Relativistic corrections to the Zeeman effect in heliumlike atoms

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An approximately relativistic theory of bound states which ensures Poincaré invariance of the atomic system to relative order $(v/c)^2$ is used to derive the Zeeman interaction Hamiltonian correct to order α^3 and to all orders in m_e/m_N for an arbitrary three-body system. This approach is distinctly different from methods used in the past. The terms of order m_e/m_N, α^2, and α^3 agree with previous results. The terms of order $\alpha^2 m_e/m_N$ and smaller do not agree with previous results. The terms of order m_e/m_N, α^2, α^3, and $\alpha^2 m_e/m_N$ are used to calculate the g factors for $n=2$ ^{4}He and ^{3}He. The corrections of order α^3 and $\alpha^2 m_e/m_N$ have not previously been calculated for the P-state g factors. Our results for the ^{4}He $2\,^3S_1$ g_J factor $[g_e(1-40.9158\times10^{-6})]$ can be compared with the result of Grotch and Hegstrom [Phys. Rev. A **8**, 1166 (1973)] $[g_e(-40.9157\times10^{-6})]$. We calculate the ratio of this g factor to the g factor of $1\,^2S_{1/2}$ hydrogen to be $1-23.211\times10^{-6}$. This agrees with the result of Grotch and Hegstrom [Phys. Rev. A **8**, 1166 (1973)], $1-23.211\times10^{-6}$, and the best experimental result [G. M. Keiser, H. G. Robinson, and C. E. Johnson, Phys. Rev. A **16**, 822 (1977)], $1-23.214(50)\times10^{-6}$. We also find that including the mass polarization in the $2\,^3S_1$ wave function contributes a negligible amount, 1.4×10^{-10}, to the ^{4}He $2\,^3S_1$ g_J factor. We use 125-term variational wave functions in a configuration-interaction basis and explicitly examine the effect of configuration mixing on the g factors. We find the ^{4}He $2\,^3P_J$ g_s' factor to order $\alpha^2 m_e/m_N$ to be $g_e-80.4010\times10^{-6}$. This agrees (to order α^2) with the results of Lewis and Hughes [Phys. Rev. A **8**, 2845 (1973)]. We also calculate radiative corrections of order α^3 that contribute to the $2\,^3P_J$ g_L' factor $(g_L'=1-m_e/m_N+8.838\times10^{-6})$ and find that they are too small (1.79×10^{-7}) to resolve a long-standing discrepancy between theory and experiment for the $2\,^3P_J$ g_L' factor. These radiative corrections have not previously been calculated. Our value for the ^{4}He g_L' factor is 1.36 standard deviations above the best experimental value. This represents a significant improvement over the results of Lewis and Hughes which is 1.97 standard deviations above the best experimental value. The ^{4}He $2\,^3P_J$ g_X factor is found to be -5.344×10^{-6}. We have also calculated the ^{4}He $2\,^1P_1$ g_L' factor $(g_L'=1-m_e/m_N-15.771\times10^{-6})$. This g factor has not previously been calculated. Finally, we have to introduce a g factor for the helium $2\,^3P$ states in the $|Jm_JLS\rangle$ representation: $g_y=1.08\times10^{-8}$ for ^{4}He and $g_y=1.06\times10^{-8}$ for ^{3}He. This g factor comes from terms of the order α^3 and $\alpha^2(m_e/m_N)$.

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I. INTRODUCTION

Since precise atomic-energy-level measurements of helium are made in constant magnetic fields, a precise understanding of the Zeeman effect for helium is important [1]. The motional corrections of order m_e/m_N were first obtained quite some time ago by Phillips [2]. The relativistic corrections of order α^2 were first obtained by Perl and Hughes [3]. These terms were then verified by Hegstrom [4], who used an extended Breit equation to derive a Zeeman Hamiltonian including terms up to order $\alpha^2 m_e/m_N$ for an arbitrary many-particle atomic system.

The agreement between the best experimental result $[1-23.214(50)\times10^{-6}]$ Ref. [5] and the most accurate theoretical result $(1-23.211\times10^{-6})$ [6] for the $g_J(^4\mathrm{He}\,2\,^3S_1)/g_J(\mathrm{H}1\,^2S_{1/2})$ ratio is quite good. For the ^{4}He $2\,^3P_J$ states the agreement between theory and experiment for the atomic g factors is not as good. We work in a $|Jm_JLS\rangle$ representation where L, S, and J are the total orbital angular momentum, total spin angular momentum, and total angular momentum, respectively. There are four g factors for the $2\,^3P_J$ states: a g_S' factor resulting from terms which act only in the Sm_s subspace, a g_L' factor from terms which act only in the Lm_L subspace, a g_X factor which results from terms which couple a Pauli spinor of one of the electrons with a second-rank spherical tensor, and a g_γ factor which results from terms which couple a Pauli spinor of one of the electrons with an orbital angular momentum vector. The g_γ factor, which comes from terms of the order α^3 and $\alpha^2 m_e/m_N$, has not been considered in previous work [7,10], which only included terms to order α^2. Table I displays the published experimental and theoretical results for the helium $2\,^3P_J$ and $2\,^1P_1$ state g factors. The results of our work are also included in Table I.

The largest discrepancy between theory and experiment exists for the $2\,^3P_J$ g_L' factor, which turns out to be sensitive to the atomic wave function used to evaluate the Zeeman Hamiltonian. The first entries of Table I are the results which use simple hydrogenic wave functions which assume a pure sp configuration. We are in agreement with Lewis and Hughes [7] in the results of this later calculation. Lewis and Hughes [7] also used a very

accurate 165-term variational wave function which utilized a Hylleraas basis and two nonlinear parameters to get the results in the ninth row of entries of Table I. These results include contributions from motional corrections of order m_e/m_N and relativistic corrections of order α^2. Their result, however, for the g_L' factor (0.999 837 5) is 1.97 standard deviations above the best experimental value [0.999 867 8(29)] Ref. [8]. An attempt to resolve this discrepancy was one of the goals of our work.

We will use an approximately relativistic theory of bound states developed by one of us (K.J.S.) [9], which ensures Poincaré invariance of the atomic system to relative order $(v/c)^2$. It describes the interaction of the composite system with an external electromagnetic field [9]. This theory allows us to calculate relativistic corrections to the Zeeman effect to order α^3 and motional corrections to all orders in m_e/m_N. In this work we will use all the corrections of order m_e/m_N, α^2, α^3, and $\alpha^2 m_e/m_N$ [all those which are larger than corrections of order α^4 which cannot be calculated using an approximately relativistic theory which is correct only to order $(v/c)^2$]. This is more than sufficient, however, since the experimental level of uncertainty is at the α^2 level [10].

There are two ways in which one can try to improve upon the results of Lewis and Hughes [7]: (i) include higher-order corrections (α^3 and $\alpha^2 m_e/m_N$) and (ii) evaluate the Zeeman Hamiltonian with different wave functions. We have utilized both of these options. The only α^3 corrections to the orbital g factor are radiative corrections due to the self-energies of the two electrons individually and single transverse photon exchange between the two electrons. Using nonrelativistic perturbation theory, Hegstrom correctly gives the result [4]

$$\Delta E_R = \frac{2\alpha}{3\pi m_e^2 c^2}\int_0^\infty \frac{dk}{1+\frac{2k}{m_e c^2}} \sum_{n'} \frac{\langle n|\Pi_1+\Pi_2|n'\rangle\cdot\langle n'|\Pi_1+\Pi_2|n\rangle(E_{n'}-E_n)}{k+E_{n'}-E_n}\ , \tag{1}$$

where $\Pi_i = \mathbf{p}_i + (e/c)\mathbf{A}_i$ is the mechanical momentum for electron i, we choose $\mathbf{A}_i = \frac{1}{2}\mathbf{B}\times\mathbf{r}_i$ for a constant external magnetic field, and we set $\hbar = 1$ in this paper. The constituent position and momentum variables are denoted as $\mathbf{r}_i$ and $\mathbf{p}_i$. This expression, however, must be multiplied by $\frac{3}{4}$ to account for the fact that the self-energy contributions in a nonrelativistic perturbative approach are twice as large as the (presumably more correct) results of Grotch and Kashuba [11]. Grotch correctly gives the result based upon the nonrelativistic limit of the formal covariant gauge-invariant expression for the self-energy of a fermion in an external electromagnetic field [11]. The contributions of Eq. (1) have never been calculated in the past because of the internal sum on states is difficult to evaluate. The evaluation of this contribution is outlined in Appendix A. It provides a contribution of 1.79×10^{-7} to the orbital g_L' factor for the $2\,^3P_J$ states of ^{4}He and ^{3}He.

TABLE I. Relativistic and motional corrections to the helium $2\,^3P_J$ and $2\,^1P_1$ g factors. All entries are to be multiplied by 10^{-6}. The upper entry of a double row includes m_e/m_N and α^2 corrections. The lower entry also includes α^3 and $\alpha^2\, m_e/m_N$ corrections. $g_e = 2(1+a_e)$, $g_L = 1 - m_e/m_N$.

		^{4}He				^{3}He
		$2\,^3P_J$			$2\,^1P_1$	$2\,^3P_J$
Reference	$g_s'-g_e$	$g_L'-g_L$	g_x	g_y	$g_L'-g_L$	$g_L'-g_L$
			Theoretical			
This work[a]	−80.264	3.840	−5.600		−14.760	7.840
	−80.236		−5.571	0.010		
This work[b]	−80.430	13.013	−5.640		−10.062	20.122
	−80.399		−5.594	0.011		
This work[c]	−80.461	8.656	−5.394		−15.773	14.399
	−80.428		−5.345	0.011		
This work[d]	−80.401	8.838	−5.344	0.011	−15.771	14.578
Ref. [7][e]	−80.46(1)	10.6(4)	−3.5(2.5)			
			Experimental			
Ref. [10][f]	−76.0(2.4)	3.8(9.0)	4.04(25.0)			
Ref. [8][g]		4.9(2.9)				
Ref. [27][g]						10.5(2.0)

[a]Using a simple hydrogenic wave function.
[b]Using the best wave function of a pure *sp* configuration.
[c]Using a 125-term configuration-interaction wave function.
[d]Same as (c) but also includes α^3 radiative corrections and reduced-mass corrections.
[e]Includes only terms of order m_e/m_N and α^2.
[f]Cannot measure the effect of configuration mixing.
[g]Measures the effect of configuration mixing.

Although there are no explicit Zeeman interaction terms of order $\alpha^2 m_e/m_N$ which contribute to g_L', corrections of this order arise from using wave functions for a helium atom with a finite nuclear mass when taking the expectation value of the α^2 contributions. The total $\alpha^2 m_e/m_N$ contribution to the $2\,^3P_J$ g_L' factor is 2.37×10^{-9}. Thus we see that higher-order corrections will not bring us far in resolving the discrepancy between the experimental and theoretical g_L' values.

The wave function used by Lewis and Hughes [7] provided an accurate energy eigenvalue ($-2.133\,164$ a.u.) and correspondingly accurate values for radial expectation values. The inclusion of r_{12} (the interelectron distance) directly in the Hylleraas basis used by Lewis and Hughes [7] is equivalent to configuration mixing. With a Hylleraas-type wave function, the integrals which are used to evaluate the g factors include r_{12} and are not simply the product of their radial and angular parts [7]. The evaluation of these integrals turns out to be a highly numerical procedure [7]. We used a distinctly different procedure to evaluate the helium $2\,^3P$ and $2\,^1P$ g factors. We used 125-term variational wave functions in a configuration-interaction basis with 12 nonlinear parameters. This wave function provided an energy eigenvalue of $-2.133\,160$ a.u. Instead of including r_{12} as part of the radial basis functions, the wave functions explicitly mix other configurations with the pure sp configuration of the P states and use a simple radial basis including only r_1 and r_2. This allows for a straightforward evaluation of the g factors using the Zeeman Hamiltonian recoupled in terms of spherical tensors. The results for the g factors using these wave functions are also listed in Table I. The final result is a significant improvement in the agreement between the theoretical and experimental values for the g factors, especially the g_L' factor, which is now 1.36 standard deviations above the experimental value. Here the α^3 corrections are responsible for an increase of the discrepancy by 0.06 standard deviations.

The rest of the paper is as follows. In Sec. II we present the derivation of the Zeeman Hamiltonian. The $2\,^3S_1$ g_J factor is derived in Sec. III. The $2\,^3P_J$ and $2\,^1P_1$ g factors are derived in Sec. IV. A concise summary of the paper and conclusions are given in Sec. V.

II. ZEEMAN HAMILTONIAN

The total Hamiltonian for the isolated composite system can be written to order $1/c^2$ as

$$H=\sum_{\mu=1}^{n}\left[\frac{p_\mu^2}{2m_\mu}-\frac{P_\mu^4}{8m_\mu^3c^2}\right]+U^{(0)}+U^{(1)}\ , \tag{2}$$

where $U^{(0)}$ and $U^{(1)}$ are the internal interactions of the zeroth and second order in v/c, respectively. For atomic systems and nonrelativistic interaction ($U^{(0)}$) is simply the Coulomb interactions between the constituent particles. We shall take $U^{(1)}$ to be given by the sum of the well-known Fermi-Breit intereactions between the constituent particles [12]. The Fermi-Breit intereactions include all of the $(Z\alpha)^4$ contributions to the zero-field energy-level splittings and with the phenomenological introduction of the anomalous magnetic moments of the constituent particles it also includes some of the $\alpha(Z\alpha)^4$ contributions and even terms of order $\alpha^2(Z\alpha)^4$ coming from terms which contain the product of the two anomalous magnetic-moment parameters. These terms represent the lowest-order contributions from the self-energies of the bound constituent particles.

