Recoil corrections to the Lamb shift in helium

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Abstract.
Nuclear recoil corrections to the energies of helium S levels of order $m^2/M\,\alpha^5$ are presented. They are shown to contribute only a small amount to the ionization energies of the 2^1S and 2^3S states, but to contribute significantly on the scale of accuracy of modern ^{4}He-^{3}He isotope shift experiments.

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Recoil corrections, the effect of the nucleus having a finite mass M on atomic energy levels, can be accounted for at the nonrelativistic level by replacing the electron mass m with the reduced mass $\mu = mM/(m+M)$ and including the mass-polarization (MP) Hamiltonian

$$H_{MP} = \sum_{i<j} \frac{\vec{p}_i \cdot \vec{p}_j}{M}. \tag{1}$$

The situation is more complicated for higher order relativistic and quantum electrodynamic recoil corrections. While these have been studied in considerable detail for hydrogenic atoms, in other systems, such as the helium atom, only the leading recoil effects, namely up to order $m\,\alpha^4$ have been calculated in a complete way. The corresponding operators can be derived from a nonrelativistic expansion of the Breit interaction [1]. The purpose of this paper is the presentation of a complete calculation of recoil effects at order $m^2/M\,\alpha^5$ for helium S levels

For the ground state of hydrogenic (H) atoms, the Lamb shift including recoil corrections can be written as

$$E^H = \frac{\mu}{m} E_L^H + E_{R1}^H + E_{R2}^H, \tag{2}$$

where

$$E_L^H = m \frac{4Z^4\alpha^5}{3\pi} \left[\ln(Z\alpha)^{-2} - \ln k_0(1s) + \frac{19}{30} \right], \tag{3}$$

$$E_{R1}^H = -2\frac{m}{M} E_L^H + \frac{m^2}{M} \frac{4Z^4\alpha^5}{3\pi}, \tag{4}$$

and

$$E^H_{R2} = \frac{m^2}{M}\,\frac{Z^5\alpha^5}{\pi}\,\frac{2}{3}\Big[-\ln(Z\alpha) - 4\,\ln k_0(1s) + \frac{31}{3} + 7\,\ln 2\Big]. \qquad (5)$$

The ground state Bethe logarithm, $\ln k_0(1s)$, is 2.984 128 555 766. We have divided the recoil corrections E^H_R into two parts and adopted the convention, useful for later comparison with helium, of associating a single power of the reduced mass, $\mu/m \approx 1 - m/M$ with the Lamb shift E^H_L. The first term of E^H_{R1} accounts for the fact that the s-state Lamb shift involves only operators that scale as $(\mu/m)^3 \approx 1 - 3m/M$, which leads to an overall factor of $-2m/M$ because of the convention just mentioned, and the second term accounts for the presence of a factor of μ/m in the argument of the logarithmic term. E_{R2} is a dynamical effect we will refer to as the Salpeter correction [2].

For the case of helium the theory was described in [3], where these recoil corrections were derived in an effective Hamiltonian approach. We begin by presenting the formula for the Lamb shift of S states in two electron atoms without recoil:

$$\begin{aligned} E_L = {} & \left[\frac{164}{15} + \frac{14}{3}\,\ln\alpha\right]\frac{\alpha^2}{m^2}\,\langle\delta^3(r_{12})\rangle - \frac{14}{3}\,m\,\alpha^5\left\langle\frac{1}{4\,\pi}\,P\left(\frac{1}{(m\,\alpha\,r_{12})^3}\right)\right\rangle \\ & + \left[\frac{19}{30} + \ln(\alpha^{-2}) - \ln k_0\right]\frac{4\,\alpha^2\,Z}{3\,m^2}\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle. \end{aligned} \qquad (6)$$

Here Z is the atomic number, P is a distribution defined as the limit

$$\begin{aligned} \langle\phi|P\left(\frac{1}{r^3}\right)|\psi\rangle = {} & \lim_{a\to 0}\int \mathrm{d}^3r\,\phi^*(\boldsymbol{r})\,\psi(\boldsymbol{r}) \\ & \left[\frac{1}{r^3}\,\Theta(r-a) + 4\,\pi\,\delta^3(r)\,(\gamma + \ln a)\right], \end{aligned} \qquad (7)$$

and the two-electron Bethe logarithm, $\ln k_0$, is defined by

$$\ln k_0 = \frac{1}{D}\Big\langle(\boldsymbol{p}_1 + \boldsymbol{p}_2)\,(H - E)\,\ln\Big[\frac{2\,(H-E)}{\alpha^2\,m}\Big]\,(\boldsymbol{p}_1 + \boldsymbol{p}_2)\Big\rangle, \qquad (8)$$

$$D = 2\,\pi\,\alpha\,Z\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle. \qquad (9)$$

