factor of 1.5. For the higher order QED contributions, we are not even able to present approximate formulas based on, for example, hydrogenic contributions, because the theory of the Zeeman effect has not been developed until now to this order. Therefore, we use the combined value from the relativistic correction multiplied by a factor α^2, and the leading QED correction multiplied by a factor α, to obtain a conservative estimate of the uncertainty due to the uncalculated higher order effects. We employ an additional conservative enlargement factor of 5 in order to estimate the size of the effects of order α^3.

As evident from Tables II and III, agreement of theory and experiment is rather satisfactory for a number of contributions, with the exception of a 2σ discrepancy for δg_S (comparing our result to that of Ref. [9]) for the $2\,^3P$ state and a $3\,\sigma$ discrepancy for δg_L (comparing our result to that of Ref. [1]). It would be very interesting to remeasure the effect and clarify the status of the experimental results.

VI. CONCLUSIONS

In the calculation of the g_J factor of excited states of helium, all aspects of atomic physics play a role: electron correlation, relativity, and QED radiative corrections. Furthermore, these effects are all intertwined; that is, there are QED radiative corrections multiplying the relativistic effects, contributing in higher order. We here carry out a theoretical analysis of the P-state g factor of singlet and triplet helium states, with a special emphasis on relativistic, radiative, and finite-mass corrections. The effects are calculated through order α^2 (for the relativistic effects), and we also include radiative effects of order α^3. Furthermore, finite-mass corrections of order λ and λ^2 are included, while available partial results for the effects of relative order $\alpha^2\,\lambda$ are used in order to estimate the theoretical uncertainty in this order. Results are summarized in Tables II and III; a 2σ discrepancy for δg_S in comparison to Ref. [9] and a now-famous 3σ discrepancy for δg_L in comparison to Ref. [1] highlight the need for additional experimental evidence before definitive conclusions can be drawn.

With regard to the QED self-energy correction to the g factor, one encounters a peculiar situation for P states: Namely, both the high-energy part as well as the low-energy part are separately finite, while the low-energy part is given by a Bethe-logarithm term and the high-energy part is given by the anomalous magnetic moment. Both terms are finite, and it is easy to overlook one of the contributions. For atomic hydrogen, this has been verified both numerically [7] and analytically [8]. For helium singlet versus triplet states, we find that the low-energy part of the self-energy correction to the bound-state g factor is spin dependent.

Our calculations are performed in an angular-momentum coupling scheme which allows us to separate the internal degrees of freedom of the atom from the interaction with the external magnetic field. The angular momentum algebra can become rather involved for helium P states. We fully confirm the relativistic treatment of Ref. [4] using our mixed approach. In a more general context, one may recall that the contribution of the anomalous magnetic moment to the P-state lifetime in few-electron systems has recently given rise to interesting experimental-theoretical discrepancies [36] which remain to be fully resolved.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation (Grant No. PHY-1068547) and by a precision measurement grant from the National Institute of Standards

and Technology. The authors acknowledge helpful conversations with K. Pachucki. Support from Poznań Networking and Supercomputing Center also is gratefully acknowledged.

APPENDIX: NONRELATIVISTIC TREATMENT

The nonrelativistic Hamiltonian of an n-electron atom is given as (in atomic units)

$$H = \frac{\vec{p}_N^{\,2}}{2M} + \sum_a \left(\frac{\vec{p}_a^{\,2}}{2m} - \frac{Z}{r_a} \right) + \sum_{a>b} \frac{1}{r_{ab}}, \tag{A1}$$

where we keep the electron mass m and the nucleus mass M in symbolic form. In the center-of-mass system, we have $\vec{p}_N = -\sum_a \vec{p}_a$, and therefore

$$H = \sum_a \left(\frac{\vec{p}_a^{\,2}}{2\mu} - \frac{Z}{r_a} \right) + \sum_{a>b} \left(\frac{1}{r_{ab}} + \frac{\vec{p}_a \cdot \vec{p}_b}{M} \right), \tag{A2}$$

where the latter term corresponds to the mass polarization. The reduced mass μ is given as

$$\frac{1}{\mu} = \frac{1}{m} + \frac{1}{M}. \tag{A3}$$

If we define the ratio $\lambda = -\mu/M$ as in Eq. (4), then an important identity is

$$1 + \lambda = 1 - \frac{\mu}{M} = \frac{\mu}{m}. \tag{A4}$$

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