In a previous paper [9], one of us (K.J.S.) has shown that the interaction of an arbitrary composite system with an external electromagnetic field can be written as the sum of two terms:

$$H_I=H_{I1}+H_{I2}\ . \tag{3}$$

Here H_{I1} is the interaction resulting from a minimal substitution in the total Hamiltonian of the isolated composite system. Retaining only the terms that are linear in the external magnetic field, we have

$$H_{I1}=i\sum_{\mu=1}^{n}\frac{e_\mu}{2c}\{[\mathbf{r}_\mu,H]\cdot\mathbf{A}_\mu+\mathbf{A}_\mu\cdot[\mathbf{r}_\mu,H]\}\ , \tag{4}$$

where e_μ and $\mathbf{r}_\mu$ are the charge and constituent position vector of particle μ, respectively. The second term H_{I2} includes the sum of spin-dependent terms resulting from the Foldy-Wouthuysen reduction of single Dirac particles with anomalous magnetic moments in an external electromagnetic field. For the case of a constant external magnetic field and no electric field we have retained only terms linear in the magnetic field and obtain

$$H_{I2}=-\sum_{\mu=1}^{n}\frac{e_\mu}{m_\mu c}(1+a_\mu)\mathbf{s}_\mu\cdot\mathbf{B}_\mu+\sum_{\mu=1}^{n}\frac{e_\mu}{4m_\mu^3c^3}[p_\mu^2,\mathbf{s}_\mu\cdot\mathbf{B}_\mu]_+ +\sum_{\mu=1}^{n}\frac{a_\mu e_\mu}{2m_\mu^3c^2}(\mathbf{s}_\mu\cdot\mathbf{p}_\mu)(\mathbf{p}_\mu\cdot\mathbf{B}_\mu)\ , \tag{5}$$

where a_μ, $\mathbf{s}_\mu$, and $\mathbf{p}_\mu$ are the anomalous magnetic-moment parameter, spin, and momentum of the μth particle. In addition to H_1+H_2 we must add $\frac{3}{4}\Delta E_R$ in Eq. (1).

Now the relations of Krajcik and Foldy [13] must be used to express the Zeeman Hamiltonian $H_I=H_{I1}+H_{I2}$ in terms of the center of mass and internal variables. The radiative and recoil corrections of Eq. (1) are of order α^3 and are already relativistically correct to order $(v/c)^2$. Therefore, the usual nonrelativistic transformations from the constituent to center of mass and internal variables are used in Appendix A to evaluate this contribution. The Krajcik and Foldy relations are [13]

$$\mathbf{r}_\mu=\boldsymbol{\rho}_\mu+\mathbf{R}-\frac{1}{2c^2}\left[\frac{\boldsymbol{\rho}_\mu\cdot\mathbf{P}}{M}\left[\frac{\boldsymbol{\pi}_\mu}{m_\mu}+\frac{\mathbf{P}}{2M}\right]+\text{H.c.}\right]-\frac{1}{2c^2}\sum_v\left[\frac{\pi_v^2\boldsymbol{\rho}_v}{2m_vM}+\text{H.c.}\right]+\sum_v\frac{(\boldsymbol{\rho}_v\times\boldsymbol{\pi}_v)}{2M^2c^2}\times\mathbf{P} -\frac{\boldsymbol{\sigma}_\mu\times\mathbf{P}}{2m_\mu Mc^2}+\sum_v\frac{\boldsymbol{\sigma}_v\times\boldsymbol{\pi}_v}{2m_vMc^2}+\sum_v\frac{\boldsymbol{\sigma}_v\times\mathbf{P}}{2M^2c^2}-\frac{1}{M}\mathbf{W}^{(1)}-\frac{i}{m}\left[\int_0^P d\mathbf{p}\cdot\mathbf{W}^{(1)},\boldsymbol{\rho}_\mu\right]\ , \tag{6}$$

$$\mathbf{p}_\mu=\boldsymbol{\pi}_\mu+\frac{m_\mu}{M}\mathbf{P}+\left[\frac{\pi_\mu^2}{2m_\mu}-\frac{m_\mu}{M}\sum_v\frac{\pi_v^2}{2m_v}+\frac{\boldsymbol{\pi}_\mu\cdot\mathbf{P}}{2M}\right]\frac{\mathbf{P}}{Mc^2}-\frac{i}{M}\left[\int_0^P d\mathbf{p}\cdot\mathbf{W}^{(1)},\boldsymbol{\pi}_\mu\right], \tag{7}$$

$$\mathbf{s}_u=\boldsymbol{\sigma}_\mu-\frac{\boldsymbol{\sigma}_\mu\times(\boldsymbol{\pi}_\mu\times\mathbf{P})}{2m_\mu Mc^2}-\frac{i}{M}\left[\int_0^P d\mathbf{p}\cdot\mathbf{W}^{(1)},\boldsymbol{\sigma}_\mu\right], \tag{8}$$

where $\boldsymbol{\rho}_\mu$, $\boldsymbol{\pi}_\mu$, and $\boldsymbol{\sigma}_\mu$ are the internal position, momenta, and spin variables. The position and momentum variables of the center of mass are denoted by $\mathbf{R}$ and $\mathbf{P}$. The interaction-dependent part of the Lorentz boost operator which determines the form of the constituent to center of mass and relative variables relations for a heliumlike atom is

$$\mathbf{W}^{(1)}=\frac{Ze^2}{2c^2}\left[\frac{m_N}{M}\right]\left[-\frac{\mathbf{q}_1}{q_1}-\frac{\mathbf{q}_2}{q_2}+\left[\frac{2m_e}{m_N}\right]\left[\frac{\mathbf{q}_1}{q_2}+\frac{\mathbf{q}_2}{q_1}\right]\right]+\frac{e^2}{2c^2}\left[\frac{m_N}{M}\right]\frac{\mathbf{q}_1+\mathbf{q}_2}{|q_1-q_2|}, \tag{9}$$

where Ze and $(-e)$ are the nuclear and electronic charges, the total atomic mass is the sum of the electronic and nuclear masses $M=m_N+2m_e$, $\mathbf{q}_1\equiv\boldsymbol{\rho}_1-\boldsymbol{\rho}_3$, $\mathbf{q}_2\equiv\boldsymbol{\rho}_2-\boldsymbol{\rho}_3$, and $\boldsymbol{\rho}_1$, $\boldsymbol{\rho}_2$, and $\boldsymbol{\rho}_3$ are the position vectors of the two electrons and the nucleus relative to the center of mass, respectively. This result has not previously been found and is derived in Appendix B.

The matrix elements of the resulting interaction Hamiltonian contain factors of $\mathbf{R}$ and $\mathbf{P}$. Matrix elements of $\mathbf{R}$ in states of definite momenta are ambiguous. Therefore, before we go to the $\mathbf{P}\rightarrow\mathbf{0}$ limit we must take the expectation values of these operators using a symmetric normalized wave packet

$$\Psi=\frac{1}{(\pi\lambda)^{3/4}}e^{-R^2/2\lambda}, \tag{10}$$

which in the $\lambda\rightarrow\infty$ limit is equivalent to the $\mathbf{P}=\mathbf{0}$ plane wave. Once this is done we get an unambiguous operator (H_I) in the $\mathbf{P}=\mathbf{0}$ frame.

After much algebra and retaining terms of order m_e/m_N, α^2, α^3, and $\alpha^2 m_e/m_N$ and neglecting nuclear spin-dependent terms we obtain for the Zeeman Hamiltonian $H_z=H_I+\Delta E_R$ the expression

$$H_z=\sum_{i=0}^{9}H_i+\Delta E_R, \tag{11}$$

$$H_0=\mu_B\mathbf{B}\cdot(\mathbf{L}+g_e\mathbf{S}), \tag{12}$$

$$H_1=-\mu_B\mathbf{B}\cdot\sum_{i=1}^{2}(\boldsymbol{l}_i+2\boldsymbol{\sigma}_i)\frac{\pi_i^2}{2m_e^2c^2}, \tag{13}$$

$$H_2=\frac{Ze^2}{2m_ec^2}\left[1+2a_e-\frac{m_e}{m_N}\right]\times\mu_B\mathbf{B}\cdot\sum_{i=1}^{2}[\boldsymbol{\sigma}_i\times\nabla_i(q_i^{-1})]\times\mathbf{q}_i, \tag{14}$$

$$H_3=\frac{-e^2}{m_ec^2}\left[1+2a_e+\frac{m_e}{m_N}\right]\mu_B\mathbf{B}\cdot[\boldsymbol{\sigma}_1\times\nabla_1(q_{12}^{-1})]\times\mathbf{q}_1, \tag{15}$$

$$H_4=\frac{-2e^2}{m_ec^2}\left[1+a_e-\frac{m_e}{2m_N}\right]\mu_B\mathbf{B}\cdot[\boldsymbol{\sigma}_1\times\nabla_1(q_{12}^{-1})]\times\mathbf{q}_1, \tag{16}$$

$$H_5=\frac{-e^2}{m_ec^2}\mu_B\mathbf{B}\cdot[q_{12}^{-1}(\mathbf{q}_1\times\boldsymbol{\pi}_2)+q_{12}^{-3}(\mathbf{q}_1\times\mathbf{q}_2)(\mathbf{q}_{12}\cdot\boldsymbol{\pi}_2)], \tag{17}$$

$$H_6=-\left[\frac{m_e}{m_N}\right]\mu_B\mathbf{B}\cdot\left[\mathbf{L}+\sum_{i\neq j}(\mathbf{q}_i\times\boldsymbol{\pi}_j)\right], \tag{18}$$

$$H_7=\frac{-a_e}{m_e^2c^2}\mu_B\mathbf{B}\cdot\sum_{i=1}^{2}\boldsymbol{\pi}_i(\boldsymbol{\sigma}_i\cdot\boldsymbol{\pi}_i), \tag{19}$$

$$H_8=\frac{-Ze^2}{2m_ec^2}\left[\frac{m_e}{m_N}\right]\mu_B\mathbf{B}\cdot\sum_{i\neq j}(\boldsymbol{\sigma}_i\times\nabla_i q_i^{-1})\times\mathbf{q}_j, \tag{20}$$

$$H_9=\frac{1}{2m_em_Nc^2}\mu_B\mathbf{B}\cdot\sum_{i\neq j}(\boldsymbol{\pi}_i+\boldsymbol{\pi}_j)\times(\boldsymbol{\pi}_i\times\boldsymbol{\sigma}_i), \tag{21}$$

where μ_B is the Bohr magneton, $g_e=2(1+a_e)$ is the free-electron g factor, a_e is the electronic anomalous magnetic-moment parameter, $\mathbf{L}=\sum_i\boldsymbol{l}_i$, $\mathbf{S}=\sum_i\boldsymbol{\sigma}_i$, $q_{12}\equiv|q_1-q_2|$, and $\boldsymbol{l}_i$, $\boldsymbol{\pi}_i$, and $\boldsymbol{\sigma}_i$ are the orbital angular momenta, momenta conjugate to $\mathbf{q}_i$, and spin variables of the ith electron relative to the nucleus in the center-of-mass frame, respectively. The radiative and recoil corrections of Eq. (1) are denoted as ΔE_R.

