Precision spectroscopy of H_2^+ and antiprotonic helium atoms. Theory.

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Expansion in terms of α

Hydrogen atom (Dirac energy):

$$E_{nj}(\alpha) = \frac{m}{\sqrt{1+(Z\alpha)^2/\left(n-(j+1/2)+\sqrt{(j+1/2)^2-(Z\alpha)^2}\right)^2}}$$

$$\approx m\left[1 - \frac{(Z\alpha)^2}{n^2} + \frac{(Z\alpha)^4}{2n^3}\left(\frac{3}{4n}-\frac{1}{j+1/2}\right)\right.$$

$$\left. -\frac{(Z\alpha)^6}{8n^3}\left(\frac{5}{2n^3}-\frac{6}{n^2(j+1/2)}+\frac{3}{n(j+1/2)^2}+\frac{1}{(j+1/2)^3}\right) + \dots\right]$$

General quantum electrodynamics case:

$$E(\alpha) = M + \alpha^2 E_{nr} + \alpha^4 F_{40} + \alpha^5 \left(\ln\alpha F_{51} + F_{50}\right)$$

$$+\alpha^6 \left(\ln^2\alpha F_{62} + \ln\alpha F_{61} + F_{60}\right) + \dots$$

Nonrelativistic energies.
Modern status of ”computer“ limits.

Nonrelativistic energies

Helium ground state

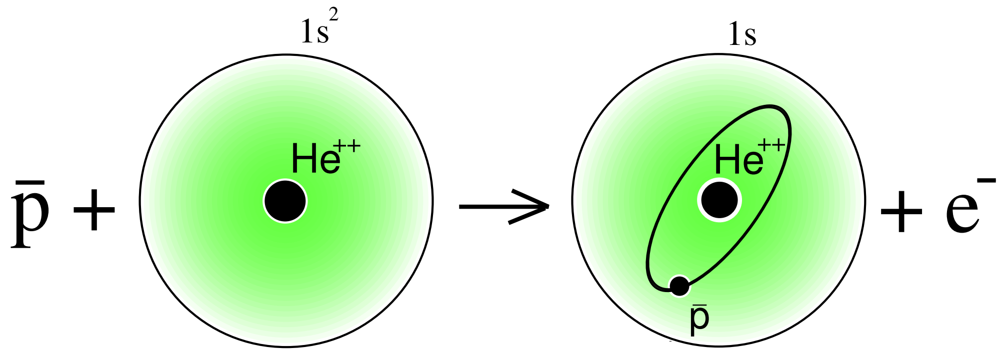
$E_{\mathrm{He}} = -2.90372\,43770\,34119\,59831\,11592\,45194\,40444_6$ Schwartz, 2002

Hydrogen molecular ion H_2^+ ground state

$E_{\mathrm{H}_2^+} = -0.59713\,90631\,23405\,07483\,41340\,9602_6$ Yan, 2007

Constants used: $M_p = 1\,836.152\,701\;m_e$.

Antiprotonic helium



Formation of an antiprotonic helium atom, $\bar{p}$He$^+$.

In [Phys. Lett. **9**, 65 (1964)] Condo suggested that some part of negatively charged massive particles occupies circular or nearly circular orbits, (n, l) with $l \approx n - 1$.

In this case, in order to remove the ≈ 25 eV binding energy of the electron, $\bar{p}$ has to change orbital angular momentum by several units. This makes such states stable against Auger decay

$$\bar{p}\text{He}^+ \to \bar{p}\text{He} + e^- .$$

Thus the only channel to cascade down for an atom is the slow radiative decay (∼1–3 μs).

The strong interaction plays no role.

Leading relativistic and radiative corrections.

