

Helium fine structure

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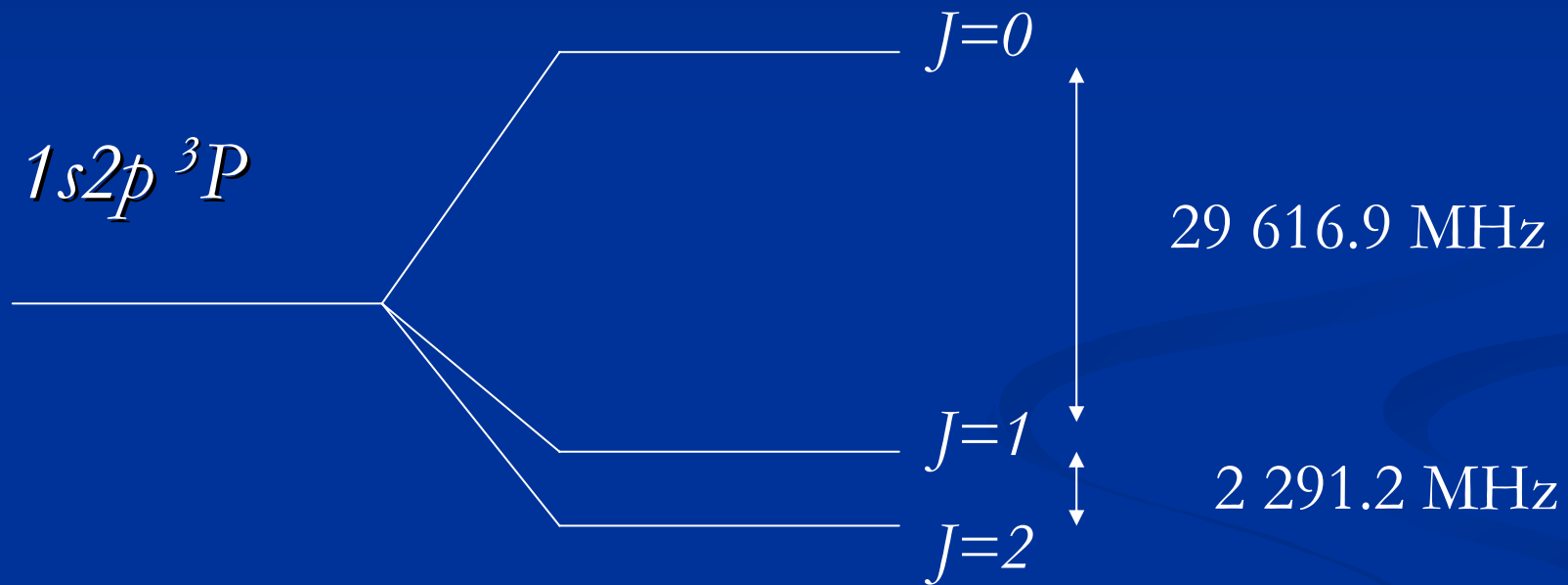
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Fine-structure splitting of the $1s2p\ ^3P_J$ state of helium



Why helium and why fine structure?

- Helium is the simplest many-body system $\Rightarrow$ accurate theoretical description is possible.
Small natural line width of the $2^3P_J-2^3S$ transitions $\Rightarrow$ superb experimental precision (accuracy up to 7×10^{-12}).
- Theory of the fine structure is simpler than that of the separate energy levels ($m\alpha^6$ correction for FS – Douglas and Kroll 1974; $m\alpha^6$ correction for energy – Pachucki 2006); complete treatment of $m\alpha^7$ correction is possible.
- For decades theoretical and experimental investigations of the helium fine structure were motivated by perspectives for the determination of the fine structure constant. Current experimental accuracy $\Leftrightarrow$ 14 ppb determination of α . (The best determination is from the electron g factor, 0.37 ppb, 2008).

Theory and experiment, status 2006: serious disagreement (12σ and 24σ)

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Improved Theory of Helium Fine Structure

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Improved theoretical predictions for the fine-structure splitting of 2^3P_J levels in helium are obtained by the calculation of contributions of order α^5 Ry. New results for transition frequencies $\nu_{01} = 29\,616\,943.01(17)$ kHz and $\nu_{12} = 22\,911\,611.13(30)$ kHz disagree significantly with the experimental values, indicating an outstanding problem in bound state QED.