The terms of order m_e/m_N and α^2 in Eqs. (11)–(21) above agree with previous results [2–4,7]. The terms of order m_e/m_N are equivalent to the motional corrections resulting from a minimal substitution in the nonrelativistic Hamiltonian for a heliumlike atom with a finite nuclear mass [2]. The α^2 terms are purely relativistic terms which one would obtain from the appropriate reduction of any extended two-particle bound-state wave equation correct to relative order $[(v/c)^2]$ [3,4]. The terms of order α^3 also agree with the results of Hegstrom and coworkers [4,6]. These terms account for the other radiative corrections (to α^3) beyond Eq. (1). They result from accounting for the anomalous magnetic moments of the electrons. The terms of order $\alpha^2 m_e/m_N$, however, are different from the results of Hegstrom [4]. The appropriate accounting of these relativistic motional corrections was precisely the intent in using an approximately relativistic theory of bound states which is Poincaré invariant to relative order $(v/c)^2$. Hegstrom derived his Zeeman Hamiltonian by performing a Charaplyvy-Barker-Glover

reduction of a unitarily transformed extended Breit equation [4]. Discussions and comparisons of the two methods have been given by Grotch and Kashuba [14] and Grotch and Hegstrom [15]. The $\alpha^2 m_e/m_N$ contributions in H_3 and H_4 agree with the results of Hegstrom [4]. The $\alpha^2 m_e/m_N$ contribution in H_2+H_8 is exactly half of the spin-other-orbit contributions in Hegstrom's Eq. (21) [4]. These are the only contributing forms of order $\alpha^2 m_e/m_N$ in Hegstrom[s Hamiltonian [4]. In addition to these we have the contributions from Eq. (21) above. So we lose a contribution in H_2+H_8 but pick up a contribution in H_9. This is the result of the algebra which is necessary to ensure Poincaré invariance of the atomic system to relative order $(v/c)^2$. It amounts exactly to the replacement

$$-\sum_{\substack{i,j\\(i\neq j)}}\frac{Ze^2}{2q_i^3}\left[\frac{m_e}{m_N}\right]\frac{\mu_B}{m_e c^2}\mathbf{B}\cdot[(\mathbf{q}_i+\mathbf{q}_j)\times(\boldsymbol{\sigma}_i\times\mathbf{q}_i)]$$

$$\Longrightarrow-\sum_{\substack{i,j\\(i\neq j)}}\left[\frac{m_e}{m_N}\right]\frac{\mu_B}{2m_e^2c^2}\mathbf{B}\cdot[(\boldsymbol{\pi}_i+\boldsymbol{\pi}_j)\times(\boldsymbol{\sigma}_i\times\boldsymbol{\pi}_i)] \tag{22}$$

in Hegstrom's [4] spin-other-orbit terms of order $\alpha^2 m_e/m_N$. These terms contribute to the g_s' and g_x factors. To facilitate the extraction of the g factors it is useful to recouple the Zeeman Hamiltonian in terms of spherical tensors

$$H_0'=\mu_B\mathbf{B}\cdot(g_L\mathbf{L}+g_e\mathbf{S})\ , \tag{23}$$

$$H_1=-\mu_B\mathbf{B}\cdot\sum_{i=1}^{2}(l_i+2\sigma_i)\frac{\pi_i^2}{2m_e c^2}\ , \tag{24}$$

$$H_2=\frac{2Ze^2}{3m_e c^2}\left[1+2a_e-\frac{m_e}{m_N}\right]\mu_B\mathbf{B}\cdot\sum_{i=1}^{2}\frac{1}{q_i}[\boldsymbol{\sigma}_i+(\tfrac{5}{2})^{1/2}\{\boldsymbol{\sigma}_i C_i^{(2)}\}^{(1)}]\ , \tag{25}$$

$$\begin{aligned}H_3+H_4=\frac{2e^2}{m_e c^2}\mu_B\mathbf{B}\cdot\Bigg[\Bigg[&\boldsymbol{\sigma}_1+2\boldsymbol{\sigma}_2+2a_e\mathbf{S}+\left[\frac{m_e}{m_N}\right](\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)\Bigg]\\&\times\sum_k(-1)^k(2k+1)^{1/2}\Bigg\{\frac{1}{3}\left[k\frac{q_1^k}{q_2^{k+1}}-(k+1)\frac{q_2^k}{q_1^{k+1}}\right]\{C_1^{(k)}C_2^{(k)}\}^{(0)}\\&+\frac{[k(k+1)]^{1/2}}{2\sqrt{6}}\left[\frac{q_1^k}{q_2^{k+1}}+\frac{q_2^k}{q_1^{k+1}}\right]\{C_1^{(k)}C_2^{(k)}\}^{(1)}\\&-\frac{[k(k+1)]^{1/2}}{6\sqrt{2}}\left[\left[\frac{2k+3}{2k-1}\right]^{1/2}\frac{q_1^k}{q_2^{k+1}}-\left[\frac{2k-1}{2k+3}\right]^{1/2}\frac{q_2^k}{q_1^{k+1}}\right]\\&\times\{C_1^{(i)}C_2^{(k)}\}^{(2)}+\frac{1}{2\sqrt{3}}\left[\frac{k(k-1)(2k-3)}{2k-1}\right]^{1/2}\frac{q_1^k}{q_2^{k+1}}\{C_1^{(k-2)}C_2^{(k)}\}^{(2)}\\&-\frac{1}{2\sqrt{3}}\left[\frac{(k+1)(k+2)(k+5)}{2k+3}\right]^{1/2}\frac{q_2^k}{q_1^{k+1}}\{C_1^{(k+2)}C_2^{(k)}\}^{(2)}\Bigg\}\Bigg]\ ,\end{aligned} \tag{26}$$

$$\begin{aligned}H_5=\frac{1}{m_e c^2\sqrt{3}}\mu_B\mathbf{B}\cdot\sum_k(-1)^k\Bigg[&\left[\frac{q_2^k}{q_1^{k+1}}+\frac{q_1^{k+2}}{q_2^{k+3}}\right]\Bigg\{\frac{k(k+3)}{2k+3}[(2k+1)^{1/2}\times\{C_1^{(k)}\{C_2^{(k)}l_2\}^{(k)}\}^{(1)}\\&-(2k+5)^{1/2}\{C_1^{(k+2)}\{C_2^{(k+2)}l_2\}^{(k+2)}\}^{(1)}]\\&-2\left[\frac{2k+1}{2k+3}\right]^{1/2}\Bigg[(2k+1)^{1/2}\{C_1^{(k)}\{C_2^{(k)}l_2\}^{(k+1)}\}^{(1)}\\&+\left[\frac{(k+1)(2k+5)}{k+2}\right]^{1/2}\\&\times\{C_1^{(k+2)}\{C_2^{(k)}l_2\}^{(k+1)}\}^{(1)}\Bigg]\Bigg\}\end{aligned}$$

$$+\left[(k+3)\frac{q_1^{k+2}}{q_2^{k+2}}\frac{\partial}{\partial q_2}-k\frac{q_2^{k+1}}{q_1^{k+1}}\frac{\partial}{\partial q_2}\right]\frac{1}{2k+3}$$
$$\times([k(k+1)(2k+1)]^{1/2}\{C_1^{(k)}C_2^{(k)}\}^{(1)}$$
$$-[(k+2)(k+3)(2k+5)]^{1/2}\{C_1^{(k+2)}C_2^{(k+2)}\}^{(1)})\Bigg], \tag{27}$$

$$H_6'=-2\left[\frac{m_e}{m_N}\right]\mu_B\mathbf{B}\cdot\left[2\frac{q_1}{q_2}\{C_1^{(1)}\{C_2^{(1)}l_2\}\}^{(1)}-\sqrt{2}q_1\frac{\partial}{\partial q_2}\{C_1^{(1)}C_2^{(1)}\}^{(1)}\right], \tag{28}$$

$$H_7=\frac{-a_3}{m_e^2c^2}\mu_B\mathbf{B}\cdot\sum_{k=1}^{2}\left[\tfrac{1}{3}\pi_i^2\sigma_i+\frac{\sqrt{10}}{3}\{\sigma_iC_i^{(2)}\}^{(1)}\left[\frac{\partial^2}{\partial^2 q_i}-\frac{1}{q_i}\frac{\partial}{\partial q_i}\right]\right.$$
$$-(\tfrac{5}{3})^{1/2}\{\sigma_i\{C_i^{(2)}l_i\}^{(2)}\}^{(1)}\left[\frac{2}{q_i}\frac{\partial}{\partial q_i}-\frac{2}{q_i^2}\right]+\frac{1}{\sqrt{6}}\frac{1}{q_i^2}\{\sigma_il_l\}^{(1)}$$
$$\left.+\tfrac{1}{3}(\tfrac{70}{3})^{1/2}\frac{1}{q_i^2}\{\sigma_i\{C_i^{(2)}l_i^{(2)}\}^{(2)}\}^{(1)}+\frac{\sqrt{10}}{9q_i^2}l^2\{\sigma_iC_i^2\}^{(1)}+(\tfrac{5}{3})^{1/2}\frac{1}{3q_i^2}\{\sigma_il_i^{(2)}\}^{(1)}\right], \tag{29}$$

$$H_8=\frac{-Ze^2}{2m_ec^2}\left[\frac{m_e}{m_N}\right]\mu_B\mathbf{B}\cdot\sum_{i\neq j}\frac{q_j}{q_i^2}\left[\frac{-2}{\sqrt{3}}\{C_j^{(1)}C_i^{(1)}\}^{(0)}\sigma_i-\{\sigma_i\{C_j^{(1)}C_i^{(1)}\}^{(1)}\}^{(1)}+(\tfrac{5}{3})^{1/2}\{\sigma_i\{C_j^{(1)}C_i^{(1)}\}^{(2)}\}^{(1)}\right], \tag{30}$$

$$H_9=\frac{1}{2m_em_Nc^2}\mu_B\mathbf{B}\cdot\sum_{i\neq j}\left\{-\tfrac{2}{3}\pi_i^2\sigma_i+\frac{\sqrt{10}}{3}\{\sigma_iC_l^{(2)}\}^{(1)}\left[\frac{\partial^2}{\partial^2 q_i}-\frac{1}{q_i}\frac{\partial}{\partial q_i}\right]\right.$$
$$-(\tfrac{5}{3})^{1/2}\{\sigma_i\{C_i^{(2)}l_i\}^{(2)}\}^{(1)}\left[\frac{2}{q_i}\frac{\partial}{\partial q_i}-\frac{2}{q_i^2}\right]+\tfrac{1}{3}(\tfrac{70}{3})^{1/2}\frac{1}{q_i^2}\{\sigma_i\{C_i^{(2)}l_i^{(2)}\}^{(2)}\}^{(1)}$$
$$+\frac{\sqrt{10}}{9q_i^2}l_i^2\{\sigma_iC_i^2\}^{(1)}+(\tfrac{5}{3})^{1/2}\frac{1}{3q_i^2}\{\sigma_il_i^{(2)}\}^{(1)}+\frac{1}{\sqrt{6}}\frac{1}{q_i^2}\{\sigma_il_l\}^{(1)}$$
$$+\frac{2\sqrt{3}}{q_iq_j}\left[-\tfrac{2}{3}\sigma_i\{\{C_j^{(1)}l_j\}^{(1)}\{C_i^{(1)}l_i\}^{(1)}\}^{(0)}\right.$$
$$\left.-\frac{1}{\sqrt{3}}\{\sigma_i\{\{C_j^{(1)}l_j\}^{(1)}\{C_i^{(1)}l_i\}^{(1)}\}^{(1)}\}^{(1)}+\frac{\sqrt{5}}{3}\{\sigma_i\{\{C_j^{(1)}l_j\}^{(1)}\{C_i^{(1)}l_i\}^{(1)}\}^{(2)}\}^{(1)}\right]$$
$$+\frac{\sqrt{3}\partial^2}{\partial q_i\partial q_j}\left[-\tfrac{2}{3}\sigma_i\{C_j^{(1)}C_i^{(1)}\}^{(0)}-\frac{1}{\sqrt{3}}\{\sigma_i\{C_j^{(1)}C_i^{(1)}\}^{(1)}\}^{(1)}+\frac{\sqrt{5}}{3}\{\sigma_i\{C_j^{(1)}C_i^{(1)}\}^{(2)}\}^{(1)}\right]$$
$$-\frac{\sqrt{6}\partial}{q_i\partial q_j}\left[-\tfrac{2}{3}\sigma_i\{C_j^{(1)}\{C_i^{(1)}l_i\}^{(1)}\}^{(0)}\right.$$
$$\left.-\frac{1}{\sqrt{3}}\{\sigma_i\{C_j^{(1)}\{C_i^{(1)}l_i\}^{(1)}\}^{(1)}\}^{(1)}+\frac{\sqrt{5}}{3}\{\sigma_i\{C_j^{(1)}\{C_i^{(1)}l_i\}^{(1)}\}^{(2)}\}^{(1)}\right]$$
$$-\frac{\sqrt{6}\partial}{q_j\partial q_i}\left[-\tfrac{2}{3}\sigma_i\{C_i^{(1)}\{C_j^{(1)}l_j\}^{(1)}\}^{(0)}\right.$$
$$\left.\left.-\frac{1}{\sqrt{3}}\{\sigma_i\{C_i^{(1)}\{C_j^{(1)}l_j\}^{(1)}\}^{(1)}\}^{(1)}+\frac{\sqrt{5}}{3}\{\sigma_i\{C_i^{(1)}\{C_j^{(1)}l_j\}^{(1)}\}^{(2)}\}^{(1)}\right]\right\}, \tag{31}$$

where $C_i^{(k)}$ is a spherical tensor of rank k for the ith electron. The recoupling of two tensors to form another tensor of rank f is denoted by encasing the two tensors in curly brackets: $\{\ \}^{(f)}$. The α^2 contributions were first recoupled by Innes and Ufford [16]. In order to recouple H_9 we had to define a second-rank angular momentum tensor ($l_i^{(2)}$). The evaluation of the reduced matrix elements of this tensor is presented in Sec. IV. We have defined $g_L=1-m_e/m_N$ and combined the m_e/m_N term proportional to L in H_6 with H_0 in conformity with the conventions of Lewis, Pichanick, and Hughes [10] and Lewis and Hughes [7].

