Numerical results for Lamb Shift

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1 Introduction

Lamb shift [1], the energy splitting between the $2S_{1/2}$ and $2P_{1/2}$ states, is one of the most important experiments in history. As is known, the fine structure, witch is of $\mathcal{O}(\alpha^4)$, does not split states of the same j with different l:

$$\Delta E_{\text{fine structure}} = \frac{(Z\alpha)^2}{n}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right)E_n. \tag{1}$$

For $n = 2$ and $Z = 1$, the fine structure splitting of the $2P_{1/2}$ (or $2S_{1/2}$) and $2P_{3/2}$ states:

$$\Delta E(2P_{3/2}) - \Delta E(2P_{1/2}) \approx 4.5 \times 10^{-5}\ \text{eV} = 10948.8\ \text{MHz}. \tag{2}$$

But in Lamb's experiments, the energy of $2S_{1/2}$ and $2P_{1/2}$ is not exactly the same. In this note, I will give a numeric result of the Lamb shift based on the results of [2].

2 Details of numeric calculations of Lamb shift

2.1 Contribution from the Bethe's log in $\Delta E(2S_{1/2})$

The main contribution of Lamb shift comes form the Bethe's log[1]:

$$\Delta E_1 = \frac{2\alpha^3}{3\pi}\sum_{m\neq n}\left|\langle n|\boldsymbol{v}|m\rangle\right|^2(E_m - E_n)\ln\frac{E_r}{|E_m - E_n|}. \tag{3}$$

It is easy to check:

$$\Delta E_1 = \frac{2\alpha^3}{3\pi}\sum_{m\neq n}\left|\langle n|\boldsymbol{x}|m\rangle\right|^2(E_m - E_n)^3\ln\frac{E_r}{|E_m - E_n|}. \tag{4}$$

Here, we have used the elementary commutation relation:

$$[\boldsymbol{x},\boldsymbol{v}] = i, \qquad \left[\boldsymbol{x},\hat{h}_0\right] = i\boldsymbol{v}.$$

$$\hat{h}_0 = \frac{\boldsymbol{v}^2}{2} - \frac{Z}{r},$$

and the E_r above represents the energy of electron at rest:

$$E_r = m_e c^2 = \frac{1}{\alpha^2}\ \text{a.u.},$$

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[1]In this note, I adopt the atom unite (a.u.) for convenience, details of a.u. are listed in Appendix.

and the energy level for the bound states:

$$E_n = -\frac{1}{2}\frac{Z^2}{n^2} \text{ a.u..}$$

It is easy to check $E_n \sim \alpha^2 E_r$ and we expect the Lamb shift $\Delta E(2S_{1/2}) - \Delta E(2P_{1/2}) \sim \alpha^5 E_r$ in our results. For the discrete states:

$$\psi_{nlm}(r,\theta,\phi) = Y_{lm}(\theta,\phi)R_{nl}(r).$$

where:

$$R_{nl}(r) = \frac{1}{(2n+1)!}\sqrt{\frac{(n+l)!}{(n-l-1)!2n}}\left(\frac{2Z}{n}\right)^{\frac{3}{2}} e^{-\frac{Zr}{n}}\left(\frac{2Zr}{n}\right)^{l} F\left(-(n-l-1), 2l+2, \frac{2Zr}{n}\right), \tag{5}$$

and

$$\int_0^{+\infty} drr^2 R_{ml}(r)R_{nl}(r) = \delta_{mn}.$$

When we take $n = 2$ in (3), the transition matrix elements:

$$\int_0^{+\infty} drr^3 R_{20}(r)R_{m1}(r) = \frac{256\sqrt{2}}{Z}\left(\frac{m-2}{m+2}\right)^m \frac{\sqrt{m^7(m^2-1)}}{(m^2-4)^3}.$$