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The fine-structure splitting of the helium 2^3P_J states is an intrinsically relativistic effect and arises from the inter-

terms, and I will explicitly demonstrate its cancellation in their sum. Natural relativistic units will be used with $\hbar =$

Theory and experiment: status 2006

in kHz

	$0 \rightarrow 1$	$1 \rightarrow 2$	
up to $m\alpha^6$	29 616 871.67(6)	2 291 163.69(12)	KP
	29 616 871.21	2 291 163.68	Drake
$m\alpha^7, \log$	82.59	-10.09	KP; Zhang 1996
$m\alpha^7, \text{Bethe}$	-29.76(16)	-12.51(27)	KP&Sapirstein 2000
$m\alpha^7, \text{other}$	28.89	10.22	KP 2006
$m\alpha^6 m/M$	-10.38	9.82	Drake 2002
Theory	29 616 943.01(17)	2 291 161.13(30)	
Experiment	29 616 951.66(70)	2 291 175.59(51)	Zelevinsky 2005
	29 616 950.9(9)		George 2001
	29 616 952.7(1.0)		Giusfredi 2005

not checked independently

K. Pachucki (KP), Phys. Rev. Lett. 97, 013002 (2006)

Theory of the fine structure: orientation

The fine structure intervals of light atoms are described by expanding all relativistic and QED effects in powers of α ,

$$E_{\text{fs}} = E^{(4)} + E^{(5)} + E^{(6)} + E^{(7)} + \dots,$$

where $E^{(i)}$ is the contribution of order $m\alpha^i$ (and may contain powers of $\ln \alpha$). In turn, each $E^{(i)}$ is expanded in powers of the electron-to-nuclear mass ratio, $E^{(i)} = E_{\infty}^{(i)} + E_M^{(i)} + E_{M^2}^{(i)} + \dots$.

- $E^{(4)}$ is induced by the (spin-dependent part of the) Breit-Pauli Hamiltonian $H^{(4)}$.
- $E^{(5)}$ is due to the anomalous magnetic moment correction to the Breit-Pauli Hamiltonian.
- $E^{(6)} = \langle H^{(6)} \rangle + \left\langle H^{(4)} \frac{1}{(E_0 - H_0)'} H^{(4)} \right\rangle$. $H^{(6)}$ is derived by Douglas and Kroll in 1974. Calculation is done by Lewis and Serafino in 1978 and more accurately by Yan and Drake in 1995.

Theory of the fine structure: higher-order corrections

- $E_M^{(6)}$ (i.e., correction of order $m^2/M\alpha^6$) was studied by Zhang in 1997 (mistakes!!) and by Pachucki and Sapirstein in 2003.
- logarithmic part of $E^{(7)}$ was calculated by Zhang et al. in 1996 and by Pachucki in 1999.
- nonlogarithmic part of $E^{(7)}$: derivation by Zhang 1997 (mistakes!!), Pachucki and Sapirstein in 2000 (a part of correction), Pachucki in 2006 (the complete correction).

Nonrelativistic wave function: helium

Korobov 2000, 2002

The spatial part of the triplet P wave function is represented as

$$\vec{\phi}(\vec{r}_1, \vec{r}_2) = \sum_i c_i \left[\vec{r}_1 \exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}) - (1 \leftrightarrow 2) \right].$$

Real nonlinear parameters α_i , β_i , and γ_i are chosen quasirandomly from the intervals $\alpha_i \in [A_1, A_2]$, $\beta_i \in [B_1, B_2]$, $\gamma_i \in [C_1, C_2]$, with the parameters $A_{1,2}$, $B_{1,2}$, and $C_{1,2}$ determined by a variational optimization.

All integrals for evaluation of matrix elements of various operators are obtained from the single master integral

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

by formal differentiation or integration over the parameters.

Our result for the nonrelativistic energy obtained with $N = 6600$ basis functions:

$$E(2^3P) = -2.133\,164\,190\,779\,283\,205\,146\,96 \stackrel{+0}{-10}.$$

Bethe logarithm for helium

Two calculational approaches:

I) Sum over the spectrum (Drake and Goldman 1999 , Korobov 2004):

$$\ln k_0 = \frac{\sum_n |\langle 0 | \vec{\nabla} | n \rangle|^2 (E_n - E_0) \ln |E_n - E_0|}{\sum_n |\langle 0 | \vec{\nabla} | n \rangle|^2 (E_n - E_0)},$$

where $\vec{\nabla} \equiv \vec{\nabla}_1 + \vec{\nabla}_2$.

II) The integral representation (Schwartz 1961, Korobov and Korobov 1999):

$$\ln k_0 \stackrel{K \rightarrow \infty}{=} \int_0^K dk k J(k) - A K - B \ln K, \quad J(k) = \frac{1}{\mathcal{D}} \left\langle \vec{\nabla} \frac{1}{E_0 - H_0 - k} \vec{\nabla} \right\rangle,$$

where $\mathcal{D} = 2\pi Z \langle \delta^3(r_1) + \delta^3(r_2) \rangle$.

Bethe logarithm in more detail

$$\ln k_0 = R(\kappa_1) + \int_0^{\kappa_1} dk \, k \, J(k) + \left(\int_{\kappa_1}^{\kappa_2} + \int_{\kappa_2}^{\infty} \right) dk \, \frac{w(k)}{k^2},$$

where $w(k) = k^3 J(k) - A k^2 - B k - C\sqrt{k} - D \ln k$, and A , B , C , and D are known.

$$J(k) = \frac{1}{\mathcal{D}} \left\langle \vec{\nabla} \frac{1}{E_0 - H_0 - k} \vec{\nabla} \right\rangle$$

has a definite sign (for $k > E_0 - \min(E_n)$) and obeys the variational principle.