III. $2\,^3S_1$ g_J FACTOR

The techniques used to evaluate the $2\,^3S_1$ g factor are well known [3,4]. The only terms which do not contribute to the g_J factor are H_5, H_6, and ΔE_R, which act only in the Lm_L subspace of the $|JM_JLS\rangle$ representation. For S states $L=0$, $J=S$, and $g_J=g_S$. Using the projection theorem, we define the g_J factor

$$g_J\equiv\frac{1}{\mu_B B}\langle Sm_s=1|H_z|Sm_s=1\rangle\ . \tag{32}$$

Using the fact that $\langle\sigma_i\rangle=\delta_{i,z}$ for $S=1$, $\langle(\pi_i)^2\rangle=\frac{1}{3}\langle\pi^2\rangle$ (for $i=x$, y, and z), and similar results for the expectation value of the square of a Cartesian component of any operator in a spherically symmetric state, it is easy to see $\langle\boldsymbol{\pi}\times(\boldsymbol{\sigma}\times\boldsymbol{\pi})\rangle=\frac{2}{3}\langle\pi^2\rangle$ and similarly for all the other triple cross products in H_z. We now need to consider the effect of the finite mass of the heliumlike nucleus on the $2\,^3S_1$ wave function and expectation values of π_1^2, $1/q_1$, $\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_2$, $1/q_{12}$, and $(\mathbf{q}_1\cdot\mathbf{q}_2)/q_1^3$. The nonrelativistic Hamiltonian for a heliumlike atom with finite nuclear mass is [17]

$$H_f=\frac{\pi_1^2}{2\mu}+\frac{\pi_2^2}{2\mu}+\frac{(\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_2)}{m_N}-\frac{Ze^2}{q_1}-\frac{Ze^2}{q_2}+\frac{e^2}{q_{12}}\ , \tag{33}$$

where $\mu=(m_e m_N)/(m_e+m_N)$ is the reduced mass for the helium atom. This Hamiltonian is different from the nonrelativistic Hamiltonian for the helium atom with an infinitely massive nucleus in two respects: (i) the replacement of the electronic mass by the reduced mass in the electronic kinetic energy operators and (ii) the addition of the third term, which is referred to as the mass polarization term. If we first set the mass polarization term to zero the effect of the reduced mass in Eq. (33) is such that for an operator which has dimensions of (length)$^{-n}$, $\langle\hat{o}\rangle=\mu^n\langle\hat{o}\rangle_\infty$ (the operator scales as μ^n), where $\langle\hat{o}\rangle_\infty$ and $\langle\hat{o}\rangle$ are the expectation values using wave functions for the case of an infinitely massive nucleus and wave functions of H_f without the mass polarization term, respectively [18]. The operators π_1^2, $1/q_1$, $\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_2$, and $1/q_{12}^3$, are of degrees 2, -1, 2, and -3, respectively. To first order in m_e/m_N,

$$\mu^n=m_e[1-n(m_e/m_N)]\ , \tag{34}$$

$m_e/m_n=1.370\,933\,54\times10^{-4}$ for ^{4}He [19] and $m_e/m_N=1.818\,881\,21\times10^{-4}$ for ^{3}He [20]. Therefore, scaling affects the expectation values at the 10^{-4} level. If we now explicitly include the mass polarization term in the Hamiltonian when determining the variational wave functions, the expectation values will be affected at the 10^{-6} and 10^{-5} level for the $2S$ and $2P$ states of helium, respectively [21,22]. The largest contributions to the Zeeman Hamiltonian for which the form of the wave function can have an influence are of the order α^2 for the S states and m_e/m_N for P states and we are neglecting terms of order α^4 (3×10^{-9}) and smaller. Thus, we can neglect the effect of mass polarization completely. Scaling the α^2 terms with μ is equivalent to adding terms of the order $\alpha^2 m_e/m_N$. Note that the motional corrections of order m_e/m_N in H_6 are of degree 0 and do not scale with the reduced mass.

We can also reach the same conclusions via a different route. Application of the virial theorem to the Hamiltonian for an infinitely massive nucleus leads to the well-known results $\langle T\rangle=-E$ and $\langle V\rangle=2E$, where T, V, and E are the total kinetic-energy operator, potential-energy operator, and energy eigenvalue, respectively. Application of the virial theorem to Eq. (33) leads to the same relations where now the total kinetic-energy operator includes the mass polarization operator and the electronic mass is replaced by the reduced mass. Treating mass polarization in first-order perturbation theory, scaling with the reduced mass, and using the virial theorem, we can write

$$\left\langle-\frac{Ze^2}{q_1}-\frac{Ze^2}{q_2}+\frac{e^2}{q_{12}}\right\rangle=2E_f=2\mu\left[E_\infty+\left\langle\frac{(\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_2)}{m_N}\right\rangle\right]\ ,$$
$$\left\langle\frac{\pi_1^2}{2\mu}\right\rangle=\frac{-E_f}{2}=\frac{-\mu}{2}\left[E_\infty+\mu\left\langle\frac{(\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_2)}{m_N}\right\rangle\right]\ , \tag{35}$$

where E_f is the energy eigenvalue of H_f for the state under consideration. Using Eqs. (32), (34), (35), factoring $1=\frac{1}{2}g_e(1-a_e)$ to first order in a_e, and setting $a_e=\alpha/2\pi$ here and in H_1–H_9 we get the $n\,^3S_1$ g_J factor for an arbitrary heliumlike atom:

$$\begin{aligned}g_J=g_e\Bigg\{&1+\frac{E_\infty}{3m_ec^2}-\frac{1}{6m_ec^2}\left\langle\frac{e^2}{q_{12}}\right\rangle_\infty\\&-\frac{\alpha E_\infty}{4\pi m_ec^2}-\frac{E_\infty}{2m_Nc^2}-\frac{Ze^2}{6m_Nc^2}\left\langle\frac{\mathbf{q}_1\cdot\mathbf{q}_2}{q_1^3}\right\rangle_\infty\\&+\frac{1}{12m_Nc^2}\left\langle\frac{e^2}{q_{12}}\right\rangle_\infty+\frac{1}{6m_ec^2}\left\langle\frac{(\boldsymbol{\pi}_1\cdot\boldsymbol{\pi}_2)}{m_N}\right\rangle_\infty\Bigg\}\ .\end{aligned} \tag{36}$$

The α^2 and α^3 corrections agree with the results of Grotch and Hegstrom [6]. The $\alpha^2 m_e/m_N$ terms are not in agreement with their results. It is important to note here that Lewis and Hughes [23] used the above result correct to order α^3 (from Ref. [6]) to calculate numerically the g_J factors for many $n\,^3P_1$ states of heliumlike

atoms. Clearly that work is not correct since the P states are not spherically symmetric and $\langle(\pi_i)^2\rangle \neq \frac{1}{3}\langle\pi^2\rangle$ for the P states. If it was correct then all the contributions of the form $\{\sigma_i C_i^{(2)}\}^{(1)}$ would have to vanish for the $n\,^3P_1$ states and they do not. Furthermore, they erroneously claim that the α^3 contributions only affect the g_s factor, which is fallacious precisely because $\{\sigma_i C_i^{(2)}\}^{(1)}$ and similar forms do not vanish for any of the P states. These terms contribute to g_x.

We use the very accurate results of Pekeris [21]:

$$E_\infty = -2.175\,229\,378\,24\alpha^2 m_e c^2 ,$$

$$\langle e^2/q_{12}\rangle_\infty = 0.268\,197\,855\,3\alpha^2 m_e c^2 ,$$

$$\langle e^2/q_1\rangle_\infty - 1.154\,664\,153\alpha^2 m_e c^2 ,$$

$$\langle(\pi_1\cdot\pi_2)/m_N\rangle_\infty = 1.020\,109\,2\times 10^{-6}\alpha^2 m_e c^2 ,$$

and the five-figure-accurate result of Barkley and Hegstrom [6]:

$$\langle \mathbf{q}_1\cdot\mathbf{q}_2/q_1^3\rangle_\infty = -0.149\,860\alpha m_e c$$

to get

$$g_J = g_e[1-(40.991\,63-0.067\,27-0.008\,47 -0.000\,05)\times 10^{-6}] = 2.002\,237\,377\,8$$

for $2\,^3S_1$ ^{4}He and

$$g_J = g_e[1-(40.991\,63-0.067\,27-0.011\,23 -0.000\,01)\times 10^{-6}] = 2.002\,237\,383\,4$$

for $2\,^3S_1$ ^{3}He. The first three terms in the parentheses are contributions of order α^2, α^3, and $\alpha^2 m_e/m_N$, respectively. The last contribution is that due to mass polarization, which is negligible as expected. The above result for ^{4}He can be compared with the result of Barkley and Hegstrom [6]:

$$g_J = g_e[1-(40.991\,63-0.067\,27 -0.008\,67)\times 10^{-6}] = 2.002\,237\,378\,2 ,$$

which does not include mass polarization. Correspondingly, we get $1-23.211\times 10^{-6}$ and $1-23.208\times 10^{-6}$ for ratio of the helium $2\,^3S_1$ g_J factor to the hydrogen $1\,^2S_{1/2}$ g_J factor for ^{4}He and ^{3}He, respectively. The former is in excellent agreement with the best experimental value [5] $1-23.214(50)\times 10^{-6}$ and Barkely and Hegstrom [6], $1-23.211\times 10^{-6}$.

IV. $2\,^3P_J$ AND $2\,^1P_1$ g FACTORS

We have used three different types of wave functions to evaluate the g'_L, g'_s, g_x, and g_γ factors for the $2\,^3P_J$ and $2\,^1P_1$ states of ^{4}He and ^{3}He in a $|Jm_J LS\rangle$ representation. We have not retained the nuclear-spin-dependent terms in the Zeeman Hamiltonian and therefore will not calculate the ^{3}He g_I factor. All of the wave functions used are for an infinitely massive nucleus. Mass polarization is completely negligible and terms of the order α^2 have been scaled with the reduced mass to account for the effect of the finite mass of the nucleus on the wave function. The wave functions can be written as [22]

$$\begin{aligned}\psi &= A\sum_{\substack{m,n,\\ l_1 l_2}} C^{mn}_{l_1 l_2} q_1^m q_2^n e^{-(\alpha_i q_1+\beta_i q_2)} Y^{LM}_{l_1 l_2}\chi(1,2)\\ &\equiv A\sum_{\substack{m,n,\\ l_1 l_2}} C^{mn}_{l_1 l_2}\phi^{mn}_{l_1 l_2}\chi(1,2) ,\\ Y^{LM}_{l_1 l_2} &\equiv \sum_{m_1 m_2}\langle l_1 l_2 m_1 m_2|LM\rangle Y_{l_1 m_1}(\hat{\mathbf{q}}_1) Y_{l_2 m_2}(\hat{\mathbf{q}}_2) ,\end{aligned} \tag{37}$$

where A is the antisymmetrization operator $[1\pm(\text{exchange})]$, $\chi(1,2)$ is the spin function for either the triplet or the singlet state, $Y_{lm}(\hat{\mathbf{q}}_i)$ is a spherical harmonic, and $\langle l_1 l_2 m_1 m_2|LM\rangle$ is a Clebsch-Gordan coefficient. The coefficients $C^{mn}_{l_1 l_2}$ are determined by performing a Raleigh-Ritz variational calculation with the nonrelativistic Hamiltonian for a helium atom with an infinitely massive nucleus. These wave functions, which do not explicitly include q_{12} (the interaction distance) in the radial

TABLE II. Energy eigenvalues (in a.u.) and radial expectation values (in a.u.) for the $2\,^1P_1$ and $2\,^3P_J$ wave functions. The radial coordinate is that of an electron relative to the nucleus. The four entries are results for a hydrogenic wave function. A 50-term best wave function of a pure sp configuration, a 125-term best configuration-interaction wave function, and the wave function of Pekeris (Ref. [19]) in descending order. Pekeris does not have a value for $1/r^2$.

Operator	$2\,^2P_1$	$2\,^3P_J$
$-E$	2.122 390	2.130 691
	2.122 595	2.132 370
	2.123 828	2.133 160
	2.123 843	2.133 164
$\frac{1}{r}$	1.222 125	1.131 250
	1.122 243	1.132 800
	1.123 189	1.133 232
	1.123 178	1.133 242
r	2.965 112	2.670 463
	2.941 291	2.688 850
	2.910 521	2.674 230
	2.910 684	2.673 962
r^2	16.481 69	13.003 98
	16.108 50	13.374 83
	15.759 73	13.214 70
	15.769 58	13.211 74
$\frac{1}{r^2}$	4.050 810	4.009 604
	4.047 058	4.107 441
	4.043 083	4.014 629

basis, account for electronic correlation through configuration mixing. The nonlinear parameters $(\alpha_i\beta_i)$ are optimized for each different configuration. The dominant configuration for the P states is $l_1=0$, $l_2=1$ (sp). We obtained the first wave function by retaining only the dominant radial contribution $m=0$, $n=1$ for the pure sp configuration. This is the hydrogenic wave function of Eckart [24]. Expanding the radial basis to 50 terms, we then found the best possible wave function of a pure sp configuration. Finally, the most accurate wave function was obtained by mixing 30 $l_1=1$, $l_2=2$; 20 $l_1=2$, $l_2=3$; 10 $l_1=3$, $l_2=4$; 10 $l_1=4$, $l_2=5$; and 5 $l_1=5$, $l_2=6$ terms to the best pure sp wave function and then optimizing the 12 nonlinear parameters separately. The energy and radial expectation values for the above three wave functions are listed in Table II for comparison with each other and the very accurate results of Accad, Pekeris, and Schiff [25].