The symbol $\langle\hat{Q}\rangle$ denotes the expectation value of the operator $\hat{Q}$ between eigenstates of the Schrödinger equation in the limit of *infinite* nucleus mass, with the Hamiltonian

$$H = \frac{p_1^2}{2\,m} + \frac{p_2^2}{2\,m} + \frac{\alpha}{r} - \frac{Z\,\alpha}{r_1} - \frac{Z\,\alpha}{r_2}. \qquad (10)$$

We note that while the first two terms in Eq. (6) are specific to the two-electron case, the third term can be obtained from the hydrogenic Lamb shift through the substitutions

$$\begin{aligned} & \frac{(mZ\alpha)^3}{n^3\pi} \to \langle\delta^3(r_1) + \delta^3(r_2)\rangle, \\ & \ln k_0(1s) \to \ln k_0 + \ln Z^2. \end{aligned} \qquad (11)$$

The values of the operators needed to evaluate the Lamb shift for $n = 1$ and $n = 2$ S levels of helium, along with other operators needed to evaluate recoil corrections, discussed below, are presented in Table 1. Values of Bethe logarithms are taken from recent papers of Korobov *et al.* [4] and Baker *et al.* [5].

We now consider recoil corrections. Following the convention used in hydrogen, we define the total energy in order $m\,\alpha^5$ to be

$$E^{(5)} = \frac{\mu}{m}\,E_L + E_R, \tag{12}$$

where now the recoil correction E_R of order m^2/M is a sum of three terms:

$$E_R = E_{R1} + E_{R2} + E_{R3}. \tag{13}$$

E_{R1} comes from the same scaling arguments as in the hydrogenic case, and is given by a similar formula,

$$E_{R1} = -2\frac{m}{M}E_L + \frac{4Z\alpha^2}{3mM}\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle. \tag{14}$$

E_{R2} describes the physics of the Salpeter correction. This requires a full QED treatment [3], and the result is

$$\begin{aligned} E_{R2} = {} & \frac{(Z\,\alpha)^2}{M\,m}\left(\frac{2}{3}\,\ln(\alpha^{-1}) + \frac{62}{9} - \frac{8}{3}\,\ln k_0\right)\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle \\ & - \frac{7}{6\,\pi}\,\frac{Z^2\,\alpha^5\,m^2}{M}\,\left\langle P\left(\frac{1}{(m\,\alpha\,r_1)^3}\right) + P\left(\frac{1}{(m\,\alpha\,r_2)^3}\right)\right\rangle. \end{aligned} \tag{15}$$

Finally, the term E_{R3} accounts for the effect of mass polarization term $\boldsymbol{p}_1 \cdot \boldsymbol{p}_2/M$ on the wave function ϕ, Hamiltonian H and energy E in Eqs. (6-9). Numerical results for the correction to expectation value of all operators involved in the Lamb shift formula (6) are presented in the rows labeled 'δ_{MP}' in Table 1, which give the coefficient of the factor m/M in atomic units. Many of these corrections have already been calculated [7], but the correction to the Bethe logarithm, which even in the non-recoil limit is quite difficult to accurately evaluate, has not until now been determined.

In order to carry out the numerical calculations of recoil corrections we used wave functions similar to those used by Frolov [6] and Korobov *et al* [4]. In this approach the helium wave function is expanded in a basis set of exponential functions of the form

$$\phi(r_1, r_2, r_{12}) = \sum_i v_i[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}} \pm (r_1 \leftrightarrow r_2)], \tag{16}$$

where α_i, β_i and γ_i are real and chosen in a uniform and random way with the conditions:

$$A_1 < \alpha_i < A_2, \;\; \beta_i + \gamma_i > 0, \tag{17}$$

$$B_1 < \beta_i < B_2, \;\; \alpha_i + \gamma_i > 0, \tag{18}$$

$$C_1 < \gamma_i < C_2, \;\; \alpha_i + \beta_i > 0. \tag{19}$$

The parameters A_i, B_i, C_i are determined by minimization of the energy of the state of interest. The second conditions are necessary for the normalizability of the wave function in (16). The coefficients v_i form a vector v which is a solution of the generalized eigenvalue problem

$$H v = E N v, \tag{20}$$

where H is a matrix of the Hamiltonian in this basic set, N is a normalization matrix, and E an eigenvalue, the energy of the state corresponding to v. The calculation of all matrix elements can be performed with the use of one formula:

$$\frac{1}{16\,\pi^2}\int d^3r_1\int d^3r_2\,\frac{e^{-\alpha r_1-\beta r_2-\gamma r_{12}}}{r_1\,r_2\,r_{12}}=\frac{1}{(\alpha+\beta)(\beta+\gamma)(\gamma+\alpha)}. \tag{21}$$

