Antiprotonic Helium Structure and Spectroscopy

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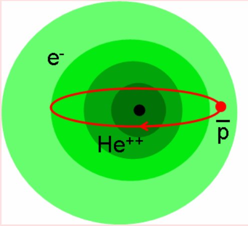

EXA11, September 2011

Structure of States

Structure. Naive picture

- Antiproton orbiting around He^{+} *quasinucleus* with effective charge $Z_{eff} \approx 1.7$

$$E(n,l) = R_\infty Z_{eff}^2 \frac{M^*}{n^2}, \qquad n \sim \sqrt{M^*} \approx 37$$

- Accounting finite size of an electronic cloud one gets that $Z_{eff}(l)$ depends on l (growing with l)

$$E(n,l-1) < E(n,l)$$

- *Configuration Interaction* (CI):

$$\Psi(\mathbf{r}_e,\mathbf{r}_{\bar p}) = \psi_0^e(\mathbf{r}_e)\varphi^{\bar p}_{nlm}(\mathbf{r}_{\bar p}) + \sum_i c_i \left\{ Y_{l_i^e} \otimes Y_{l_i^{\bar p}} \right\}_{lm} \psi_i^e(r_e)\varphi_i^{\bar p}(r_{\bar p})$$

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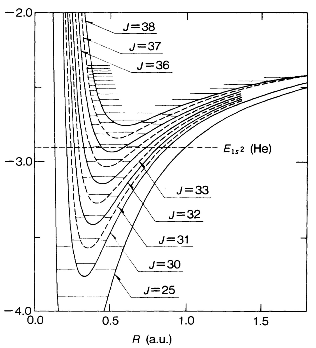
The Adiabatic Approximation



The wave function is taken in a separable form

$$\Psi_{vJM}(\mathbf{r},\mathbf{R}) = \psi_0^e(\mathbf{r};R)R^{-1}\chi_{vJ}(R)Y_{JM}(\hat{\mathbf{R}})$$

where the vibrational wave function $\chi_{vJ}(R)$ satisfies the Schrödinger equation

$$\left\{\frac{1}{2M^*}\left[-\frac{d^2}{dR^2}+\frac{J(J+1)}{R^2}\right]+V(R)-E_{vJ}\right\}\chi_{vJ}=0$$

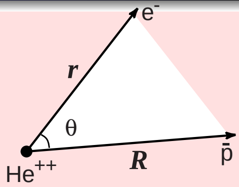
Relation between quantum numbers:

$$J=l, \qquad v=n-l-1$$

Molecular Expansion

The wave function:

$$\Psi_{vLM}(\mathbf{r},\mathbf{R}) = \sum_{m=0}^{L} \mathcal{D}^L_{Mm}(\Phi,\Theta,\varphi) F^L_m(r_e, R_{\bar{p}}, \theta)$$



Here $\mathcal{D}^L_{Mm}(\Phi,\Theta,\varphi)$ is a symmetrized Wigner D-function of Euler angles of a molecular moving frame.

For the particular state, when m_{max} is smaller than Δl, the multipolarity of the Auger transition, the Hamiltonian projected onto the subspace

$$\mathcal{H}_{m_{max}} = \sum_{m=0}^{m_{max}} \mathcal{D}^L_{Mm}(\Phi,\Theta,\varphi) F^L_m(r_e, R_{\bar{p}}, \theta)$$

has this state bound (or pure discrete spectrum state).

$\mathcal{H}_0$ contains the adiabatic solution.

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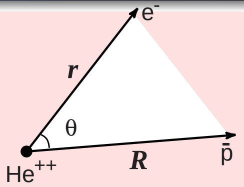

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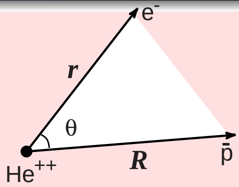

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Convergence of Molecular Expansion

Contribution of σ, π and δ components into the nonrelativistic energies of ${}^4\mathrm{He}^+\bar{p}$ ($L = 36$).