The benefit of using a configuration-interaction basis is that l_1 and l_2 are specified for each term of the wave function. This is not true for a wave function expanded in terms of a Hylleraas-type basis, which explicitly includes q_{12}. With l_1 and l_2 specified, general theorems of angular momentum can then be used to evaluate the expectation value of the Zeeman Hamiltonian [10,26]. The g factors in the $|Jm_JLS\rangle$ are then defined as

$$\langle {}^3P_j m_J|H_z|{}^3P_{J'}m_{J'}\rangle=(-1)^{1-J'}\sqrt{(2J'+1)}6\langle J'1m_J'0|Jm_J\rangle \times\left[W(JJ'11;11)[g_s'(-1)^{J+J'}g_L'](-1)^{j'}\left\{\begin{Bmatrix} J & J' & 1\\ 1 & 1 & 2\\ 1 & 1 & 1\end{Bmatrix}g_x+\begin{Bmatrix} J & J' & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{Bmatrix}g_\gamma\right\}\right]\mu_B B\ , \tag{38}$$

$$\langle {}^1P_1 m_J|H_z|{}^1P_1 m_J\rangle=\sqrt{2}\langle 11m0|1m\rangle g_L'\mu_B B\ ,$$

where $\langle J'1m_{J'}0|Jm_J\rangle$, $W(JJ'11;11)$, and

$$\begin{Bmatrix} J & J' & 1\\ 1 & 1 & 2\\ 1 & 1 & 1\end{Bmatrix}$$

are Clebsch-Gordan coefficients, Racca W functions, and nine-j symbols, respectively [26]. This is equivalent to the definition of Lewis, Pichanick, and Hughes [10]. The g_x and g_γ factors result from terms in the Zeeman Hamiltonian which do not act in either the Lm_L or the Sm_S subspaces separately. The terms which contribute to g_x couple a Pauli spin vector with a second-rank spherical tensor, e.g., $\{\sigma_i C_i^{(2)}\}^{(1)}$. The terms which contribute to g_γ couple a Pauli spin vector with an orbital-angular-momentum vector $\{\sigma_i l_i\}^{(1)}$. The g_γ factor was not included in the work of Lewis, Pichanick, and Hughes [10] or Lewis and Hughes [7] since these authors did not consider the contributions of orders α^3 and $\alpha^2 m_e/m_N$ which give rise to g_γ. In Eq. (38) $g_s'=g_e+[(\alpha^2+\alpha^3+\alpha^2 m_e/m_N)$ corrections] and $g_L'=1-m_e/m_N+[(m_e/m_N+\alpha^2+\alpha^3+\alpha^2 m_e/m_N)$ corrections]. The expectation value of the Zeeman Hamiltonian using the wave functions of Eq. (37) can be written symbolically as

$$\langle\psi|H_z|\psi'\rangle=AA'\sum_{\substack{m,m,\\ l_1,l_2}}\sum_{\substack{m',n',\\ l_1',l_2'}}C_{l_1l_2}^{mn}C_{l_1'l_2'}^{m'n'}\langle\phi_{l_1l_2}^{mn}|H_z|\phi_{l_1'l_2'}^{m'n'}\rangle\ , \tag{39}$$

where the sum are over all the terms of a wave function and contain both direct and exchange contributions. We define

$$\begin{aligned} c_a\equiv\frac{\alpha^2}{4}m_e/m_N[(2l_1+1)(2l_2+1)]^{1/2}&\langle l_1100l_1'0\rangle\langle l_2100|l_2'0\rangle\\ \times\Big\{&2[l_2'(l_2'+1)(2l_2'+1)(l_1'+1)(2l_1'+1)351]^{1/2}W(l_1l_1'11;1l_1')W(l_2l_2'1l;1l_2')\left\langle mn\left|\frac{1}{q_1q_2}\right|m'n'\right\rangle\\ &+[l_1'(l_1'+1)(2l_1'+1)18[^{1/2}W(l_1l_1'1l;1l_1')\left\langle mn\left|\frac{\partial}{q_1\partial q_2}\right|m'n'\right\rangle+[l_2'(l_2'+1)(2l_2'+1)18]^{1/2}\\ &\times W(l_2l_2'11;1l_2')\left\langle mn\left|\frac{\partial}{q_2\partial q_1}\right|m'n'\right\rangle-\left\langle mn\left|\frac{\partial^2}{\partial q_1\partial q_2}\right|m'n'\right\rangle\Big\}\ , \end{aligned} \tag{40}$$

where the bracketed terms are the radial matrix elements of an operator between the radial basis terms of the variational wave function:

$$\langle mn|\hat{0}(q_1q_2)|m'n'\rangle \equiv \int_0^\infty q_1^2 dq_1 \int_0^\infty q_2^2 dq_2 \hat{0}(q_1q_2) q_1^{m+m'} q_2^{n+n'} \ . \tag{41}$$

We also define radial integrals for which $q_1 \geq q_2$:

$$\langle mn|\hat{0}(q_1q_2)|m'n'\rangle_{\geq} \equiv \int_0^\infty q_1^2 dq_1 \int_0^{q_1} q_2^2 dq_2 \hat{0}(q_1q_2) q_1^{m+m'} q_2^{n+n'} \ . \tag{42}$$

and similarly for those in which $q_2 \geq q_1$. The g factors are explicitly found to be

$$\begin{aligned} g_s' = g_e + AA' \sum_{\substack{m,n,\\ l_1,l_2}} \sum_{\substack{m',n',\\ l_1',l_2'}} C_{l_1l_2}^{mn} C_{l_1'l_2'}^{m'n'} \Bigg\{ & -\alpha^2 \left[1+\frac{\alpha}{6\pi}-\frac{11}{3}m_e/m_N\right]\langle mn|T_1|m'n'\rangle \\ & +\frac{\alpha^2}{3}\left[1+\frac{\alpha}{\pi}-2m_e/m_N\right]\left\langle mn\left|\frac{1}{q_1}\right|m'n'\right\rangle \\ & +\frac{\alpha^2}{6}m_e/m_N(-1)^{l_1+l_2'}[(2l_1+1)(2l_2+1)]^{1/2}\langle l_1100|l_1'0\rangle\langle l_2100|l_2'0\rangle W(l_1l_2l_1'l_2';11) \\ & \times\left\langle mn\left|\frac{q_2}{q_1^2}\right|m'n'\right\rangle + \tfrac{2}{3}c_a(-1)^{l_1+l_2'}W(l_1l_1'l_2l_2';11) \\ & -\sum_{k=0}^{\infty}\left[\frac{\alpha^2}{2}\left[k\left\langle mn\left|\frac{q_1^k}{q_2^{k+1}}\right|m'n'\right\rangle_{\geq} -(k+1)\left\langle mn\left|\frac{q_2^k}{q_1^{k+1}}\right|m'n'\right\rangle_{\geq}\right](-1)^{l_1+l_2'}\right. \\ & \times[(2l_1+1)(2l_2+1)]^{1/2}\langle l_1100|l_1'0\rangle\langle l_2100|l_2'0\rangle \\ & \left.\left.\times W(l_1l_2l_1'l_2';1k)\left[1+\frac{2\alpha}{3\pi}-m_e/m_N\right]\right]\right\}, \end{aligned} \tag{43}$$

$$\begin{aligned} g_L' = 1-m_e/m_N + AA' \sum_{\substack{m,n,\\ l_1,l_2}} \sum_{\substack{m',n',\\ l_1',l_2'}} C_{l_1l_2}^{mn} C_{l_1'l_2'}^{m'n'} \Bigg[& m_e/m_N \begin{Bmatrix} 1 & 1 & 1 \\ l_1 & l_1' & 1 \\ l_2 & l_2' & 1 \end{Bmatrix} [(2l_1+1)(2l_2+1)]^{1/2}\langle l_1100|l_1'0\rangle\langle l_2100|l_2'0\rangle 3 \\ & \times\left[\left\langle mn\left|\frac{q_{1\partial}}{\partial q_2}\right|m'n'\right\rangle + (-1)^{l_2'+l_2'}[(2l_2'+1)(l_2'+1)l_2'6]^{1/2}\right. \\ & \left.\times W(l_2'l_2'11;1l_2)\left\langle mn\left|\frac{q_1}{q_2}\right|m'n'\right\rangle\right] \\ & -\alpha^2(1-2m_e/m_N)(-1)^{l_1'+l_2}[\tfrac{3}{2}(l_1)(l_1+1)(2l_1+1)]^{1/2}W(11l_1l_1';1l_2)\langle mn|T_1|m'n'\rangle \\ & +\sum_{k=0}^{\infty}\alpha^2(1-m_e/m_N)[(2l_1+1)(2l_2+1)]^{1/2} \\ & \times\begin{Bmatrix} 1 & 1 & 1 \\ l_1 & l_1' & k+2 \\ l_1 & l_2' & k+2 \end{Bmatrix}\langle l_1k+200|l_1'0\rangle\langle l_2k+200|l_2'0\rangle \\ & \times\left[(-1)^{k+1}\left[\frac{(k+3)\left\langle mn\left|\frac{q_1^{k+2}\partial}{q_2^{k+2}\partial q_2}\right|m'n'\right\rangle_{\geq} - k\left\langle mn\left|\frac{q_2^{k+1}\partial}{q_1^{k+1}\partial q_2}\right|m'n'\right\rangle_{\geq}}{(2k+3)}\right]\right. \\ & \left.\times[\tfrac{3}{8}(k+2)(k+3)(2k+5)]^{1/2} + (-1)^{1+l_2+l_2'}W[l_2'l_2'(k+2)(k+2);1l_2]\right] \end{aligned}$$

$$
\times\left[\frac{k(k+3)(2k+5)}{(2k+3)6}l_2'(l_2'+1)(2l_2'+1)(2k+5)\right]^{1/2}
$$

$$
\times\tfrac{3}{2}\left[\left\langle mn\left|\frac{q_2^k}{q_1^{k+1}}\right|m'n'\right\rangle_{\geq}+\left\langle mn\left|\frac{q_1^{k+2}}{q_2^{k+3}}\right|m'n'\right\rangle_{\geq}\right]\Bigg]
$$

$$
+\langle l_1k00|l_1'0\rangle\langle l_2k00|l_2'0\rangle
$$

$$
\times\frac{(-1)^{l_2+l_2'}}{2}\begin{Bmatrix}1 & 1 & 1\\ l_1 & l_1' & k\\ l_2 & l_2' & k\end{Bmatrix}
$$

$$
\times\left[\frac{k(k+3)(2k+1)3}{(2k+3)2}l_2'(l_2'+1)(2l_2'+1)(2k+1)\right]^{1/2}W(l_2'l_2'kk;1l_2)
$$

$$
\times\left[\left\langle mn\left|\frac{q_2^k}{q_1^{k+1}}\right|m'n'\right\rangle_{\geq}+\left\langle mn\left|\frac{q_1^{k+2}}{q_2^{k+3}}\right|m'n'\right\rangle_{\geq}\right]
$$

$$
+(-1)^{l_2+l_2'+1}\begin{Bmatrix}1 & 1 & 1\\ l_1 & l_1' & k\\ l_2 & l_2' & k+1\end{Bmatrix}3[\tfrac{1}{6}l_2'(l_2'+1)(2l_2'+1)]^{1/2}
$$

$$
\times W(l_2'l_2'k(k+1);1l_2)(2k+1)
$$

$$
\times\left[\left\langle mn\left|\frac{q_2^k}{q_1^{k+1}}\right|m'n'\right\rangle_{\geq}+\left\langle mn\left|\frac{q_1^{k+2}}{q_2^{k+3}}\right|m'n'\right\rangle_{\geq}\right]+(-1)^k\begin{Bmatrix}1 & 1 & 1\\ l_1 & l_1' & k\\ l_2 & l_2' & k\end{Bmatrix}
$$

$$
\times\left[\frac{(k+3)\left\langle mn\left|\frac{q_1^{k+2}\partial}{q_2^{k+2}\partial q_2}\right|m'n'\right\rangle_{\geq}-k\left\langle mn\left|\frac{q_2^{k+1}\partial}{q_1^{k+1}\partial q_2}\right|m'n'\right\rangle_{\geq}}{(2k+3)}\right]
$$

$$
\times[k(k+1)(2k+1)]^{1/2}\Bigg]
$$

$$
+(-1)^{l_2+l_2'}\langle l_2k00|l_2'0\rangle\langle l_1(k+2)00|l_1'0\rangle\begin{Bmatrix}1 & 1 & 1\\ l_1 & l_1' & k+2\\ l_2 & l_2' & k+1\end{Bmatrix}
$$

$$
\times W[l_2'l_2'k(k+1);1l_2]\left[\frac{(2k+1)(k+1)(2k+5)3}{(k+2)2}l_2'(l_2'+1)(2l_2'+1)\right]^{1/2}
$$

$$
\times\left[\left\langle mn\left|\frac{q_2^k}{q_1^{k+1}}\right|m'n'\right\rangle_{\geq}+\left\langle mn\left|\frac{q_1^{k+2}}{q_2^{k+3}}\right|m'n'\right\rangle_{\geq}\right]\Bigg]\Bigg]+g_{LR}\ , \tag{44}
$$

$$
g_x=AA'\sum_{\substack{mn\\ l_1l_2}}\sum_{\substack{m',n'\\ l_1'l_2'}}C_{l_1l_2}^{mn}C_{l_1'l_2'}^{m'n'}\left[\alpha^2\left[1-2m_e/m_N+\frac{\alpha}{\pi}\right]\langle l_1200|l_1'0\rangle W(21l_1l_2;1l_1')\left\langle mn\left|\frac{1}{q_1}\right|m'n'\right\rangle\right.
$$