Nonrelativistic QED

The Lagrangian for NRQED is built out nonrelativistic (two-component) Pauli spinor fields ψ for each of the electron, positron, muon, proton, etc. Photons are treated in the same fashion as in QED.

$$L_{\text{eff}} = -\frac{1}{2}(E^2 - B^2) + \psi_e^* \left(i\partial_t - e\varphi + \frac{\mathbf{D}^2}{2m} + \frac{\mathbf{D}^4}{8m^3} + \dots \right) \psi_e$$

$$+\psi_e^* \left(c_F \frac{e}{2m} \boldsymbol{\sigma}\mathbf{B} + c_D \frac{e}{8m^2} \{\mathbf{DE}\} + c_S \frac{ie}{8m^2} \{\mathbf{D}\cdot\mathbf{E}\times\boldsymbol{\sigma}\} \right) \psi_e$$

$$+ \text{ higher order terms } + \text{ muon, proton, etc.}$$

$$-\frac{d_1}{m_e m_\mu} (\psi_e^* \boldsymbol{\sigma} \psi_e) (\psi_\mu^* \boldsymbol{\sigma} \psi_\mu) + \frac{d_2}{m_e m_\mu} (\psi_e^* \psi_e) (\psi_\mu^* \psi_\mu) + \dots$$

where $\mathbf{D} = \boldsymbol{\nabla} + ie\mathbf{A}$.

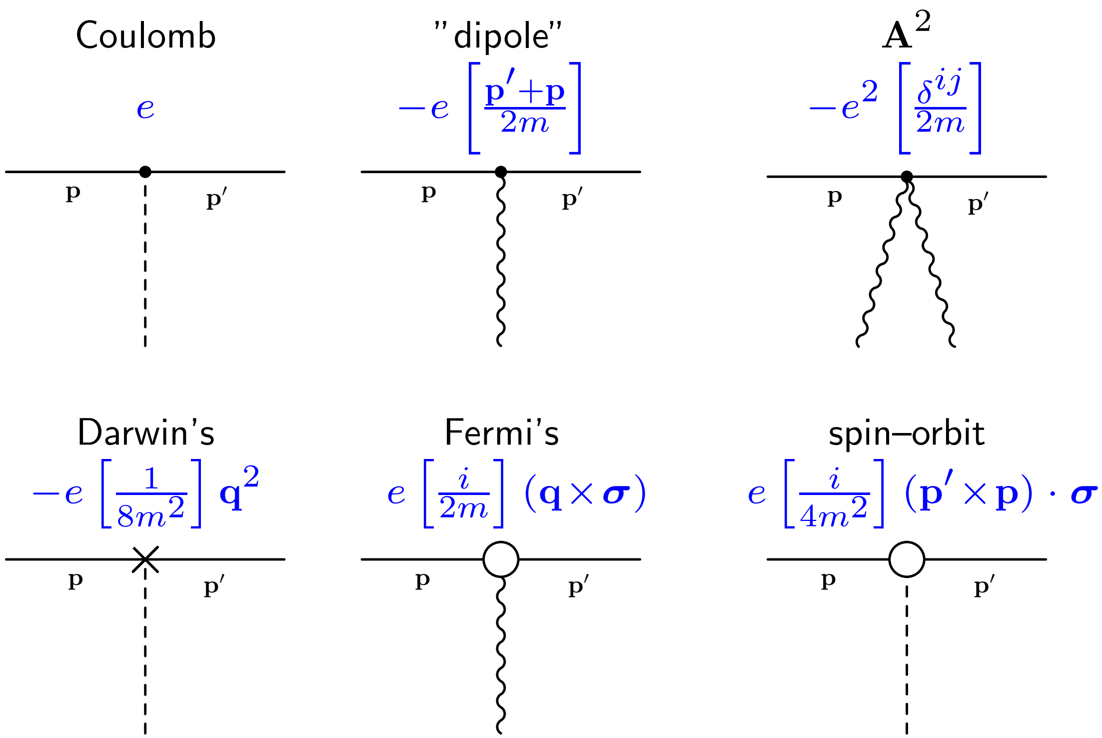
Requirements:

- coupling constants are determined by requiring that predictions of QED and NRQED agree to a desired order in (v/c);
- gauge invariance, hermiticity, locality, time reversal symmetry, parity conservation

Contributions from QED that involve relativistic loop momenta are absorbed into NRQED in a form of various local interactions.