	$v = 0$	$v = 1$	$v = 2$	$v = 3$
$m = 0$	-2.88618457	-2.81268193	-2.74848146	-2.69229316
$m = 0, 1$	-2.88668231	-2.81311531	-2.74885983	-2.69262473
$m = 0, 1, 2$	-2.88668236	-2.81311437	-2.74885989	-2.69262479

Exponential basis set

The wave function is taken in the form

$$\Psi_{LM}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{l_1+l_2=L \text{ or } L+1} C_{l_1 l_2 n}\, \mathcal{Y}^{l_1 l_2}_{LM}(\mathbf{r}_1,\mathbf{r}_2) e^{-\alpha_n r_1 - \beta_n r_2 - \gamma_n r_{12}},$$

where α_n, β_n, and γ_n are randomly generated (complex or real) parameters:

$$\alpha_i = \left[\left\lfloor \frac{1}{2} i(i+1)\sqrt{p_\alpha} \right\rfloor (A_2 - A_1) + A_1\right] + \\ +i\left\{\left[\left\lfloor \frac{1}{2} i(i+1)\sqrt{q_\alpha} \right\rfloor (A'_2 - A'_1) + A'_1\right]\right\},$$

$\lfloor x \rfloor$ designates the fractional part of x, p_α and q_α are some prime numbers. Parameters β_i and γ_i are obtained in a similar way.

As it has been discovered "experimentally" this method has in general very good convergence.

CCR Resonances

The Coulomb Hamiltonian is analytic under dilatation transformations

$$\left(U(\theta)f\right)(\mathbf{r}) = e^{m\theta/2} f(e^{\theta}\mathbf{r}),$$

for real θ and can be analytically continued to the complex plane.

The CCR method "rotates" the coordinates of the dynamical system

$$r_{ij} \to r_{ij}e^{i\varphi}, \qquad \theta = i\varphi$$

where φ is the parameter of the complex rotation.

Under this transformation the Hamiltonian changes as a function of φ

$$\boxed{H_\varphi = Te^{-2i\varphi} + Ve^{-i\varphi},}$$

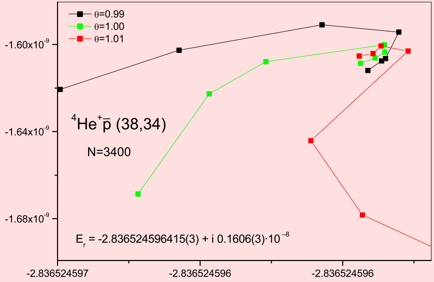
and the continuum spectrum of H_φ rotates on the complex plane around branch points ("thresholds") to "uncover" resonant poles.

CCR Resonances

The resonance energy is determined by solving the complex eigenvalue problem for the "rotated" Hamiltonian

$$(H_\varphi - E)\Psi_\varphi = 0,$$

The eigenfunction Ψ_φ obtained from this equation is square-integrable and the corresponding complex eigenvalue $E = E_r - i\Gamma/2$ defines the energy E_r and the width of the resonance, Γ.



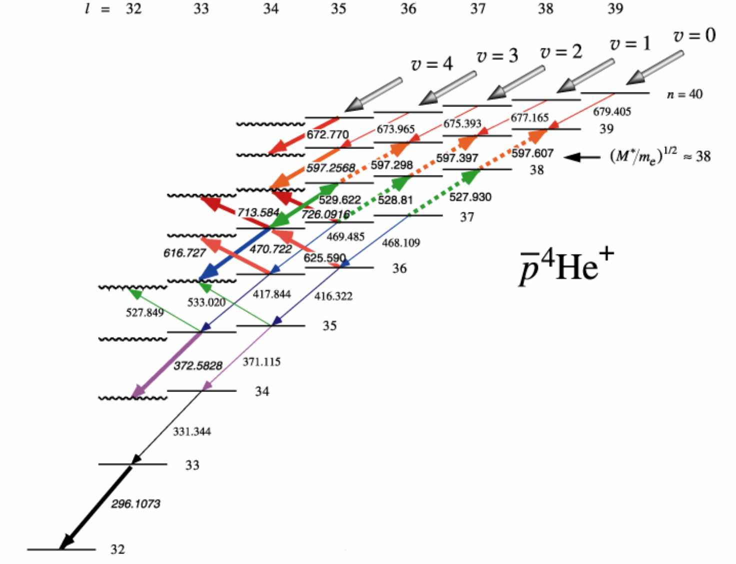
Results

Nonrelativistic energies, E_{nr}, half-widths, $\Gamma/2$, for the states of $^4\mathrm{He}^+\bar{p}$.