$$
\left.\times[\tfrac{15}{2}(2l_1+1)]^{1/2}\delta_{l_2l_2'}+\frac{\alpha^2}{4}\left[\frac{\alpha}{\pi}-m_e/m_N\right]\delta_{l_2l_2'}W(12l_2l_1';1l_1)(-1)^{l_1+l_1'}\right.
$$

$$\times\langle l_1 200|l_1' 0\rangle(2l_1+1)^{1/2}$$
$$\times\left[\sqrt{30}\left\langle mn\left|\frac{\partial^2}{\partial^2 q_1}-\frac{\partial}{q_1\partial q_1}\right|m'n'\right\rangle+\sqrt{45}(-1)^{l_1+l_1'}[5l_1'(2l_1'+1)(l_1'+1)]^{1/2}\right.$$
$$\times W(22l_1'l_1';1l_1)\left[2\left\langle mn\left|\frac{\partial}{q_1\partial q_1}\right|m'n'\right\rangle 2+\left\langle mn\left|\frac{2}{q_1^2}\right|m'n'\right\rangle\right]$$
$$+\left\langle mn\left|\frac{1}{q_1^2}\right|m'n'\right\rangle\delta_{l_1l_1'}\left[-\sqrt{70}[2l_1'+1)5]^{1/2}W(l_1l_1'22;2l_1')\right.$$
$$\times\langle l_1\|l_1^2\|l_1'\rangle-(\tfrac{10}{3})^{1/2}l_1(l_1+1)$$
$$\left.\left.-\frac{\sqrt{5}}{\langle l_1 200|l_1' 0\rangle}\langle l_1\|l_1^2\|l_1'\rangle\right]\right]+\alpha^3 m_e/m_N\begin{Bmatrix}1 & 1 & 2\\ l_1 & l_1' & 1\\ l_2 & l_2' & 1\end{Bmatrix}$$
$$\times\left[\sqrt{75}c_a\tfrac{15}{4}\langle l_1 100|l_1' 0\rangle\langle l_1 200|l_2' 0\rangle[(2l_1+1)(2l_2+1)]^{1/2}\left\langle mn\left|\frac{q_2}{q_1^2}\right|m'n'\right\rangle\right]$$
$$+\alpha^2\left[1-\frac{2\alpha}{3\pi}-m_3/m_N\right]$$
$$\times\sum_{k=0}^{\infty}(-1)^k\langle l_2 k00|l_2' 0\rangle[(2l_1+1)(2l_2+1)(k+1)]^{1/2}$$
$$\times\left[-\tfrac{45}{8}\sqrt{k(k+1)}\left[\frac{(2k+3)}{(2k-1)}\left\langle mn\left|\frac{q_1^k}{q_2^{k+1}}\right|m'n'\right\rangle_{\geq}-\frac{(2k-1)}{(2k+3)}\left\langle mn\left|\frac{q_2^k}{q_1^{k+1}}\right|m'n'\right\rangle_{\geq}\right]\right.$$
$$\times\begin{Bmatrix}1 & 1 & 2\\ l_1 & l_1' & k\\ l_2 & l_2' & k\end{Bmatrix}\langle l_1 k00|l_1' 0\rangle$$
$$+\tfrac{9}{4}\langle l_1(k-2)00|l_1' 0\rangle\begin{Bmatrix}1 & 1 & 2\\ l_1 & l_1' & k-2\\ l_2 & l_2' & k\end{Bmatrix}\left[\frac{k(k-1)(2k-3)5}{(2k-1)}\right]^{1/2}$$
$$\times\left\langle mn\left|\frac{q_1^k}{q_2^{k+1}}\right|m'n'\right\rangle_{\geq}-\tfrac{9}{4}\langle l_1(k+2)00|l_1' 0\rangle\begin{Bmatrix}1 & 1 & 2\\ l_1 & l_1' & k+2\\ l_2 & l_2' & k\end{Bmatrix}$$
$$\left.\times\left[\frac{(k+1)(k+2)(2k+5)5}{(2k+3)}\right]\left\langle mn\left|\frac{q_2^k}{q_1^{k+1}}\right|m'n'\right\rangle_{\geq}\right]\Bigg], \tag{45}$$

$$g_\gamma=AA'\sum_{\substack{m,n,\\ l_1l_2}}\sum_{\substack{m',n',\\ l_1'l_2'}}C_{l_1l_2}^{mn}C_{l_1'l_2'}^{m'n'}\left\{\frac{\alpha^2}{4}\left[\frac{\alpha}{\pi}-m_e/m_N\right]\left\langle mn\left|\frac{1}{q_1^2}\right|m'n'\right\rangle 3\delta_{l_1l_1'}\delta_{l_2l_2'}W(11l_2l_1';1l_1)(-1)^{l_1+l_2}\right.$$
$$\left.\times[2l_1(2l_1+1)(l_1+1)]^{1/2}\right\}, \tag{46}$$

where g_{LR} is the contribution to the g_L' factor coming from the radiative corrections of Eq. (1) derived in Appendix A, $T_1 \equiv \pi_1^2/2m_e$, and $\langle l_1 \| l_1^2 \| l_1' \rangle$ is the reduced matrix element for l_1^2 which is a second-rank angular-momentum tensor operator built from the components of the angular momentum vector in the usual way:

$$l_m^2 = \sum_{m_1,m_2} \langle 11 m_1 m_2 | 2m \rangle l_{m_1}^1 l_{m_2}^1 . \tag{47}$$

The fact that the components of $\boldsymbol{l}$ do not commute is not a problem since the components of l^2 are symmetric. Using $l_\pm^1 = \mp 1/\sqrt{2} L_\pm$, $L_0^1 = L_0$, $L_0 |Lm\rangle = m|Lm\rangle$, and $L_\pm |Lm\rangle = [l(l+1) - m(m\pm 1)]^{1/2} |Lm \pm 1\rangle$ the reduced matrix elements are found to be

$$\langle l_1 \| l_1^2 \| l_1' \rangle = \delta(l_1, l_1') \begin{cases} 1.290\,994\,448\,735\,806 & (l_1 = 1) \\ 4.582\,575\,694\,955\,841 & (l_1 = 2) \\ 9.486\,832\,980\,505\,138 & (l_1 = 3) \\ 16.020\,819\,787\,597\,219 & (l_1 = 4) \\ 24.186\,773\,244\,895\,647 & (l_1 = 5) \\ 33.985\,290\,935\,932\,859 & (l_1 = 6) \\ 45.416\,590\,214\,002\,923 & (l_1 = 7) . \end{cases} \tag{48}$$

Equations (43)–(45) contain the $\alpha^2 m_e/m_N$ corrections due to the scaling of the α^2 terms with the reduced mass, thus accounting for the effect of the finite mass of the nucleus on the wave function to the precision we require. The numerical contributions of order m_e/m_N, α^2, α^3, and $\alpha^2 m_e/m_N$ to the $2\,^3P_J$ and $2\,^1P_1$, g_L', g_s', g_x, and g_γ factors of ^{4}He and ^{3}He are listed in Tables III and IV for each of the three wave functions that we used. The results using the simple hydrogenic wave function agree (to α^2) exactly with the results of Lewis and Hughes [7]. The expectation value of the m_e/m_N corrections of H_6 [Eq. (28)] is sensitive to the form of the wave function. Using an accurate wave function expanded in a configuration-interaction basis, we get a substantial improvement between the experimental g_L' factor and the theoretical g_L' factor over the results of Lewis and Hughes [7]. However, our result for the ^{4}He g_L' factor is still 1.36 standard deviations above the experimental value [8] when including the α^3 radiative corrections of Eq. (1).

Here we would like to comment on the accuracy of the results of our work using a configuration-interaction wave function in contrast to the accuracy of the results of Lewis and Hughes [7], who used a Hylleraas-type wave function. Our best $2\,^3P$ energy is accurate to 2 ppm and the $2\,^3P$ energy of Lewis and Hughes [7] is accurate about to 20 ppb. Since the error in the energy of a variational calculation is proportional to the square of the error in the wave function, we would roughly expect our wave functions and matrix elements to be accurate to 10^{-3} and those of Lewis and Hughes [7] to be accurate to 10^{-4}. This, in fact, corresponds to the error that Lewis and Hughes associate with their value for g_s' (not a single matrix element) by means of extrapolation [7]. The errors that Lewis and Hughes [7] associate with g_L' and g_x (by extrapolation) are much worse: 3.7% and 71.4%, respectively. If our wave function was only correct to 1 ppt we

TABLE III. Individual theoretical motional and relativistic corrections to the ^{4}He $2\,^3P_J$ and $2\,^1P_1$ g factors. All entries are to be multiplied by 10^{-6}. Of the three entries for each g factor, the upper entry is the result using a simple hydrogenic wave function. The middle entry is the result using the best wave function of a pure sp configuration. The lowest entry is the result using a 125-term configuration-interaction wave function. Only the lowest entries include α^3 radiative and reduced-mass corrections $g_e = 2(1+a_e)$ and $g_L = 1 - m_e/m_N$.

g factor	m_e/m_N	α^2	α^3	$\alpha^2 m_e/m_N$	Total
		$2\,^3P_J$			
$g_s' - g_e$	0.000 00	−80.264 14	0.038 45	−0.009 91	−80.236
	0.000 00	−80.430 14	0.038 47	−0.007 71	−80.399
	0.000 00	−80.460 58	0.038 48	0.021 08	−80.401
$g_s' - g_e$	12.242 76	−8.402 59	0.000 00	0.000 00	3.840
	21.756 27	−8.743 39	0.000 00	0.000 00	13.013
	17.565 97	−8.909 70	0.178 90	0.002 37	8.838
g_x	0.000 00	−5.596 53	0.014 82	0.005 22	−5.577
	0.000 00	−5.640 40	0.016 77	0.023 01	−5.600
	0.000 00	−5.393 72	0.017 56	0.026 22	−5.350
g_γ	0.000 00	0.000 00	0.009 45	0.000 93	0.010
	0.000 00	0.000 00	0.009 58	0.001 26	0.011
	0.000 00	0.000 00	0.009 61	0.001 38	0.011
		$2\,^1P_1$			
$g_L' - g_L$	−8.161 55	−6.598 41	0.000 00	0.000 00	−14.760
	−3.463 32	−6.598 43	0.000 00	0.000 00	−10.062
	−8.969 73	−6.802 75	0.000 00	0.001 81	−15.773

TABLE IV. Individual theoretical motional and relativistic corrections to the ^{3}He $2\,^3P_J$ and $2\,^1P_1$ g factors. All entries are to be multiplied by 10^{-6}. Of the three entries for each g factor, the upper entry is the result using a simple hydrogenic wave function. The middle entry is the result using the best wave function of a pure sp configuration. The lowest entry is the result using a 125-term configuration-interaction wave function. Only the lowest entries include α^3 radiative and reduced mass corrections $g_e=2(1+a_e)$ and $g_L=1-m_e/m_N$.

g factor	m_e/m_N	α^2	α^3	$\alpha^2 m_e/m_N$	Total
		$2\,^3P_J$			
$g_s'-g_e$	0.000 00	−80.264 14	0.038 45	−0.013 15	−80.394
	0.000 00	−80.430 14	0.038 47	−0.010 23	−80.402
	0.000 00	−80.460 58	0.038 48	0.027 97	−80.394
$g_L'-g_L$	16.243 04	−8.402 59	0.000 00	0.000 00	7.840
	28.865 05	−8.743 39	0.000 00	0.000 00	20.122
	23.305 59	−8.909 70	0.178 90	0.003 14	14.578
g_x	0.000 00	−5.596 53	0.014 82	0.006 93	−5.575
	0.000 00	−5.640 40	0.016 77	0.030 53	−5.593
	0.000 00	−5.393 72	0.017 56	0.034 79	−5.341
g_γ	0.000 00	0.000 00	0.009 45	0.000 32	0.010
	0.000 00	0.000 00	0.009 58	0.001 04	0.011
	0.000 00	0.000 00	0.009 61	0.001 15	0.011
		$2\,^1P_1$			
$g_L'-g_L$	−10.828 31	−6.598 41	0.000 00	0.000 00	−17.427
	−4.594 95	−6.598 43	0.000 00	0.000 00	−11.193
	−11.900 56	−6.802 75	0.000 00	0.002 40	−18.701

would expect the error in g_s' to be at least $\pm 0.08\times 10^{-6}$, yet we obtain exact agreement (to terms of order α^2) with the results of Lewis and Hughes [7]. In fact, Lewis and Hughes [7] obtain the same result ($g_s'-g_e=-80.46\times 10^{-6}$) with Hylleraas-type wave functions of 35, 56, 84, 120, and 165 terms. This is because the terms which contribute to g_s' are scalar operators in the Lm_L subspace. They are not sensitive to the exact form of the wave function. The terms which contribute to g_L' and g_x have a more complicated angular structure. As a consequence the g_L' and g_x factors depend more on the exact form of the wave function. If we compare the convergence of the energy and g factors of Lewis and Hughes [7] with our results in Tables I and II we can only conclude that the main difference between our results and the results of Lewis and Hughes [7] cannot be due to the order-of-magnitude error in the wave function or the slow convergence of the configuration-interaction basis. We expect that the simplicity of our approach in separating the radial and angular integrals has facilitated in the calculation of more accurate values of g_L' and g_x. Looking at Tables III and IV we note that the only contribution which depended critically on choice of each of the wave functions that we used was the expectation value of H_6' [Eq. (28)], which is responsible for the range of values for g_L' in Tables I, II, and IV. Furthermore, to get an idea of the magnitude of error in our g factors we have recalculated the $2\,^3P$ g factors for configuration-interaction wave functions which yield energy eigenvalues in error by 1 and 5 ppm relative to our best wave function with an energy eigenvalue of −2.133 160 a.u. Using the latter two wave functions we have taken the average error in the g factors (for each ppm error in the energy eigenvalue) as an estimate of the error (for each ppm error in the energy eigenvalue) in our reported $2\,^3P$ g factors. In this manner we estimate the error in our ^{4}He $2\,^3P$ g factors as $g_\gamma=0.011(0)\times 10^{-6}$, $g_s'-g_e=-80.401(0)\times 10^{-6}$, $g_x=-5.344(2)\times 10^{-6}$, and $g_L'-g_L=8.838(13)\times 10^{-6}$. The error in the ^{3}He $2\,^3P$ g factors is about the same as the ^{4}He $2\,^3P$ g factors in ppm.

