Theory of light hydrogen-like atoms: status and perspectives

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Two body system with arbitrary masses

- the highest precision theoretical predictions can be achieved for simple atomic systems systems, like: hydrogenic, He, HD^+, H_2
- they serve for determination of fundamental constants: Ry, r_p, r_d, m_e/m_C, m_e/m_p, Q_D, μ_h, ...
- they could serve for determination of various nuclear properties: charge radius, polarizability, vector polarizability (hfs)
- the rotational excited states can be calculated with extreme precision $\rightarrow$ determination of Ry ? Rydberg states of heavy ions ?
- they could serve for search of unknown yet interactions by comparison with theoretical predictions: muonium, positronium

Theoretical description of energy levels

- The light particle spin $S = 1/2$, charge $= 1$, the heavy particle spin I is arbitrary, charge$= Z$.

$$H_{\rm eff} = E_0 + E_1\,\vec{L}\cdot\vec{S} + E_2\,\vec{S}\cdot\vec{I} + E_3\,\vec{L}\cdot\vec{I} + E_4\,I^i\,S^j\,(L^i\,L^j)^{(2)} + E_5\,(L^i\,L^j)^{(2)}\,(I^i\,I^j)^{(2)} + E_6\,L^i\,S^j\,(I^i\,I^j)^{(2)} + E_7\,(L^i\,L^j\,L^k)^{(3)}\,(I^i\,I^j)^{(2)}\,S^k + (\ldots)\,(I^i\,I^j\,I^k)^{(3)} + \ldots$$

- The physical energy levels are obtained by diagonalization of this effective Hamiltonian, $\vec{J}^2 = (\vec{L} + \vec{S})^2$ is not necessarily a good quantum number.
- Each coefficient E_i is a function of $\alpha, Z\,m/M, m_e/\mu$ and possibly of nuclear structure through the charge radius, Zemach radius, and other radii.
- Determination of E_i proceeds by expansion in α and calculation of each coefficient using NRQED theory
- Rotational states $L > 1$ does not depend on nuclear structure, many QED corrections vanish, so they can be calculated with extreme precision
- What are the leading nuclear effects ?

Nuclear spin independent effects to energy levels

Simple picture:

- $\rho_E(r)$ and $\rho_M(r)$: the charge and the magnetic moment distribution within the nucleus.
- $G_E(q^2)$, $G_M(q^2)$: corresponding Fourier transform,
- $\delta E_{\rm fs} = \delta E^{(4)} + \delta E^{(5)} + \delta E^{(5)}_{\rm rec} + \delta E^{(6)}$
- $\delta E^{(4)} = \frac{2\,\pi}{3}\,\phi^2(0)\,Z\,\alpha\,r_C^2$, where $r_C^2 = \int d^3r\; r^2\,\rho_E(r)$
- $\delta E^{(5)} = -\frac{\pi}{3}\,\phi^2(0)\,(Z\,\alpha)^2\,m\,r_F^3$, where $r_F^3 = \int d^3r_1\,d^3r_2\;\rho(r_1)\,\rho(r_2)\,|\vec{r}_1 - \vec{r}_2|^3$
- $\delta E^{(5)}_{\rm rec} = -\frac{m}{M}\,\phi^2(0)\,(Z\,\alpha)^2\,r_C^2\left(\frac{7}{6} - 2\,\gamma - 2\,\ln(m\,r_L)\right)$, where

  $\int d^3r_1 \int d^3r_2\,\rho(\vec{r}_1)\,\rho(\vec{r}_2)\,|\vec{r}_1 - \vec{r}_2|^2\,\ln(m\,|\vec{r}_1 - \vec{r}_2|) = 2\,r^2\,\ln(m\,r_L)$
- $\delta E^{(6)} = \ldots$ three-photon exchange