Examples of basic interactions in NRQED

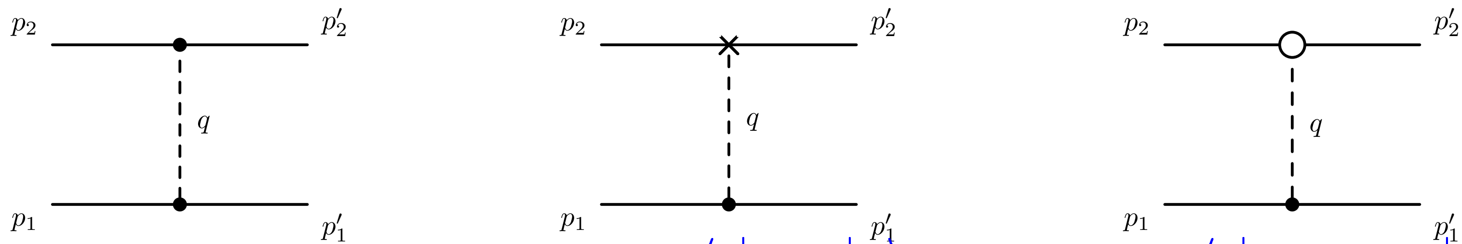
Examples of basic interactions are illustrated by Feynman diagrams for NRQED.



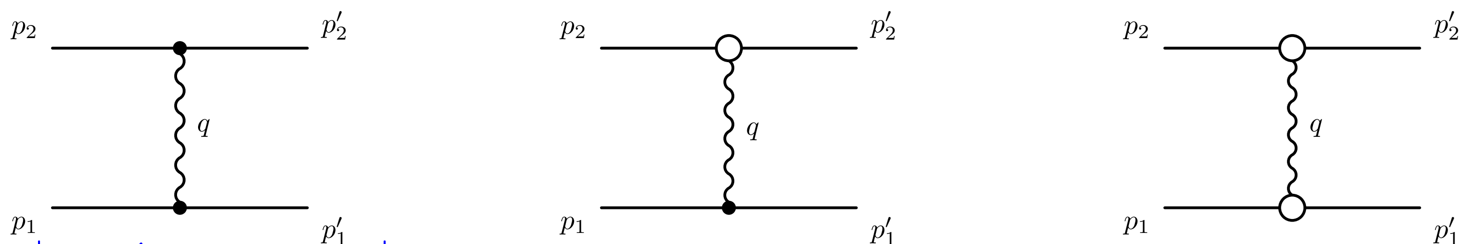
Here $\mathbf{q}=\mathbf{p}'-\mathbf{p}$ is a transferred impulse of the particle.

Breit-Pauli Hamiltonian

Let us consider diagrams of NRQED, which result in a contribution of order $m\alpha^4$:



$$e^2 \left\langle i \left| \frac{1}{\mathbf{q}^2} \right| f \right\rangle \qquad -e^2\, c_D^{(2)} \left\langle i \left| \frac{1}{8m_2^2} \right| f \right\rangle \qquad e^2\, c_S^{(2)} \left\langle i \left| \frac{i\boldsymbol{\sigma}_2[\mathbf{q}\times\mathbf{p}_2]}{4m_2^2\mathbf{q}^2} \right| f \right\rangle$$



$$-e^2 \left\langle i \left| \frac{p_1^i p_2^j}{m_1 m_2} \left(\frac{\mathbf{q}^2 - q_i q_j}{\mathbf{q}^4} \right) \right| f \right\rangle \qquad e^2\, c_F^{(2)} \left\langle i \left| \frac{i\boldsymbol{\sigma}_2[\mathbf{q}\times\mathbf{p}_1]}{2m_1 m_2\mathbf{q}^2} \right| f \right\rangle \qquad e^2\, c_F^{(1)}\, c_F^{(2)} \left\langle i \left| \frac{[\mathbf{q}\times\boldsymbol{\sigma}_1][\mathbf{q}\times\boldsymbol{\sigma}_2]}{4m_1 m_2\mathbf{q}^2} \right| f \right\rangle$$