V. SUMMARY AND CONCLUSIONS

The purely motional contributions of order m_e/m_N and relativistic contributions of order α^2 and α^3 to the Zeeman Hamiltonian for heliumlike atoms [Eqs. (11)–(21)] agree with previous calculations [2–4]. The relativistic motional corrections of order $\alpha^2 m_3/m_N$, however, do not agree with the results of Hegstrom [4].

Note added in proof. Although the terms of order $\alpha^2(m_e/m_N)$ of our Zeeman Hamiltonian [Eqs. (11)–(21)] are not the same as those of Hegstrom [4], our Zeeman Hamiltonian [Eqs. (11)–(21)] can be obtained by making a unitary transformation on the Hamiltonian [Eq. (21) of Ref. [4]] of Hegstrom [4] with the unitary operator

$$U=\exp\left[\frac{ie}{4}(\mathbf{r}_1+\mathbf{r}_2-2\mathbf{r}_3)\cdot\mathbf{B}\times\left[\frac{\boldsymbol{\sigma}_1\times\boldsymbol{\pi}_1+\boldsymbol{\sigma}_2\times\boldsymbol{\pi}_2}{2m_e m_N c^2}\right]+\text{H.c.}\right].$$

Thus our Zeeman Hamiltonian and Hegstrom's [4]

Zeeman Hamiltonian for heliumlike atoms should lead to the same value for the g factors of heliumlike atoms provided the same wave functions are used. This is exemplified in the agreement between our value for the ^{4}He $2\,^3S_1$ g_J factor and the value for this g factor obtained by Barkley and Hegstrom [6].

Our ^{4}He $2\,^3S_1$ g_J factor $[g_3(1-40.9158\times10^{-6})=2.002\,237\,377\,8]$ agrees with the results of Grotch and Hegstrom and Barkley and Hegstrom [6] $[g_e(1-40.915\,69\times10^{-6})=2.002\,237\,378\,2]$. The ratio of the above g factor to the g_J factor of $1\,^2S_{1/2}$ hydrogen [9] [2.002 283 852 451] is $1-23.211\times10^{-6}$ using our value and using the results of Barkley and Hegstrom [6]. This compares well with the most precise experimental value [5] $[1-23.214(50)\times10^{-6}]$.

We have calculated all of the corrections of order m_e/m_N, α^2, α^3, and $\alpha^2 m_e/m_N$ to the $2\,^3P_J$ ^{4}He and ^{3}He g factors. The corrections of order α^3 and $\alpha^2 m_e/m_N$ have not previously been included for these g factors. We have used wave functions for a finite nuclear mass expanded in terms of a configuration-interaction basis as opposed to a Hylleraas [7] basis. Including terms to order α^2, our result for the $2\,^3P_J$ ^{4}He g_s' factor $[g_e-80.461\times10^{-6}]$ agrees exactly with the calculation of Lewis and Hughes [7]. Including terms of orders α^3 and $\alpha^2 m_e/m_N$ changes this value to $g_s'=g_e-80.401\times10^{-6}$. This is 1.83 standard deviations below the only experimental value for the ^{4}He $2\,^3P_J$ g_s' factor $[g_e-76.0(2.4)\times10^{-6}]$ [10]. However, the experimental result cannot measure the effect of configuration mixing: it is based upon the assumption of a pure sp configuration for the $2\,^3P_J$ states [10]. Our result for the g_X factor $[-5.344\times10^{-6}]$ is in good agreement with the result of Lewis and Hughes [7] $[-3.5(2.5)\times10^{-6}]$. The only experimental value is quite imprecise $4.0(25.0)\times10^{-6}$] Ref. [10]. Better experimental results exist for the ^{4}He and ^{3}He $2\,^3P_J$ g_L' factors: $[1-m_e/m_N+4.9(2.9)\times10^{-6}]$ Ref. [8] and $[1-m_e/m_N+10.5(2.0)\times10^{-6}]$ Ref. [27], respectively. These experimental results do not assume a pure sp configuration for the $2\,^3P_J$ states. Our results for these g_L' factors are $1-m_e/m_N+8.838\times10^{-6}$ and $1-m_e/m_N+14.578\times10^{-6}$, respectively. Our ^{4}He g_L' factor is substantially closer to the experimental result than the result of Lewis and Hughes $[1-m_e/m_N+10.6(4)\times10^{-6}$ for ^{4}He] [7]. Our latter results for the g_L' factors include a contribution $[0.179\times10^{-6}]$ from radiative and recoil corrections of order α^3, which have not been calculated previously.

Some of the terms of orders α^3 and $\alpha^2 m_e/m_N$ of the Zeeman Hamiltonian are of the form $\pi_1\times(\sigma_1\times\pi_1)$. The contribution of these terms to the $2\,^3P$ and $2\,^1P$ helium g factors have not been evaluated in the past [7,10]. They give rise to another g factor defined in Eq. (38): $g_y=1.08\times10^{-8}$ for ^{4}He and $g_\gamma=1.06\times10^{-8}$ for ^{3}He.

Finally, we have calculated the ^{4}He $2\,^1P_1$ g_L' factor $1-m_e/m_N=15.771\times10^{-6}$. We have not calculated the radiative and recoil corrections of order α^3 in this case since the calculations of the radiative corrections are quite involved and this g_L' factor is not of much interest. In fact, there is no mention of this g_L' factor in the published literature.

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APPENDIX A

In this appendix we outline the calculation of the radiative corrections of Eq. (1). We only need to calculate ΔE_R accurate to three significant digits. We can therefore assume a pure sp configuration for the $2\,^3P$ state ($|n\rangle$). Neglecting terms of order $\alpha^3 m_e/m_N$, we can replace the constituent position ($\mathbf{r}_i$) and momentum ($\mathbf{p}_i$) variables by the relative (to the nucleus in the c.m. frame) variables $\mathbf{q}_i=\mathbf{r}_i-\mathbf{r}_N$ and $\boldsymbol{\pi}_i$ (conjugate to $\mathbf{q}_i$) in Eq. (1). The mechanical-momentum operators in Eq. (1) are spin-independent operators acting only on the Lm_L subspace and therefore all of the states of the internal sum on states must have the same symmetry as the end states $|n\rangle$. This allows us to make use of exchange symmetry and replace $\boldsymbol{\pi}_2$ and $\mathbf{q}_2$ by $\boldsymbol{\pi}_1$ and $\mathbf{q}_1$ in Eq. (1). This gives us eight equivalent contributions: four self-energy and four transverse. The self-energy terms are twice as large as the (presumably more correct) results of Grotch and Kashuba [11]. Therefore, to bring the self-energy contributions in agreement with the result of Grotch and Kashuba [11] we must multiply Eq. (1) by $\frac{3}{4}$. Expanding the dot product, retaining only terms linear in the magnetic field, integrating over k, and using $\langle n|\mathbf{r}_1|n'\rangle(E_{n'}-E_n)=\langle n|[\mathbf{r}_1,H]|n'\rangle=i\boldsymbol{\pi}/m_e$, Eq. (1) becomes

$$\Delta E_R=\frac{16\alpha\mu_B iB}{3\pi m_e^2c^2}\sum_{n'}\ln\left[\frac{m_ec^2}{|E_{n'}-E_n|}\right]\times[\langle n|\pi_{1x}|n'\rangle\langle n'|\pi_{1y}|n\rangle-\text{c.c.}]\,. \tag{A1}$$

Using $\pi_x=(1/\sqrt{2})(\pi_--\pi_+)$, $\pi_y=(i/\sqrt{2})(\pi_-+\pi_+)$, and $\boldsymbol{\pi}=(i\sqrt{2}/q_1)\{C_1^{(1)}l_1\}^{(1)}-i\partial C_1^{(1)}/\partial q_1$ (subscript 1 indicates electron 1), we evaluate the matrix elements in Eq. (A1) to get [26]

$$\Delta E_R=\frac{16\alpha\mu_B B}{3\pi m_e^2c^2}\sum{}'\left[\ln\left[\frac{m_ec^2}{|E_{n'}-E_n|}\right][\langle L'1m_{L'}-1|Lm_L\rangle-\langle L'1m_{L'}1|Lm_L\rangle][\langle L1m_L-1|L'm_{L'}\rangle+\langle L1m_L1|L'm_{L'}\rangle]\right.$$
$$\times\{\delta_{l_2l_2'}\delta_{l_bl_b'}(-1)^{L+L'+l_2+l_b'}(-1)^{l_a+l_1'}[(2L'+1)(2L+1)(2l_1+1)(2l_a'+1)]^{1/2}W(LL'l_1l_1';1l_2)$$
$$\left.\times W(L'Ll_a'l_a;1l_b')\}\left[\delta_{l_1l_1'}[(2l_1'+1)l_1(l_1+1)3]^{1/2}W(l_1l_1'11;1l_1')\langle l_1100|l_1'0\rangle\right.\right.$$

$$\times\left\langle l_1 l_2\left|\frac{\sqrt{2}}{q_1}\right|l_1' l_2'\right\rangle+\langle l_1 100|l_1' 0\rangle\left\langle l_1 l_2\left|\frac{\partial}{\partial q_1}\right|l_1' l_2'\right\rangle\Bigg]$$

$$\times\left[\delta_{l_a l_a'}[(2l_a+1)l_a(l_a+1)3]^{1/2}W(l_a' l_a 11;1 l_a)\langle l_a' 100|l_a 0\rangle\left\langle l_a' l_b'\left|\frac{\sqrt{2}}{q_1}\right|l_a l_b\right\rangle\right.$$

$$\left.+\langle l_a' 100|l_a 0\rangle\left\langle l_a' l_b'\left|\frac{\partial}{\partial q_1}\right|l_a l_b\right\rangle\right]\Bigg], \tag{A2}$$

where the sum extends over all primed variables. The subscripts 1 and 2 (a and b) are used for the orbitals of the first (second) matrix elements of Eq. (A1). Symbols such as $\langle l_1 l_2|(\sqrt{2}/q_1)|l_1' l_2'\rangle$ represent the radial integrals for the specified orbitals. We choose $L=1$, $l_1=l_a=0$, and $l_2=l_b=1$ for the pure sp configuration $2\,^3P$ state. The only configurations of the internal states which will connect with the pure $sp\ 2\,^3P$ state via a vector operator in the l_1 subspace are ss, pp, and sd:

$$\Delta E_R=\frac{16\alpha\mu_B B}{3\pi m_e^2 c^2}\sum{}'\left\{N_{sp}^2\ln\left[\frac{m_e c^2}{|E_{n'}-E_n|}\right](\langle L'1m_{L'}-1|1m_L\rangle-\langle L'1m_{L'}1|1m_L\rangle)\right.$$

$$\times(\langle 11m_L-1|L'm_{L'}\rangle+\langle 11m_L 1|L'm_{L'}\rangle)$$

$$\times\left[[3(2L'+1)]^{1/2}[W(1L'01;11)]^2(-1)^{L'+1}N_{pp}'^2\right.$$

$$\times\left[\left\langle s_1 p_2\left|\frac{\partial}{\partial q_1}\right|p_1' p_2'\right\rangle-\left\langle s_1 p_2\left|\frac{\partial}{\partial q_1}\right|p_2' p_1'\right\rangle\right]$$

$$\times\left[\left\langle p_1' p_2'\left|\frac{\partial}{\partial q_1}\right|s_1 p_2\right\rangle-\left\langle p_2' p_1'\left|\frac{\partial}{\partial q_1}\right|s_1 p_2\right\rangle\right]$$

$$-\frac{1}{\sqrt{3}}N_{ss}'^2\left[\left\langle p_1 s_2\left|\frac{\partial}{\partial q_1}\right|s_1' s_2'\right\rangle-\left\langle p_1 s_2\left|\frac{\partial}{\partial q_1}\right|s_2' s_1'\right\rangle\right]\left[\left\langle s_1' s_2'\left|\frac{\partial}{\partial q_1}\right|p_1 s_2\right\rangle-\left\langle s_2' s_1'\left|\frac{\partial}{\partial q_1}\right|p_1 s_2\right\rangle\right]$$

$$\left.\left.-\frac{2}{\sqrt{15}}N_{sd}'^2\left\langle p_1 s_2\left|\frac{\partial}{\partial q_1}\right|d_1' s_2'\right\rangle\left\langle d_1' s_2'\left|\frac{\partial}{\partial q_1}\right|p_1 s_2\right\rangle\right]\right\}, \tag{A3}$$

where we have used triplet wave functions of the form $\psi=N_{l_1 l_1}[f(q_1 q_2))l_1 l_2-f(q_2 q_1)l_2 l_1]$, $N_{l_1 l_2}$ is a normalization constant, and $f(q_1 q_2)$ is a radial function for the configuration $l_1 l_2$. The contributions from the matrix elements of the $\{C_1^{(1)} l_1\}^{(1)}$ tensor operator vanish. Choosing $m_L=1$ the g_{LR} factor is defined as $g_{LR}=\Delta E_R/\mu_B B$. Summing over L' and $m_{L'}$ the contributions from the pp orbitals vanish and we have

$$g_{LR}=\frac{16\alpha}{9\pi m_e^2 c^2}\sum{}'\left\{N_{sp}^2\ln\left[\frac{m_e c^2}{|E_{n'}-E_n|}\right]\left[N_{ss}'^2\left[\left\langle p_1 s_2\left|\frac{\partial}{\partial q_1}\right|s_1' s_2'\right\rangle-\left\langle p_1 s_2\left|\frac{\partial}{\partial q_1}\right|s_2' s_1'\right\rangle\right]\right.\right.$$

$$\times\left[\left\langle s_1' s_2'\left|\frac{\partial}{\partial q_1}\right|p_1 s_2\right\rangle-\left\langle s_2' s_1'\left|\frac{\partial}{\partial q_1}\right|p_1 s_2\right\rangle\right]$$

$$\left.\left.-N_{sd}'^2\left\langle p_1 s_2\left|\frac{\partial}{\partial q_1}\right|d_1' s_2'\right\rangle\left\langle d_1' s_2'\left|\frac{\partial}{\partial q_1}\right|p_1 s_2\right\rangle\right]\right\}. \tag{A4}$$

The sum in Eq. (A4) is split further into the following contributions.