Three-photon elastic photon exchange

In the infinite nuclear mass limit

$$
\begin{aligned}
E^{(6)}_{\rm fns}(nS) &= -(Z\,\alpha)^6\,m^3\,r_C^2\,\frac{2}{3\,n^3}\left[\frac{9}{4n^2}-3-\frac{1}{n}+2\,\gamma-\ln\frac{n}{2}+\Psi(n)+\ln(m\,r_{C2}\,Z\,\alpha)\right]\\
&+(Z\,\alpha)^6\,m^5\,r_C^4\,\frac{4}{9\,n^3}\left[-\frac{1}{n}+2+2\,\gamma-\ln\frac{n}{2}+\Psi(n)+\ln(m\,r_{C1}\,Z\,\alpha)\right]\\
&+(Z\,\alpha)^6\,m^5\,r_{CC}^4\,\frac{1}{15\,n^5}\,,\\
E^{(6)}_{\rm fns}(nP_{1/2}) &= (Z\,\alpha)^6\,m\left(\frac{m^2\,r_C^2}{6}+\frac{m^4\,r_{CC}^4}{45}\right)\frac{1}{n^3}\left(1-\frac{1}{n^2}\right),\\
E^{(6)}_{\rm fns}(nP_{3/2}) &= (Z\,\alpha)^6\,m^5\,r_{CC}^4\,\frac{1}{45\,n^3}\left(1-\frac{1}{n^2}\right),\\
E^{(6)}_{\rm fns}(nL_J) &= 0 \text{ for } L>1\,,
\end{aligned}
$$

where $r_{CC}^4 = \langle r^4\rangle$ and the effective nuclear charge radii r_{C1} and r_{C2} encode the high-momentum contributions and are expectedto be of the order of r_C.

In the case of the electronic atoms, the terms proportional to r_C^4 and r_{CC}^4 in these formulas are smaller than the next-order correction and thus can be neglected.

More accurate picture:

- $\delta E^{(5)} = \delta E^{(5)}_{\rm pol} + \delta E^{(5)}_{\rm nucleons}$
- $\delta E^{(5)}_{\rm nucleons} = -\frac{\pi}{3}\,\alpha^2\,\phi^2(0)\,m_e\left[Z\,R^3_{pF} + (A-Z)\,R^3_{nF}\ + \sum_{i,j=1}^{Z}\langle\phi_N||\vec{R}_i - \vec{R}_j|^3|\phi_N\rangle\right]$
- Friar radii: $R_{pF} = 1.947(75)$ fm, $R_{nF} = 1.43(16)$ fm
- $E^{(5)}_{\rm pol} = -\alpha^2\,\phi^2(0)\,\frac{2}{3}\,m_e\left\langle\phi_N\right|\vec{d}\,\frac{1}{H_N-E_N}\left[\frac{19}{6} + 5\,\ln\frac{2\,(H_N-E_N)}{m}\right]\vec{d}\left|\phi_N\right\rangle$ (electronic)
- $E^{(5)}_{\rm pol} = -\frac{4\,\pi\,\alpha^2}{3}\,\phi^2(0)\left\langle\phi_N\right|\vec{d}\,\sqrt{\frac{2\,m}{H_N-E_N}}\vec{d}\left|\phi_N\right\rangle + \ldots$ (muonic)
- $\delta E^{(6)}$ not yet calculated, only the elastic part

Nuclear structure effects in hyperfine splitting

- $\delta E_{\rm nucl} = \delta^{(1)} E_{\rm nucl} + \delta^{(2)} E_{\rm nucl} + \ldots$ where
  $\delta^{(1)} E_{\rm nucl}$ is the two-photon exchange correction of order $(Z\,\alpha)\,E_F$,
  $\delta^{(2)} E_{\rm nucl}$ is the three-photon exchange correction of order $(Z\,\alpha)^2\,E_F$,
  $E_F = -\frac{2}{3}\,\psi^2(0)\,\vec{\mu}\cdot\vec{\mu}_e$
- $\delta^{(1)} E_{\rm nucl} = -2\,m_r Z\alpha\,r_Z E_F$ where
  r_Z is the Zemach radius defined by $r_Z = \int d^3 r_1 \int d^3 r_2\, \rho_M(r_1)\,\rho_E(r_2)\,|\vec{r}_1 - \vec{r}_2|$
- nuclear recoil correction

$$\delta^{(2)} E_{\rm fns,rec} = -\,E_F\,\frac{Z\,\alpha}{\pi}\,\frac{m}{M}\,\frac{3}{8}\left\{g\left[\gamma - \frac{7}{4} + \ln(m\,r_{M^2})\right]\right.$$
$$\left. -\,4\left[\gamma + \frac{9}{4} + \ln(m\,r_{EM})\right] - \frac{12}{g}\left[\gamma - \frac{17}{12} + \ln(m\,r_{E^2})\right]\right\}$$