On these diagrams the Coulomb propagator is expressed by $G^{00} = 1/\mathbf{q}^2$, and the transverse photon propagator for the exchange photons ($q_0 \approx m\alpha^2$) can be approximated by a three-dimensional form

$$G^{ij} = \frac{\delta_{ij} - q_i q_j/\mathbf{q}^2}{q^2 + i\varepsilon} \approx -\frac{1}{\mathbf{q}^2}\left[\delta_{ij} - \frac{q_i q_j}{\mathbf{q}^2}\right], \qquad i,j = 1,2,3.$$

QED corrections of order $m\alpha^5$ and $m\alpha^5(m/M)$

The complete spin independent contributions of order $m\alpha^5$ and $m\alpha^5(m/M)$ in case of a one electron molecular system can be presented as follows:

$$\Delta E^{(3)} = \alpha^3 \sum_i \left[\frac{4Z_i}{3} \left(-\ln\alpha^2 - \beta(L,v) + \frac{5}{6} - \frac{3}{8} - \frac{1}{5} \right) \langle \delta(\mathbf{r}_i) \rangle + \frac{2Z_i^2}{3M_i} \left(-\ln\alpha - 4\,\beta(L,v) + \frac{31}{3} \right) \langle \delta(\mathbf{r}_i) \rangle - \frac{14Z_i^2}{3M_i} Q(r_i) \right],$$

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. Here $\mathbf{J} = \sum_a z_a \mathbf{p}_a / m_a$ is the electric current density operator of the system, and $Q(r)$ is the Q-term introduced by Araki and Sucher

$$Q(r) = \lim_{\rho\to 0} \left\langle \frac{\Theta(r-\rho)}{4\pi r^3} + (\ln\rho + \gamma_E)\delta(\mathbf{r}) \right\rangle.$$

Denominator in $\beta(L,v)$ can be expanded as follow:

$$\langle 0|[\mathbf{J}[H_0,\mathbf{J}]]|0\rangle = -4\pi \sum_{i>j} z_i z_j \left(\frac{z_i}{m_i} - \frac{z_j}{m_j} \right)^2 \langle \delta(\mathbf{r}_{ij}) \rangle.$$

Higher order QED corrections.

Spin averaged relativistic corrections of order $R_\infty\alpha^4$.

Effective Hamiltonian in the order $m\alpha^6$:

$$H^{(6)} = \frac{p^6}{16m^5} + \frac{(\boldsymbol{\mathcal{E}}_1+\boldsymbol{\mathcal{E}}_2)^2}{8m^3} - \frac{3\pi}{16m^4}\Big\{p^2[\rho_1+\rho_2]+[\rho_1+\rho_2]p^2\Big\}
+\frac{5}{128m^4}\left(p^4V+Vp^4\right) - \frac{5}{64m^4}\left(p^2Vp^2\right).$$

Total contribution to the energy of order $m\alpha^6$:

$$\Delta E^{(6)} = \langle H_B Q(E_0-H_0)^{-1}QH_B\rangle + \left\langle H^{(6)}\right\rangle$$

Nonrelativistic Hamiltonian:

$$H_0 = \frac{p^2}{2m}+V, \qquad V = -\frac{Z_1}{r_1}-\frac{Z_2}{r_2}.$$

Breit–Pauli Interaction:

$$H_B = -\frac{p^4}{8m^3}+\frac{\pi}{2m^2}[Z_1\delta(\mathbf{r}_1)+Z_2\delta(\mathbf{r}_2)] + \left(Z_1\frac{[\mathbf{r}_1\times\mathbf{p}]}{2m^2r_1^3}+Z_2\frac{[\mathbf{r}_2\times\mathbf{p}]}{2m^2r_2^3}\right)\mathbf{s}\,,$$

Separation of divergent terms

We apply a transformation to the Breit-Pauli second order term:

$$\begin{cases} H'_B = H_B + (H_0 - E_0)U + U(H_0 - E_0) \\ \left\langle H_B Q(E_0 - H_0)^{-1} Q H_B \right\rangle = \\ \qquad = \left\langle H'_B Q(E_0 - H_0)^{-1} Q H'_B \right\rangle + \langle U H_B + H_B U \rangle - 2\langle U \rangle \langle H_B \rangle + \langle U(H_0 - E_0)U \rangle \end{cases}$$

with $U = \frac{1}{4m}[Z_1/r_1 + Z_2/r_2] = -\frac{1}{4m}V$.