state	E_{nr}	$\Gamma/2$
$(31,30)$	$-3.6797747876576(1)$	$4.7602\cdot10^{-9}$
$(32,31)$	$-3.50763503897101(1)$	$5.4\cdot10^{-13}$
$(33,32)$	$-3.35375787083340(1)$	$1.07\cdot10^{-12}$
$(34,32)$	$-3.2276763796294(3)$	$2.7237\cdot10^{-9}$
$(35,32)$	$-3.116679795873(3)$	$6.9733\cdot10^{-8}$
$(34,33)$	$-3.21624423907002(1)$	$1.4\cdot10^{-13}$
$(35,33)$	$-3.1053826755489(3)$	$2.8\cdot10^{-12}$
$(36,33)$	$-3.0079790936832(4)$	$2.9188\cdot10^{-9}$
$(35,34)$	$-3.09346690791590(1)$	—
$(36,34)$	$-2.996335447966270(5)$	$2.3\cdot10^{-13}$
$(37,34)$	$-2.9111809394697(4)$	$2.6\cdot10^{-12}$
$(37,35)$	$-2.89928218336728(1)$	—

Ro-vibrational Spectroscopy

Schematic Diagram of the Level Structure



Leading order relativistic corrections

- Relativistic correction for the bound electron:

$$E_{rc} = \alpha^2 \left\langle -\frac{\boldsymbol{\nabla}_e^4}{8m_e^3} + \frac{1}{8m_e^2}\left[Z_{\mathrm{He}} 4\pi\delta(\mathbf{r}_{\mathrm{He}}) + Z_{\bar{p}} 4\pi\delta(\mathbf{r}_{\bar{p}})\right] \right\rangle .$$

- Corrections for the anomalous magnetic moment of an electron:

$$E_{a_e} = \alpha^2 \left\langle \frac{2a_e}{8m_e^2}\left[Z_{\mathrm{He}} 4\pi\delta(\mathbf{r}_{\mathrm{He}}) + Z_{\bar{p}} 4\pi\delta(\mathbf{r}_{\bar{p}})\right] \right\rangle ,$$

$$a_e = \frac{\alpha}{\pi}\cdot\frac{1}{2} + \left(\frac{\alpha}{\pi}\right)^2 \left[\frac{197}{144} + \frac{\pi^2}{12} - \frac{\pi^2}{2}\ln 2 + \frac{3}{4}\zeta(3)\right] = 1.1596522\cdot 10^{-3}.$$

- One transverse photon exchange correction:

$$E_{exch} = \alpha^2 \Bigg\{ -\sum_{i=1,2} \frac{Z_i}{2M_i} \left\langle \frac{\boldsymbol{\nabla}_i \boldsymbol{\nabla}_e}{r_i} + \frac{\mathbf{r}_i(\mathbf{r}_i \boldsymbol{\nabla}_i)\boldsymbol{\nabla}_e}{r_i^3} \right\rangle + \frac{Z_1 Z_2}{2M_1 M_2} \left\langle \frac{\boldsymbol{\nabla}_1 \boldsymbol{\nabla}_2}{R} + \frac{\mathbf{R}(\mathbf{R}\boldsymbol{\nabla}_1)\boldsymbol{\nabla}_2}{R^3} \right\rangle \Bigg\}.$$

- Relativistic corrections for heavy particles.

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Finite Size Corrections

The leading corrections for the finite nuclear size may be written:

$$\Delta E_{\rm nuc} = \sum \frac{2\pi Z_i (R_i/a_0)^2}{3} \langle \delta(\mathbf{r}_i) \rangle,$$

where R is *the root-mean-square radius* of the nuclear charge distribution.

The *rms radii* for He nucleus and antiproton are:

$$R(^4\mathrm{He}) = 1.6757(26)\ \mathrm{fm}, \qquad R(^3\mathrm{He}) = 1.9448(137)\ \mathrm{fm},$$

$$R(\bar{p}) \stackrel{?}{=} R(p) = 0.8750(68)\ \mathrm{fm}.$$

[$R(^4\mathrm{He})$ is taken from I.Angeli, At. Data Nucl. Data Tables **87**, 185 (2004).]