- Integral over $[0, \kappa_1]$: analytically, by using the spectral representation of the resolvent ($\kappa_1 = 100$).
- Integral over $[\kappa_1, \kappa_2]$: numerically ($\kappa_2 = 10^4 \dots 10^5$).
- Integral over $[\kappa_2, \infty]$: by fitting the asymptotic expansion of $w(k)$:

$$w(k) = \text{pol} \left(\frac{1}{\sqrt{k}} \right) + \frac{\ln k}{k} \text{pol} \left(\frac{1}{k} \right)$$

Bethe logarithm for the 2^3P state of helium, numerical results

$$\begin{aligned}\ln(k_0/Z^2) &= 2.983\,691\,003\,3(2) \quad \text{our result} \\ &\quad 2.983\,690\,995(1) \quad \text{Korobov 2004} \\ &\quad 2.983\,690\,84(2) \quad \text{Drake and Goldman 1999}\end{aligned}$$

Relativistic corrections to the Bethe logarithm

- First-order perturbation induced by the spin-dependent part of the Breit-Pauli Hamiltonian (perturbations of the wave function, the reference-state energy, and the propagator)

$$H^{(4)} = -\frac{3\alpha}{4r_{12}^3} \vec{r}_{12} \times (\vec{p}_1 - \vec{p}_2) \cdot \vec{s} + \frac{Z\alpha}{4} \left(\frac{\vec{r}_1}{r_1^3} \times \vec{p}_1 + \frac{\vec{r}_2}{r_2^3} \times \vec{p}_2 \right) \cdot \vec{s} \\ + \frac{\alpha}{2r_{12}^3} \left(\vec{s}^2 - \frac{3}{r_{12}^2} (\vec{s} \cdot \vec{r}_{12})^2 \right),$$

where $\vec{s} = (\vec{\sigma}_1 + \vec{\sigma}_2)/2$.

- Correction to the electron current (operator of emission and absorption of virtual electron)

$$\vec{p}_1 + \vec{p}_2 \rightarrow -\frac{Z\alpha}{2} \left(\frac{\vec{r}_1 \times \vec{\sigma}_1}{r_1^3} + \frac{\vec{r}_2 \times \vec{\sigma}_2}{r_2^3} \right).$$

Relativistic corrections to Bethe logarithm: a calculation

■ Correction to the current:

1. stronger cancellation in the subtraction of the ultraviolet asymptotics ($\sim k^{-5/2}$, instead of $\sim k^{-3/2}$ for the Bethe logarithm)
2. separate partial-wave contributions are divergent (!)

“unrenormalized”, for each partial wave: $k^2 \tilde{J}_l(k) \stackrel{k \rightarrow \infty}{\sim} k$

“unrenormalized”, total: $k^2 \tilde{J}(k) \stackrel{k \rightarrow \infty}{\sim} \text{const}$

“renormalized”: $k^2 \tilde{J}(k) - \tilde{A} \stackrel{k \rightarrow \infty}{\sim} k^{-3/2}$

- ## ■ Perturbation by the Breit-Pauli Hamiltonian:
- the integrand does not satisfy the variational principle

Relativistic corrections to Bethe logarithm: results

in atomic units

- Correction to the current:

$$E_{L2} = 0.067\,682\,1(5) \, u_J$$

$$E_{L2} = -0.067\,75(5) \, u_J \quad \text{KP and Sapirstein, 2000}$$

where $u_J = (1, 1/2, -1/2)$ for $J = (0, 1, 2)$. The sign error is found.

- Perturbation by the Breit-Pauli Hamiltonian:

$$E_{L1} = -0.107\,664(6) \, u_J + 0.118\,404\,4(4) \, v_J$$

$$E_{L1} = -0.082(2) \, u_J + 0.095\,9(4) \, v_J \quad \text{KP and Sapirstein, 2000}$$

where $v_J = (-1, 1/2, -1/10)$ for $J = (0, 1, 2)$.

Theory and experiment: present status

K. Pachucki and V.Yerokhin, Phys. Rev. A 79, 062516 (2009)

	0→1	1→2	in kHz
up to α^6	29 616 871.53(2)	2 291 163.74	
$\alpha^7, \log$	82.59	-10.09	
α^7, Bethe	-26.90	4.23	
α^7, other	28.95	10.25	
$\alpha^6 m/M$	-9.96	9.14	
Theory	29 616 946.2(1.6)	2 291 177.3(1.6)	Pachucki 2006
	29 616 943.01(17)	2 291 161.13(30)	
Experiment		2 291 177.53(35)	Borbely 2009
	29 616 951.66(70)	2 291 175.59(51)	Zelevinsky 2005
	29 616 950.9(9)		George 2001
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theoretical uncertainty is due to higher-order effects

Summary

- Our recalculation of the helium fine structure identified and corrected several problems present in previous evaluations. Our estimation of higher-order effects is much larger than in previous studies.
- Theoretical and experimental values are now much closer than before.
- Still, complete agreement is not achieved. For the small interval, theory agrees with experiment, but for the large interval, a deviation of about 3σ is present.