Standard numerical techniques allowed the solution of the generalized eigenvalue problem, though quadruple precision was required for matrix dimensions greater than about 100. In our calculations we used basis sets with sizes up to 600. Having now the wave function and energy the calculation of all matrix elements involved in E_R with the exception of the mass polarization correction $\delta_{MP}\ln k_0$, to be discussed below, is rather straightforward. Mass polarization corrections were calculated both by treating H_{MP} as a perturbation, also discussed below, and by including it when solving the eigenvalue problem. We checked our results for some of the well known operators against Drake's listing in [7], and found good agreement.

We have first calculated ϕ_1, defined as follows,

$$|\phi_1\rangle=\frac{1}{(E-H)'}\,\frac{\boldsymbol{p}_1\cdot\boldsymbol{p}_2}{m}\,|\phi\rangle \tag{22}$$

by expansion in the same basic set as ϕ: then the mass polarization correction to the expectation value of any operator Q is

$$\delta_{MP}Q=\frac{m}{M}\,2\,\langle\phi|Q|\phi_1\rangle. \tag{23}$$

Results are presented in Table 1. The calculation of $\delta_{MP}\ln k_0$, the correction of the Bethe logarithm due to mass polarization, is more involved, since it explicitly depends on H and E. We calculate $\delta_{MP}\ln k_0$ using the same kind of integral representation as used for $\ln k_0$ (in atomic units),

$$\delta_{MP}\,\ln k_0=\frac{m}{M}\,\frac{1}{D}\,\left[\int_0^\Lambda k\,dk\,J(k)+2\,\Lambda\,\langle\phi|\nabla^2|\phi_2\rangle+Z^2\int_\Lambda^\infty\frac{dk}{k}\,W(k)\right] \tag{24}$$

where

$$\begin{aligned}J(k)\;&=2\,\langle\phi|\,\boldsymbol{p}\,\frac{1}{H-E+k}\,\boldsymbol{p}\,|\phi_2\rangle\\&\quad+\langle\phi|\,\boldsymbol{p}\,\frac{1}{H-E+k}\,(\langle\boldsymbol{p}_1\boldsymbol{p}_2\rangle-\boldsymbol{p}_1\boldsymbol{p}_2)\,\frac{1}{H-E+k}\,\boldsymbol{p}\,|\phi\rangle,\end{aligned} \tag{25}$$

$$\begin{aligned}W(k)&=2\,\langle\phi|\left(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\right)\frac{1}{H-E+k}\left(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\right)|\phi_2\rangle+\langle\phi|\left(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\right)\\&\qquad\frac{1}{H-E+k}\,(\langle\boldsymbol{p}_1\boldsymbol{p}_2\rangle-\boldsymbol{p}_1\boldsymbol{p}_2)\,\frac{1}{H-E+k}\left(\frac{\boldsymbol{r}_1}{r_1^3}+\frac{\boldsymbol{r}_2}{r_2^3}\right)|\phi\rangle,\end{aligned} \tag{26}$$

$$|\phi_2\rangle\;=|\phi_1\rangle-|\phi\rangle\,\frac{\langle\phi|2\,\pi\,Z\,[\delta^3(r_1)+\delta^3(r_2)]|\phi_1\rangle}{D}, \tag{27}$$

where the second term in (27) is due to the mass polarization correction to D, the denominator in the expression (8) for the Bethe log. The inversion of the operator

operator	1^1S_0	2^1S_0	2^3S_1
$\delta^3(r_1)$	1.8104293	1.3094608	1.3203551
δ_{MP}	-0.0911866	-0.0004018	0.0021769
$\delta^3(r_{12})$	0.1063454	0.0086484	0
δ_{MP}	-0.0123208	0.0017677	0
$1/4\,\pi\,P(1/r_{12}^3)$	0.0787238	0.0054070	0.0030925
δ_{MP}	0.04899(2)	0.00416(1)	-0.00038
$1/4\,\pi\,P(1/r_1^3)$	$-2.4610051(1)$	$-1.8129995(1)$	$-1.8320751(1)$
$\ln k_0$	4.3701579(5)	4.3664091(5)	4.364036(1)
δ_{MP}	0.0941(2)	0.0175(2)	0.0048(2)