(i) Terms in which both electrons are bound and are of the form $1sns$. There are no triplet states of the form $(nlnl-nlnl)$. For $n=2$–6 we use variational wave functions with 30 terms for the $1sns$ states and the 50 term best pure sp wave functions for $1s2p$ to get a contribution of $0.013\,37\times10^{-6}$ to g_{LR}. It becomes very difficult to create variational wave functions for $n=7$–50. Thus, for $n=7$–50 we use $1sns$ wave functions which are simply the product of $1S(Z=2)$ and $nS(Z=1)$ hydrogen states, where the inner electron "sees" the full nuclear charge ($Z=2$) and the outer electron sees a screened nuclear charge ($Z=1$). Here and in all the following contribu-

tions we use the simple hydrogenic *sp* variational wave function for $2\,^3P$ state. Additionally, we include here the contributions from states of the form $nsms(n,m\geq 1)$. These contributions converge well before $n=50$ to give $0.000\,02\times10^{-6}$ to g_{LR}.

(ii) For the other doubly discrete states (*nsmd*) we use the aforementioned screened hydrogen product approximation, which is a very good approximation since even for the $1s3d$ (3^3D) state the screened hydrogen product approximation gives an energy eigenvalue correct to five figures. Again, these contributions converge quickly and provide a contribution of $-0.000\,35\times10^{-6}$ to the g_{LR} factor.

(iii) There are also contributions for which one electron is bound and one is in the continuum. Here, the screened product hydrogen approximation should be excellent. In agreement with similar calculations of the average excitation energy and the helium Lamb shift [28], these contributions are the dominant ones. They provide $0.166\,35\times10^{-6}$ to the g_{LR} factor.

(iv) Finally, there are contributions from states in which both electrons are in the continuum. Again we have no choice but to use the product hydrogen approximation which is expected to be excellent in this case. Here, however, both electrons see the full nuclear charge ($Z=2$). They provide a contribution of $-0.000\,52\times10^{-6}$ to the g_{LR} factor.

This method of explicitly splitting the internal sum into the above contributions was previously used for Kabir and Salpeter [28] to evaluate the average excitation energy used in the helium Lamb shift. Their results agreed to four ppt with more accurate results employing a different method [29]. They, however, neglected contributions from doubly continuous states. We expect the same level of accuracy from our calculation. It has recently been brought to our attention that the doubly discrete excited states (*nsms* and *nsmd*; $n\geq1$, $m\geq1$) are not actually eigenstates of the nonrelativistic Schrödinger equation for the helium atom. These states are autoionizing and only a few have experimentally observable decay spectra [39]. The actual eigenstates of the system are linear combinations of these states with the states in which one electron is bound and one is in the continuum. The linear coefficients of these combinations are time dependent and give a nonvanishing amplitude for the doubly discrete state only if the state is prepared as such and only for a very brief period of time. At any rate, the total contribution from these doubly excited discrete states is $0.000\,008\times10^{-6}$, which is quite negligible. The dominant error in the calculation of these radiative corrections will come from the $1sns$ ($n\geq7$) doubly discrete contributions. We thus estimate our calculation of g_{LR} to have a maximum error of one half of the $1sns$ doubly discrete contribution ($\pm0.007\times10^{-6}$) and get $g_{LR}=0.0179(7)\times10^{-6}$. Had we used Eq. (1) as is, not multiplying by $\frac{3}{4}$, we wold have $g_{LR}=0.0239(9)\times10^{-6}$.

APPENDIX B

In this appendix we derive the interaction-dependent part of the Lorentz boost operator for a heliumlike atom. Our starting point in Eq. (33) of Ref. [12]:

$$[W_i^{(1)},h^{(0)}]=\frac{-i}{Mc^2}U^{(0)}P_i-M[R_i,U^{(1)}]-\frac{1}{2c^2}\sum_{\mu=1}^{3}\left\{\left[\rho_{\mu,i}\left[\frac{\pi_\mu^2}{2m_\mu}+\frac{\pi_\mu\cdot P}{M}\right]+\left[\frac{\pi_\mu^2}{2m_\mu}+\frac{\pi_\mu\cdot P}{M}\right]\rho_{\mu,i}-\left[\frac{\sigma_\mu\times\pi_\mu}{m_\mu}\right]_i\right],U^{(0)}\right\}, \tag{B1}$$

where $h^{(0)}=H_f$ is the Hamiltonian of Eq. (33) and $U^{(0)}$ is the potential-energy operator of that Hamiltonian. Making use of the commutation relations [12]

$$[R_i,(\rho_\mu,\pi_\mu,\sigma_\mu)]=[P_i,(\rho_\mu,\pi_\mu,\sigma_\mu)]=[R_i,R_j]=[P_i,P_j]=0\ ,\quad [\rho_\mu^i,\rho_\nu^j]=[\pi_\mu^i,\pi_\nu^j]=0\ ,$$
$$[\rho_\mu^i,\pi_\nu^j]=i\left[\delta_{\mu\nu}-\frac{m_\nu}{M}\right]\delta_{ij}\ ,\quad [\sigma_\mu^i,\sigma_\nu^i]=i\delta_{\mu\nu}\epsilon_{ijk}\sigma_\mu^k\ , \tag{B2}$$

we obtain the right-hand side of Eq. (B1):

$$[W_i^{(1)},h^{(0)}]=\frac{Ze^2i}{4c^2}\sum_{\substack{\mu,\nu=1\\(\mu\neq\nu)}}^{2}\left\{\frac{\pi_\mu\cdot\mathbf{q}_\mu}{q_\mu^3}\left[\left[\frac{(M-m_e)(m_e-m_N)+m_N^2}{Mm_em_N}\right]q_\mu^i+\frac{(m_e-m_N)}{Mm_N}q_\nu^i\right]\right.$$
$$\left.+\frac{\pi_\nu\cdot\mathbf{q}_\mu}{q_\mu^3}\left[\left[\frac{(M-m_e)}{Mm_N}\right]q_\mu^i-\frac{m_e}{Mm_N}q_\nu^i\right]+\frac{1}{q_\mu}\left[\pi_\mu^i\left[\frac{(m_e-m_N)}{m_Nm_e}\right]+\frac{\pi_\nu^i}{m_N}\right]\right\}$$
$$+\frac{e^2i}{4c^2}\sum_{\substack{\mu,\nu=1\\(\mu\neq\nu)}}^{2}\left\{\frac{\pi_\mu\cdot(\mathbf{q}_\mu-\mathbf{q}_\nu)}{q_{\mu\nu}^3}\left[\left[\frac{M-m_e+m_N}{Mm_e}\right]q_\mu^i+\frac{(m_e-M)}{Mm_e}q_\nu^i\right]+\frac{\pi_\mu^i}{m_eq_{\mu\nu}}\right\}, \tag{B3}$$

where $\mathbf{q}_\mu\equiv\boldsymbol{\rho}_\mu-\boldsymbol{\rho}_N$. If we assume that $\mathbf{W}^{(1)}$ is only a function of $\mathbf{q}_1$ and $\mathbf{q}_2$ (and not $\boldsymbol{\pi}_1$ and $\boldsymbol{\pi}_2$), we obtain the left-hand side of Eq. (B1):

$$[W_i^{(1)},h^{(0)}]=\sum_{\substack{\mu,\nu=1\\(\mu\neq\nu)}}^{2}\frac{i}{2}(\nabla_{q_\mu}W_i^{(1)})\cdot\left[\frac{(m_N+m_e)}{m_e m_N}\pi_\mu+\frac{\pi_\nu}{m_N}\right]. \tag{B4}$$

Equating the coefficients of π_1 and π_2 in Eqs. (B3) and (B4) we have two coupled sets of vector differential equations for each of the components of $\mathbf{W}^{(1)}$:

$$\frac{1}{\mu}\frac{\partial W_i^{(1)}}{\partial q_{ij}}+\frac{1}{m_N}\frac{\partial W_i^{(1)}}{\partial q_{2j}}=C_d(q_1q_2)_i^j\ ,\quad \frac{1}{m_N}\frac{\partial W_i^{(1)}}{\partial q_{1j}}+\frac{1}{\mu}\frac{\partial W_i^{(1)}}{\partial q_{2j}}=C_e(q_1q_2)_i^j\ , \tag{B5}$$

with

$$\begin{aligned}C_d(q_1q_2)_i^j\equiv\frac{Ze^2}{2c^2}&\left\{\frac{q_1^j}{q_1^3}\left[\left[\frac{(M-m_e)(m_e-m_N)+m_N^2}{Mm_em_N}\right]q_1^i+\frac{(m_e-m_N)}{Mm_N}q_2^i\right]+\frac{q_2^j}{q_2^3}\left[\left[\frac{(M-m_e)}{Mm_N}\right]q_2^i-\frac{m_e}{Mm_N}q_1^i\right]\right.\\&\left.+\frac{1}{q_1}\left[\frac{(m_e-m_N)}{m_Nm_e}\right]\delta_{i,j}+\frac{\delta_i^j}{m_Nq_2}\right\}\\&+\frac{e^2}{2c^2}\left\{\frac{(q_1^j-q_2^j)}{q_{12}^3}\left[\left[\frac{M-m_e+m_N}{Mm_e}\right]q_1^i+\frac{(m_e-M)}{Mm_e}q_2^i\right]+\frac{\delta_i^j}{m_eq_{12}}\right\},\end{aligned} \tag{B6}$$

and $C_e(q_1q_2)_i^j$ is obtained from $C_d(q_1q_2)_i^j$ by interchanging the labels 1 and 2. Solving the algebraic Eqs. (B5) we obtain the 18 differential equations for the three components of $\mathbf{W}^{(1)}$:

$$\begin{aligned}\frac{\partial W_i^{(1)}}{\partial q_{1j}}&=\frac{(m_e+m_N)m_e}{M}C_d(q_1q_2)_i^j-\frac{m_e^2}{M}C_e(q_1q_2)_i^j\ ,\\\frac{\partial W_i^{(1)}}{\partial q_{2j}}&=\frac{(m_e+m_N)m_e}{M}C_e(q_1q_2)_i^j-\frac{m_e^2}{M}C_d(q_1q_2)_i^j\ .\end{aligned} \tag{B7}$$

Equations (B7) can be integrated directly to obtain Eq. (5). If we assume the $\mathbf{W}^{(1)}$ is a function of π_1 and π_2 instead of $\mathbf{q}_1$ and $\mathbf{q}_2$, the resulting solution contradicts the original assumption and $\mathbf{W}^{(1)}$ turns out to be a function of $\mathbf{q}_1$, $\mathbf{q}_2$, π_1, and π_2. If we assume that $\mathbf{W}^{(1)}$ is a function of all four variables we cannot solve the resulting equations.

The complete interaction-dependent part of the Lorentz boost operator is $\mathbf{V}^{(1)}=\mathbf{R}U^{(0)}/c^2+\mathbf{W}^{(1)}$. This operator must be separable in the following sense [13]: When the system is divided into any number of subsystems that are infinitely far removed from each other a Lorentz boost of any subsystem is independent of the dynamics of any of the other subsystems. With $\mathbf{R}=\sum_i m_i\mathbf{r}_i$, $\mathbf{q}_i=\mathbf{r}_i-\mathbf{r}_N$, and the potential-energy operator of Eq. (25), we see that with $\mathbf{W}^{(1)}$ of Eq. (2) $\mathbf{V}^{(1)}$ is indeed separable.

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