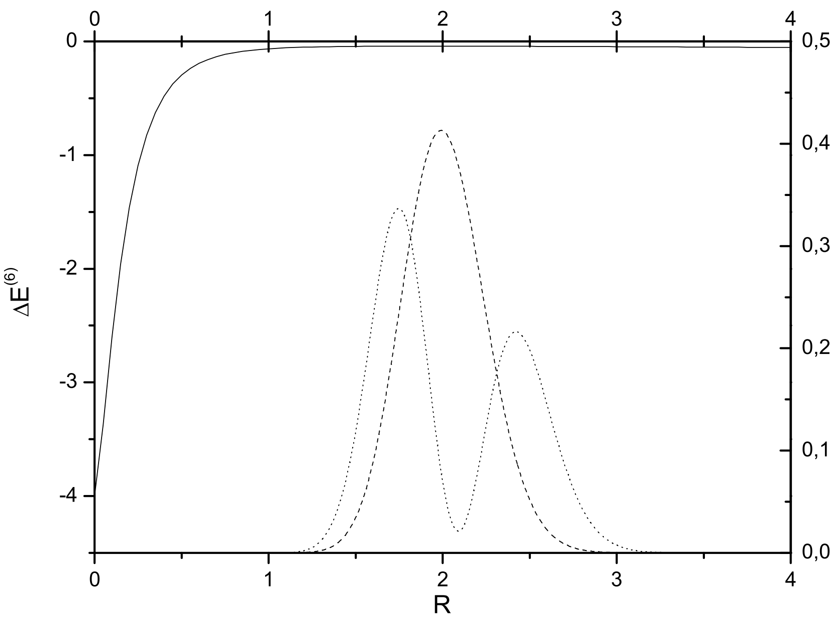
Using that Ψ_0 is a solution of the Schrödinger equation $H_0\Psi_0 = E_0\Psi_0$, one can gets:

$$\left\langle H^{(6)} \right\rangle + \left\langle H'^{(6)} \right\rangle = \frac{3E_0 \left\langle V^2 \right\rangle}{4m^2} - \frac{5E_0^2 \langle V \rangle}{4m^2} - \frac{3\pi E_0 \langle (\rho_1 + \rho_2) \rangle}{4m^3} + \frac{\left\langle \mathbf{p} V^2 \mathbf{p} \right\rangle}{8m^3} + \frac{\langle V \rangle \langle H_B \rangle}{2m} + \frac{E_0^3}{2m^2}$$

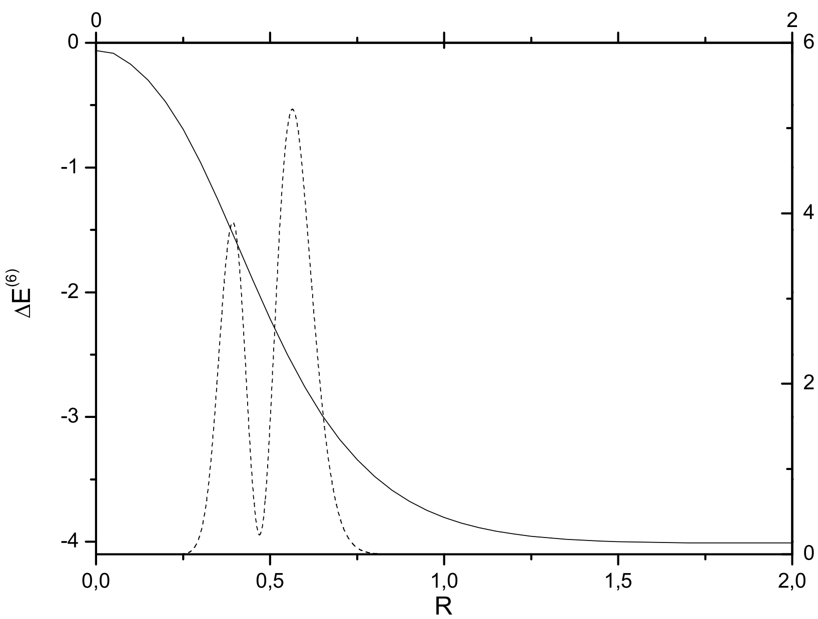
where $\rho_i = Z_i \delta(\mathbf{r}_i)$.