After integration over the azimuthal angle, θ and ϕ, we have

$$|\langle n|\boldsymbol{x}|m\rangle|^2 = \frac{131072}{Z^2}\left(\frac{m-2}{m+2}\right)^{2m}\frac{m^7(m^2-1)}{(m^2-4)^6}.$$

when $m \gg 2$,

$$|\langle n|\boldsymbol{x}|m\rangle|^2 \sim \frac{1}{m^3 Z^2}.$$

We then get the energy shift from the discrete states:

$$\Delta E_1^{dis} = 44.07 \text{ MHz}. \tag{6}$$

For the continuous states, I adopt the "k-scale" normalization:

$$\int_0^{+\infty} drr^2 R_{kl}(r)R_{k'l}(r) = \delta(k-k').$$

The k above is related to the energy of the continuous states:

$$E(k) = \frac{k^2}{2} \text{ a.u..}$$

The transition matrix element:

$$|\langle n|\boldsymbol{x}|k\rangle|^2 = \frac{131072}{Z^3}\frac{e^{-4m'\cot^{-1}\left(\frac{1}{2}m'\right)}}{(1-e^{-2\pi m'})}\frac{m'^9(m'^2+1)}{(m'^2+4)^6}.$$

where

$$m' = \frac{Z}{k}.$$

when $k \gg 1$:

$$|\langle n|\boldsymbol{x}|k\rangle|^2 \sim \frac{Z^5}{k^8}.$$

We then get the energy shift from the continuous states:

$$\Delta E_1^{con} = 1003.35 \text{ MHz}. \tag{7}$$

The the total energy shift from the Bethe's log is

$$\Delta E_1 = \Delta E_1^{dis} + \Delta E_1^{con} = 1047.42 \text{ MHz}. \tag{8}$$

2.2 Contribution from the vacuum polarization and Darwin terms in $\Delta E(2S_{1/2})$

With a.u., the contribution from the vacuum polarization and Darwin terms can be expressed as:

$$\Delta E_2 = -\frac{4Z\alpha^3}{15}\left|\phi_n(\mathbf{0})\right|^2 = -\frac{4Z^4\alpha^3}{15\pi n^3},$$

and

$$\Delta E_3 = \frac{4Z\alpha^3}{3}\left(\frac{5}{6} - \ln 2\right)\left|\phi_n(\mathbf{0})\right|^2 = \frac{4Z^4\alpha^3}{3\pi n^3}\left(\frac{5}{6} - \ln 2\right),$$

where $\left|\phi_n(\mathbf{0})\right|^2$ comes from the zero-point wave function, and only the s-wave states have non-zero value:

$$\left|\phi_n(\mathbf{0})\right|^2 = \left|R_{n0}(0)Y_{00}\right|^2 = \frac{Z^3}{\pi n^3}\frac{1}{a_0^3}.$$

Then for $n = 2$, and $l = 0$, $\Delta E_2 = -27.13$ MHz and $\Delta E_3 = 19.01$ MHz.

3 summary

The total results of energy shift for the $2S_{1/2}$ state:

$$\Delta E(2S_{1/2}) = \Delta E_1 + \Delta E_2 + \Delta E_3 = 1039.31 \text{ MHz}. \tag{9}$$

This result of $\Delta E(2S_{1/2})$ is exactly the same with that in textbook of Weinberg (see Vol. 1, *The Lamb Shift in Light Atoms*). The present experimental value gives [4]

$$\Delta E(2S_{1/2}) - \Delta E(2P_{1/2}) = 1057.845(9) \text{ MHz}.$$

Appendices

Basic facts about atom units

In this note, I adopt the Hartree atomic units, where the numerical values of the following four fundamental physical constants are all unity by definition:
Electron mass m_e;
Elementary charge e;
Reduced Planck's constant $\hbar = \frac{h}{2\pi}$;
Coulomb's constant $k_e = \frac{1}{4\pi\epsilon_0}$.

From the convention above, we can give some derived units:

Dimension	Name	Symbol	Expression
Length	Bohr radius	a_0	$\frac{\hbar}{m_e c\alpha}$
Energy	Hartree energy	E_h	$\alpha^2 m_e c^2$
Velocity			αc

Table 1: Derived atomic units

Then the speed of light:

$$c = \frac{1}{\alpha}.$$

In traditional (SI) units, the Hamiltonian is:

$$\hat{h}_0 = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}.$$

In a.u., it can be simplified as

$$\hat{h}_0 = \frac{\boldsymbol{v}^2}{2} - \frac{Z}{r}.$$

The energy spectrum for the discrete states:

$$E_n = -\frac{Z^2}{2n^2}.$$

References

[1] W. E. Lamb, R. C. Retherford, Phys. Rev. 72(1947)241.

[2] Antonio Pineda, Joan Soto, Phys. Lett. B 420(1998)391.

[3] H. A. Bethe, Phys. Rev. 72(1947)339.

[4] S. R. Lundeen, F. M. Pipkin, Phys. Rev. Lett. 46(1981)232.