Leading order radiative corrections

- The one-loop self-energy correction ($R_\infty \alpha^3$):

$$E^{(3)}_{se} = \alpha^3 \frac{4}{3}\left[\ln\frac{1}{\alpha^2} - \beta(L,v) + \frac{5}{6} - \frac{3}{8}\right]\left\langle Z_{\rm He}\delta(\mathbf{r}_{\rm He}) + Z_{\bar p}\delta(\mathbf{r}_{\bar p})\right\rangle,$$

where

$$\beta(L,v) = \frac{\langle \mathbf{J}(H_0-E_0)\ln\left((H_0-E_0)/R_\infty\right)\mathbf{J}\rangle}{\langle[\mathbf{J},[H_0,\,\mathbf{J}]]/2\rangle}$$

is the Bethe logarithm of the three-body state.

- Recoil correction of order $R_\infty\alpha^3(m/M)$:

$$E^{(3)}_{recoil} = \sum_{i=1,2}\frac{Z_i\alpha^3}{M_i}\left\{\frac{2}{3}\left(-\ln\alpha - 4\beta(L,v) + \frac{31}{3}\right)\langle\delta(\mathbf{r}_i)\rangle - \frac{14}{3}\langle Q(r_i)\rangle\right\},$$

where $Q(r)$ is the so-called Araki-Sucher term.

- One-loop vacuum polarization:

$$E^{(3)}_{vp} = \frac{4\alpha^3}{3}\left[-\frac{1}{5}\right]\left\langle Z_{\rm He}\delta(\mathbf{r}_{\rm He}) + Z_{\bar p}\delta(\mathbf{r}_{\bar p})\right\rangle.$$

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Higher order corrections in a nonrecoil limit $R_\infty\alpha^4$ order

- The one-loop self-energy and vacuum polarization contributions:

$$E^{(4)}_{se} = \alpha^4 \left[4\pi\left(\frac{139}{128}-\frac{1}{2}\ln 2\right)\right] \left\langle Z^2_{\rm He}\delta(\mathbf{r}_{\rm He})+Z^2_{\bar p}\delta(\mathbf{r}_{\bar p})\right\rangle,$$

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- The two-loop QED correction:

$$E^{(4)}_{2loop} = \alpha^4\left[\frac{1}{\pi}\left(-\frac{6131}{1296}-\frac{49\pi^2}{108}+2\pi^2\ln 2-3\zeta(3)\right)\right] \times \left\langle Z_{\rm He}\delta(\mathbf{r}_{\rm He})+Z_{\bar p}\delta(\mathbf{r}_{\bar p})\right\rangle.$$

- The $R_\infty\alpha^4$ relativistic correction is obtained using the adiabatic "effective" potential for an $m\alpha^6$ order term of the two-center Dirac energy.

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$R_\infty\alpha^5$ order corrections

A complete set of $R_\infty\alpha^5$ order corrections consist of the one- and two-loop radiative corrections only:

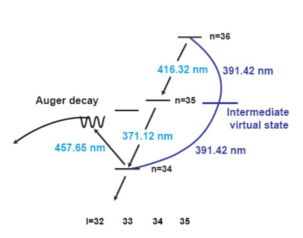
$$E_{se}^{(5)} = \alpha^5\left[-1\right]\left\{Z_{\rm He}^3\,\ln^2(Z_{\rm He}\alpha)^{-2}\langle\delta(\mathbf{r}_{\rm He})\rangle + Z_{\bar p}^3\,\ln^2(Z_{\bar p}\,\alpha)^{-2}\langle\delta(\mathbf{r}_{\bar p})\rangle\right\},$$

$$E_{se}^{(5')} = \alpha^5 Z_{\rm He}^3\left[A_{61}\ln\left(Z_{\rm He}\alpha\right)^{-2} + A_{60}\right]\langle\delta(\mathbf{r}_{\rm He})\rangle\,,$$

$$E_{2loop}^{(5)} = \frac{\alpha^5}{\pi} Z_{\rm He}^2\left[B_{50}\right]\langle\delta(\mathbf{r}_{\rm He})\rangle\,,$$

where the constants A_{61}, A_{60} were taken equal to the constants of the $1s$ state of the hydrogen atom: $A_{61} = 5.286$, $A_{60} = -30.924$, and B_{50} is known and valid for a general external field: $B_{50} = -21.556(3)$.