"Effective" potentials and wave functions.

H_2^+ molecular ion



Antiprotonic Helium



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

Some higher order corrections (radiative corrections) in the *external field* approximation are known in an analytic form [Sapirstein, Yennie, 1990]:

$$E^{(4)}_{se} = \alpha^4\frac{4\pi}{m_e^2}\left(\frac{139}{128}-\frac{1}{2}\ln 2\right)\left\langle Z_1^2\delta(\mathbf{r}_1)+Z_2^2\delta(\mathbf{r}_2)\right\rangle,$$

$$E^{(4)}_{anom} = \alpha^2\frac{\pi}{m_e^2}\left[\left(\frac{\alpha}{\pi}\right)^2\left(\frac{197}{144}+\frac{\pi^2}{12}-\frac{\pi^2}{2}\ln 2+\frac{3}{4}\zeta(3)\right)\right]\left\langle Z_1\delta(\mathbf{r}_1)+Z_2\delta(\mathbf{r}_2)\right\rangle,$$

$$E^{(4)}_{vp} = \frac{4\alpha^3}{3m^2}\left[\frac{5\pi\alpha}{64}\right]\left\langle Z_1^2\delta(\mathbf{r}_1)+Z_2^2\delta(\mathbf{r}_2)\right\rangle,$$

$$E^{(4)}_{2loop} = \frac{\alpha^4}{m_e^2\pi}\left[-\frac{6131}{1296}-\frac{49\pi^2}{108}+2\pi^2\ln 2-3\zeta(3)\right]\left\langle Z_1\delta(\mathbf{r}_1)+Z_2\delta(\mathbf{r}_2)\right\rangle.$$

The last equation includes both Dirac form factor and polarization operator contributions.

Recoil corrections of order $R_\infty\alpha^4(m/M)$ are small and may be neglected.

Higher order radiative corrections in a nonrecoil limit. $R_\infty \alpha^5$

The electron ground state wave function to a good extent may be approximated by $\psi_e(\mathbf{r}_e) = C[\psi_{1s}(\mathbf{r}_1)+\psi_{1s}(\mathbf{r}_2)]$, where ψ_{1s} is the hydrogen ground state wave function. So, the most important $R_\infty \alpha^5$ order contributions can be evaluated using this approximate wave function and the expressions:

$$E^{(5)}_{se} = \alpha^5 \sum_{i=1,2} \left\{ \frac{Z_i^3}{m_e^2} \left[-\ln^2 \frac{1}{(Z_i\alpha)^2} + A_{61} \ln \frac{1}{(Z_i\alpha)^2} + A_{60} \right] \langle \delta(\mathbf{r}_i) \rangle \right\},$$

$$E^{(5)}_{2loop} = \frac{\alpha^5}{\pi m_e^2} [B_{50}] \left\langle Z_1^2 \delta(\mathbf{r}_1) + Z_2^2 \delta(\mathbf{r}_2) \right\rangle,$$