Table 1. Operators needed for evaluation of the helium Lamb shift: all except $\ln k_0$ in atomic units: the mass polarization correction δ_{MP} is to be multiplied by m/M, δ_{MP} in $\ln k_0$ includes correction to both numerator and denominator in (8)

$H - E + k$ is performed in a basis set of the form

$$\phi(r_1, r_2, r_{12}) = \sum_i v_i[\boldsymbol{r}_1\, e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}} \pm (r_1 \leftrightarrow r_2)] \tag{28}$$

using standard Lapack routines. To find the optimized values of parameters A_i, B_i and C_i necessary for generation of ϕ, we repeated the calculation of Bethe logarithm in the way described in [4]. The cutoff Λ is chosen to be 50 in atomic units, as it was in earlier calculations [8]. The integral in k of $W(k)$ is performed up to $k = 100$. For larger k we extrapolate the fitted asymptotic behavior of function W with the form

$$W(k) \approx \frac{\ln(2k)}{k}\, 4\,\pi\,\langle\phi|\delta^3(r_1)\,\frac{\partial}{\partial r_1} + \delta^3(r_2)\,\frac{\partial}{\partial r_2}|\phi_2\rangle + \frac{A}{k} + \frac{B}{k^{3/2}} + \frac{C}{k^2} \tag{29}$$

For values of k greater than 100 our integrand was inaccurate due to inexact numerical cancellation of $1/\sqrt{k}$ term. This is the source of uncertainties in Table 1 for the correction to $\ln k_0$. However, the overall size of this correction is relatively small compared to reduced mass effects and E_{R2}, so this uncertainty is not important.

We now turn to a discussion of the impact of the recoil corrections calculated here on comparison of experiment and theory. We begin with the 2^1S_0 ionization energy, which has been found to be 960 332 041.01(15) MHz [9], [10]. The non-QED ionization energy has been accurately determined [7],[11] to be 960 334 847.71 MHz, so the inferred QED is 2806.70 MHz. We show the breakdown of the QED contributions at order $m\alpha^5$ in Table 2. Because this is an ionization energy measurement, the Lamb shift of the He^+ ion, given by Eq. (2) must be subtracted. We see that a difference of 51.5 MHz results. This is largely accounted for by a part of the as yet incompletely calculated $m\alpha^6$ terms, specifically the first binding correction to the Lamb shift, which contributes

$$E_L^{(6)} = \frac{\alpha(Z\alpha)^2}{m^2}\, A_{50}\,\langle\delta^3(r_1) + \delta^3(r_2)\rangle - \frac{m\alpha(Z\alpha)^5}{\pi}\, A_{50} \tag{30}$$

State	2^1S_0	2^3S_1
Inferred QED	2806.70	4057.27
$\frac{\mu}{m}E_L$	108 710.59	109 954.03
E_{R1}	-27.36	-27.68
E_{R2}	18.31	18.54
E_{R3}	-0.06	0.01
$-\frac{\mu}{m}E_L^H$	-105 955.14	-105 955.14
$-E_{R1}^H$	26.67	26.67
$-E_{R2}^H$	-17.79	-17.79
Theoretical QED	2755.21	3998.65

Table 2. QED corrections to the ionization energies of 2^1S_0 and 2^3S_1 in ^{4}He: units MHz

to the ionization energy, where

$$A_{50} = 4\,\pi\left[\frac{139}{128} + \frac{5}{192} - \frac{\ln 2}{2}\right]. \tag{31}$$

While the 52.0 MHz coming from this term brings theory and experiment quite close to one another, a complete calculation of terms of order $m\alpha^6$, the theory of which is discussed in Ref. [12], is still necessary. We note that a number of higher order binding corrections and the two-loop Lamb shift contributing in order $m\alpha^7$ were included in Ref. [13]: here, because the theory at order $m\alpha^6$ is still incomplete, we have chosen not to include them.

We note that the individual sizes of the various recoil terms are fairly large, though, as mentioned above, the effect of mass polarization on the Bethe logarithm, although quite difficult to calculate, is relatively small. However, there is a high degree of cancellation between the recoil terms of helium and He$^+$, so the net effect on the ionization energy is only -234 kHz, on the order of the experimental uncertainty, and much smaller than the uncalculated terms discussed above.