Two-photon spectroscopy. Year 2010.



[M. Hori *et al.* Nature **475**, 484 (2011)]

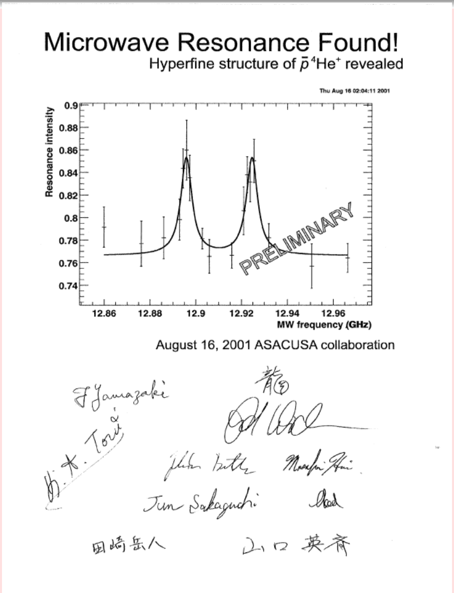
Isotope	Transition $(n, l) \to (n-2, l-2)$	Transition frequency (MHz)	
		Experiment	Theory
$\bar{p}^4\mathrm{He}^+$	$(36,34)\to(34,32)$	1,522,107,062(4)(3)(2)	1,522,107,058.9(2.1)(0.3)
	$(33,32)\to(31,30)$	2,145,054,858(5)(5)(2)	2,145,054,857.9(1.6)(0.3)
$\bar{p}^3\mathrm{He}^+$	$(35,33)\to(33,31)$	1,553,643,100(7)(7)(3)	1,553,643,100.7(2.2)(0.2)

Experimental values show respective total, statistical and systematic 1-s.d. errors in parentheses; theoretical values (ref. 3 and V. I. Korobov, personal communication) show respective uncertainties from uncalculated QED terms and numerical errors in parentheses.

$$A_r(e) = 0.000\,548\,579\,909\,1(7)[1.4\times 10^{-9}]$$

Antiprotonic Helium Hyperfine Structure

Discovery of a MW Resonance



HFS in $^4\mathrm{He}^+\bar{p}$

Effective spin Hamiltonian:

$$H_{\mathrm{eff}} = \frac{d_1}{L+1}(\mathbf{L}\cdot\mathbf{s}_e) + \frac{d_2}{L+1}(\mathbf{L}\cdot\mathbf{s}_{\bar{p}}) + d_3(\mathbf{s}_e\cdot\mathbf{s}_{\bar{p}})$$
$$+\frac{d_4}{(2L-1)(2L+3)}\left\{\frac{2L(L+1)}{3}(\mathbf{s}_e\cdot\mathbf{s}_{\bar{p}}) - \left[(\mathbf{L}\cdot\mathbf{s}_e)(\mathbf{L}\cdot\mathbf{s}_{\bar{p}}) + (\mathbf{L}\cdot\mathbf{s}_{\bar{p}})(\mathbf{L}\cdot\mathbf{s}_e)\right]\right\}$$

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Coefficients d_i for the (37,35) state (in MHz)

$$d_1 = -13087.8, \quad d_2 = 151.625, \quad d_3 = -297.018, \quad d_4 = -974.163$$

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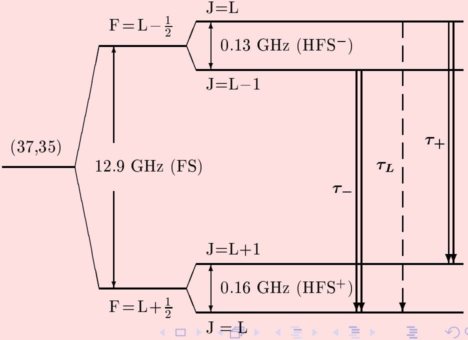
The coupling scheme is:

$$\mathbf{F} = \mathbf{L} + \mathbf{s}_e, \quad \mathbf{J} = \mathbf{F} + \mathbf{s}_{\bar{p}}$$