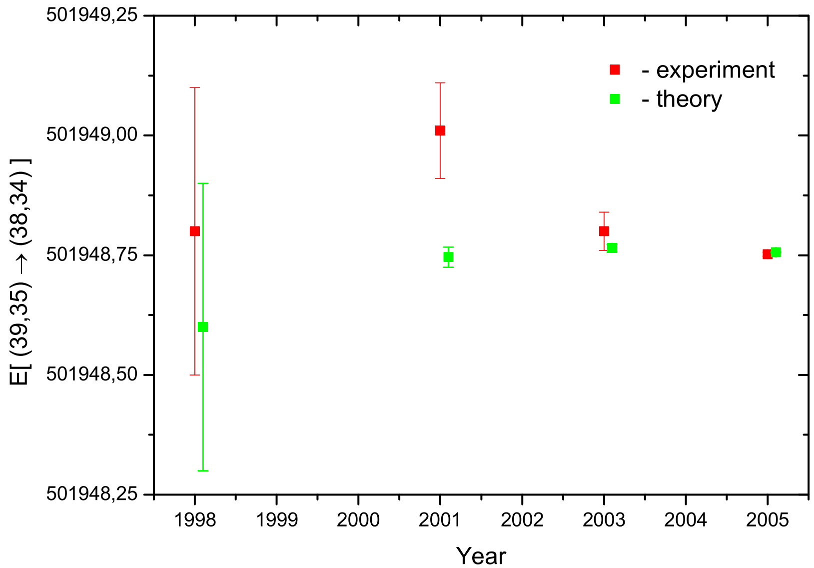
where the constants A_{61}, A_{60}, and B_{50} are taken equal to the constants of the $1s$ state of the hydrogen atom $A_{61} = 5.419\ldots$ [Lazer, 1960], $A_{60} = -30.924\ldots$ [Pachucki, 1993], and $B_{50} = -24.267\ldots$ [Pachucki, 1994; Eides, Shelyuto, 1995].

Summary

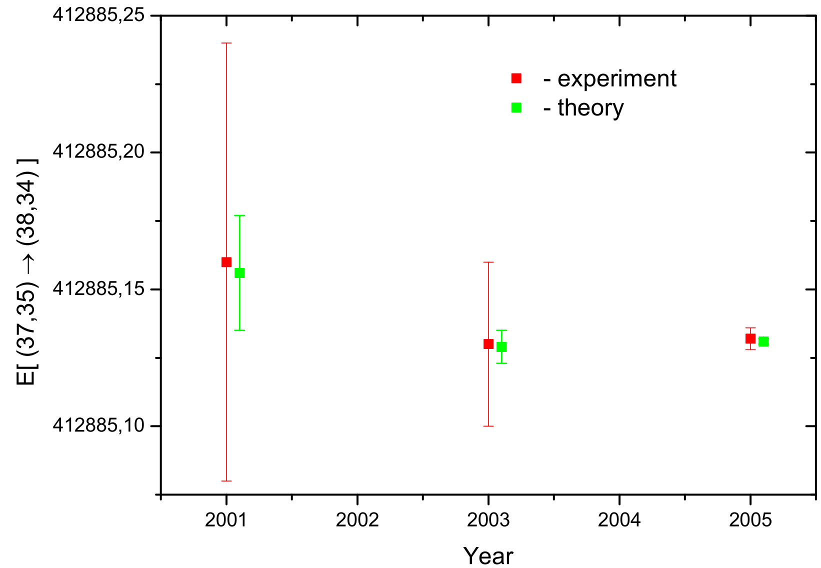
Hydrogen molecular ion. Contributions to the $(0,0)\to(0,1)$ transition energy.

	H_2^+	HD^+
ΔE_{nr}	65 687 511.0686	57 349 439.9717
ΔE_{α^2}	1091.041(03)	958.152(03)
ΔE_{α^3}	−276.544(02)	−242.118(02)
ΔE_{α^4}	−1.997	−1.748
ΔE_{α^5}	0.121(80)	0.106(70)
ΔE_{tot}	65 688 323.690(80)	57 350 154.368(70)

Improvement of theoretical and experimental precision in past years



The $(39,35) \rightarrow (38,34)$ transition



The $(37,35) \rightarrow (38,34)$ transition