The ionization energy of the 2^3S_1 state is also known from combining the experimental determination of the 2^3S_1-3^3D_1 transition energy [14] with the theoretical 3^3D_1 energy [13]. Subtracting the non-QED result [7], [11] of 1 152 846 800.14 MHz from the experimental value 1 152 842 742.87(6) MHz gives an inferred QED of 4057.27 MHz. The theory presented here accounts for 3998.65 MHz of this effect, and again the first binding correction to the Lamb shift, which in this case contributes 67.6 MHz, account for the bulk of the difference, though now a larger 9 MHz discrepancy remains to be explained by the remaining terms of order $m\alpha^6$, the theory of which is discussed in Ref. [15]. As with the singlet, we do not include any terms of order $m\alpha^7$. The strong cancellation of the recoil terms noted for the singlet state is present for the triplet also, leading to a recoil correction of only -251 kHz, which while larger than the experimental uncertainty is much less important than the uncalculated $m\alpha^6$ terms.

coefficient of	1^1S_0	2^1S_0	2^3S_1
$\mu\,\alpha^5$	15.8424	1.0778	1.5642
$m^2/M\,\alpha^5$	$-13.169(2)$	$-0.668(2)$	$-0.717(2)$
^{4}He-^{3}He [kHz]	3327.1(2)	200.2(2)	261.6(2)

Table 3. Summary of results for $m\alpha^5$ contributions to ^{3}He-^{4}He isotope shift of ionization energies. Numbers in the second and third rows are coefficients to be multiplied by the corresponding term in the first column. Numbers in the fourth row are values in kHz.

We now turn to a discussion of the isotope shift. In the above discussion we used $M/m = 7\ 294.299\ 508(16)$ for the ratio of the alpha mass to the electron mass: for the nucleus of ^{3}He one should instead use $M/m = 5\,495.885\ 238(12)$, which leads to an isotope shift that is significantly affected by the corrections calculated here, as presented in Table 3. The magnitude of these recoil effects is much larger than the precision of the isotope measurement performed by Shiner *et al.* [16]

$$E_{\rm iso}(2^3P_0\text{-}2^3S_1) = 33\,668\,074(5)\,\text{kHz} \tag{32}$$

and is of similar magnitude as the precision of measurement by Eikema *et al* [17]

$$E_{\rm iso}(2^1P_0\text{-}1^1S_0) = 263\,410(7)\,\text{MHz}. \tag{33}$$

This means that reliable theoretical predictions for isotope shifts have to include a complete treatment of recoil effects, as presented in this work. However, to compare with experiment the analogous calculation for P states is needed. As this has not yet been performed, we do not present final theoretical predictions for the isotope shift. We note also that higher order terms of order $m^2/M\,\alpha^6$ should also be included. Since they contribute only at the few kHz level, one can use an approximate treatment as done by Drake in [18].

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References

[1] A.P. Stone, Proc. Roy. Soc. (London) **77**, 786 (1961); **81**, 868 (1963).
[2] E.E. Salpeter, Phys. Rev. **87**, 328 (1952).
[3] K. Pachucki, J. Phys. B **31**, 5123 (1998).
[4] V.I. Korobov and S.V. Korobov, Phys. Rev. A **59**, 3394 (1999).
[5] J.D. Baker, R.C. Forrey, M. Jeziorska, and J.D. Morgan III, to be published.
[6] A.M. Frolov, Phys. Rev. A **57**, 2436 (1998).
[7] G.W.F. Drake, Nuclear Instruments and Methods in Physics Research B**31**, 7 (1988), G.W.F. Drake and Z.C. Yan, Phys. Rev. A **46**, 2378 (1992).

[8] C. Schwartz, Phys. Rev. **123**, 1700 (1961).
[9] C.J. Sansonetti and J.D. Gillaspy, Phys. Rev. A **45**, R1 (1992). Discussion of a slight revision of this result is given in Reference [13].
[10] W. Lichten, D. Shiner, and Zhi-Xiang Zhou, Phys. Rev. A **43**, 1663 (1991).
[11] J. Baker, Masters Thesis, University of Delaware, 1988 (unpublished).
[12] K. Pachucki, J. Phys. B **31**, 3547 (1998).
[13] G.W.F. Drake and W.C. Martin, Can. J. Phys. **76**, 679 (1998).
[14] C. Dorrer, F. Nez, B. de Beauvoir, L. Julien, and F. Biraben, Phys. Rev. Lett. **78**, 3658 (1997).
[15] K. Pachucki, J. Phys. B **31**, 2489 (1998).
[16] D. Shiner, R. Dixson, and V. Vedantham, Phys. Rev. Lett. **74**, 3553 (1995).
[17] K.S. Eikema, W. Ubachs, W. Vassen, and W. Hogervost, Phys. Rev. Lett. **76**, 1216 (1996).
[18] G.W.F. Drake, in *Long Range Casimir Forces: Theory and Recent Experiments on Atomic Systems*, ed. F.S. Levin and D.A. Micha, Plenum, New York, 1993 p.107.