- $\delta^{(2)} E_{\rm fns} = \frac{4}{3} E_F (m r_p Z\alpha)^2 \left[-\,\frac{1}{n} + 2\gamma - \ln\frac{n}{2} + \Psi(n) + \ln(m r_{pp} Z\alpha) + \frac{r_m^2}{4 r_p^2 n^2}\right]$

More accurate picture

$$\delta^{(1)} E_{\rm hfs} = E_{\rm Low} + E_{\rm 1nuc} + E_{\rm pol}$$

$$E_{\rm 1nuc} = -\frac{8\,\pi}{3}\,\alpha^2\,\frac{\psi^2(0)}{m_p + m}\,\vec{s}\cdot\langle\sum_a g_a\,\vec{s}_a\,r_{a\rm Z}\rangle$$

$$E_{\rm Low} = \frac{\alpha}{16}\,\psi^2(0)\,\vec{\sigma}\sum_{a\neq b}\frac{e_a\,e_b}{m_b}\left\langle 4\,r_{ab}\,\vec{r}_{ab}\times\vec{p}_b + \frac{g_b}{r_{ab}}\left[\vec{r}_{ab}\,(\vec{r}_{ab}\cdot\vec{\sigma}_b) - 3\,\vec{\sigma}_b\,r_{ab}^2\right]\right\rangle$$

Let us consider the special case of a spherically symmetric nucleus and neglect the proton-neutron mass difference.

$$E_{\rm Low} = -\frac{8\,\pi}{3}\,\alpha^2\,\frac{\psi^2(0)}{m_n}\sum_{a-{\rm protons}}\sum_b\langle r_{ab}\,g_b\,\vec{s}_b\rangle\,\vec{s}$$

Much better description for hfs in μD

Two-body systems with angular momentum $L > 1$

They can be calculated very accurately for an arbitrary masses:

$$E(\alpha) = E^{(0)} + E^{(2)} + E^{(4)} + E^{(5)} + E^{(6)} + o(\alpha^7)$$

where each individual term $E^{(j)}$ is of the order α^j. In particular,

$$E^{(0)} = m_1 + m_2$$

and $E^{(2)}$ is the eigenvalue of the nonrelativistic two-body Hamiltonian $H = H^{(2)}$ in the center of mass frame,

$$H = \frac{p^2}{2\,\mu} + \frac{e_1\,e_2}{4\,\pi}\,\frac{1}{r}\,.$$

When we set $e_1 = -e$, $e_2 = Z\,e$ it is equal to

$$E^{(2)} = E = -\frac{(Z\,\alpha)^2\,\mu}{2\,n^2}\,,$$

with $\mu = m_1\,m_2/(m_1 + m_2)$ being the reduced mass.

Two-body systems with angular momentum $L > 1$

$$E^{(4)} = \mu^3 (Z\alpha)^4 \biggl\{ \frac{1}{8\,n^4}\left(\frac{3}{\mu^2} - \frac{1}{m_1\,m_2}\right) - \frac{1}{\mu^2 (2l+1)\,n^3} + \frac{2\,\delta_{l0}}{3\,n^3}(r_{C1}^2 + r_{C2}^2) + \frac{\delta_{l0}}{m_1\,m_2\,n^3}$$
$$+ \frac{1}{l(l+\frac{1}{2})(l+1)n^3}\biggl[\vec{L}\cdot\vec{s}_1\left(\frac{1+2\kappa_1}{2m_1^2} + \frac{1+\kappa_1}{m_1\,m_2}\right) + \vec{L}\cdot\vec{s}_2\left(\frac{1+2\kappa_2}{2m_2^2} + \frac{1+\kappa_2}{m_1\,m_2}\right)$$
$$- \frac{6(1+\kappa_1)(1+\kappa_2)}{m_1\,m_2\,(2\,l-1)(2\,l+3)}\,s_1^i\,s_2^j (L^i L^j)^{(2)}\biggr] + \frac{8\,\delta_{l0}}{3m_1\,m_2\,n^3}(1+\kappa_1)(1+\kappa_2)\,\vec{s}_1\cdot\vec{s}_2\biggr\}$$