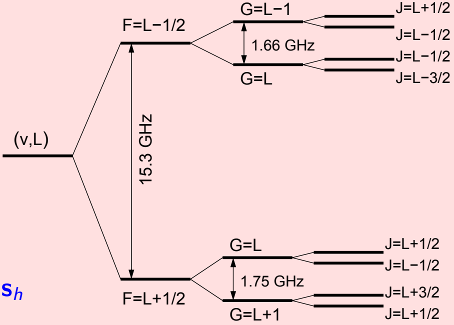
with the state vector $|vLFJJ_z\rangle$



HFS in $^3\mathrm{He}^+\bar{p}$

Magnetic moment ratios of a proton and helion to nuclear magneton are:

$$\mu_p/\mu_N = 2.792847351, \qquad \mu_h/\mu_N = -2.12762485.$$



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with the state vectors $|vLFGJJ_z\rangle$

NRQED of order $m\alpha^6$ to the $E_1(\mathbf{s}_e\cdot\mathbf{L})$ interaction

Second order term:

$$\Delta E_A = 2\alpha^4\left\langle -\frac{\mathbf{p}_e^4}{8m_e^3}+\frac{\pi}{2m_e^2}\left[Z_1\delta(\mathbf{r}_1)+Z_2\delta(\mathbf{r}_2)\right]\middle| Q(E_0-H_0)^{-1}Q\middle|\frac{(1+2a_e)Z_a}{2m_e^2}\,\frac{1}{r_a^3}(\mathbf{r}_a\times\mathbf{p}_e)\mathbf{s}_e\right\rangle$$
$$+2\alpha^4\left\langle -\frac{\mathbf{p}_e^4}{8m_e^3}+\frac{\pi}{2m_e^2}\left[Z_1\delta(\mathbf{r}_1)+Z_2\delta(\mathbf{r}_2)\right]\middle| Q(E_0-H_0)^{-1}Q\middle| -\frac{(1+a_e)Z_j}{m_em_a}\,\frac{1}{r_a^3}(\mathbf{r}_a\times\mathbf{P}_a)\mathbf{s}_e\right\rangle$$

Effective Hamiltonian $H^{(6)}$

$$\mathcal{V}_1 = e^2\left(i\frac{3\boldsymbol{\sigma}_e^P[\mathbf{q}\times\mathbf{p}_e](p_e'^2+p_e^2)}{32m_e^4}\right)\quad\frac{1}{\mathbf{q}^2}\quad(Z_a)$$
$$\mathcal{V}_2 = -e^2\left(i\frac{[\boldsymbol{\sigma}_e^P\times\mathbf{q}](p_e'^2+p_e^2)}{8m_e^3}\right)\quad\frac{1}{\mathbf{q}^2}\quad\left(Z_i\frac{\mathbf{P}_a}{M_a}\right),\qquad a=1,2\,({}^4\mathrm{he},\bar{p})$$

Seagull interaction with one Coulomb and one transverse photon lines:

$$\mathcal{V}_5 = e^4\frac{\boldsymbol{\sigma}_e^P}{4m_e^2}\left[\left\{\left[-\frac{1}{\mathbf{q}_2^2}\left(\delta^{ij}-\frac{q_2^iq_2^j}{\mathbf{q}_2^2}\right)\right]\left(-Z_2\frac{\mathbf{P}_2'+\mathbf{P}_2}{2M_2}\right)\right\}\times\left[\frac{i\mathbf{q}_1}{\mathbf{q}_1^2}\right](Z_1)\right]+(1\leftrightarrow 2)$$

Radiative corrections (from the form factors) are also included.

Comparison with experiment

- Experiment [T. Pask *et al.* PLB (2009)]:

$$\tau_+ = 12\,896.641(63)\ \text{MHz},$$
$$\tau_- = 12\,924.461(63)\ \text{MHz}.$$

- The Breit-Pauli approximation [KB, JPB (2001)] (relative accuracy $\mathcal{O}(\alpha^2)$):

$$\tau_+ = 12\,896.35(69)\ \text{MHz},$$
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- Corrections of the $m\alpha^6$ order:

$$\tau_+ = 12\,897.0(1)(3)\ \text{MHz},$$
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