In the limit of the infinite mass m_2 and the point particle "1"

$$E^{(4)} = m\,(Z\alpha)^4 \left\{\frac{3}{8\,n^4} - \frac{1}{(2j+1)\,n^3}\right\}. \tag{1}$$

coincides with the Dirac or the Klein-Gordon equation

Two-body systems with angular momentum $L > 1$

The leading QED corrections

$$E^{(5)} = -\frac{7}{3\pi}\frac{(Z\alpha)^5\mu^3}{m_1 m_2}\frac{1}{n^3\, l(2l+1)(l+1)} - \frac{4}{3\pi}\left(\frac{1}{m_1}+\frac{Z}{m_2}\right)^2\frac{\alpha(Z\alpha)^4\mu^3}{n^3}\ \ln\left[k_0(n,l)\right] + \frac{(Z\,\alpha)^5}{\pi\, n^3}\,\delta_{l0}\,(\delta_N + \delta_S\,\vec{s}_1\cdot\vec{s}_2)$$

where δ_N, δ_S are known only for spin $1/2$ particles

Two-body systems with angular momentum $L > 1$

The correction of the order $m\,\alpha^6$ for spinless particles is thus

$$\begin{aligned} E^{(6)} =& \mu(Z\alpha)^6\Big[-\frac{5}{16\,n^6}+\frac{3}{2\,(2l+1)\,n^5}-\frac{3}{2\,(2l+1)^2\,n^4}-\frac{1}{(2l+1)^3\,n^3} \\ &+\frac{\mu^2}{m_1\,m_2}\bigg(\frac{3}{16\,n^6}-\frac{(8\,l(l+1)-3)}{2\,(2l-1)(2l+1)(2l+3)\,n^5}+\frac{6}{(2l-1)(2l+1)(2l+3)\,n^3}\bigg) \\ &-\frac{\mu^4}{16\,m_1^2\,m_2^2\,n^6}+\frac{2\,\mu^3\,(\alpha_{E1}+\alpha_{E2})}{(2l-1)(2l+1)(2l+3)}\bigg(\frac{1}{n^5}-\frac{3}{l(l+1)\,n^3}\bigg)\Big] \end{aligned}$$

The limit when mass $M = m_2$ of one of the particles is infinitely heavy is in agreement with Klein-Gordon equation $j = l$:

$$\delta E^{(6,0)} = m(Z\alpha)^6\bigg(-\frac{5}{16n^6}+\frac{3}{2(1+2j)n^5}-\frac{3}{2(1+2j)^2n^4}-\frac{1}{(1+2j)^3n^3}\bigg),$$

The first-order recoil correction

$$\begin{aligned} E^{(6,1)} = (Z\alpha)^6\,\frac{m^2}{M}\bigg[&\frac{1}{2n^6}+\frac{6-10l(l+1)}{(2l-1)(2l+1)(2l+3)n^5}+\frac{3}{2(1+2l)^2n^4} \\ &+\frac{3+28l(l+1)}{(2l-1)(2l+1)^3(2l+3)n^3}\bigg] \end{aligned}$$

To do list

- two-photon exchange to hfs for light nuclei
- three-photon exchange nuclear structure correction (spin-independent)
- E^6 for $L = 0$ with arbitrary masses
- $E^{(7,1)}$ for an arbitrary state
- two-loop radiative correction $\delta E = \alpha^2 \, (Z\,\alpha)^6$
- three-loop radiative corrections $\delta E = \alpha^3 \, (Z\,\alpha)^5$
- ...