Lecture 5

Further beyound the Dirac equation: isotope shift, parity violation effects



Plan of the lecture



- Isotope shift of energy levels: Mass and volume effects
 - Isotope shift in Ca⁺ ions
 - Analysis of DR spectra of heavy ions
- Parity violation in heavy ions
 - Nuclear spin independent effect
 - Parity violation in nuclei: Anapole moment



Energy levels of hydrogen-like ions



• OK, we did a rather long way... Are there further corrections to the energy levels?



Energy

Dirac energy levels

• So far we have discussed Dirac equation for <u>point-like</u>, <u>infinitely heavy</u> nucleus:

$$\left(-i\hbar c\boldsymbol{a}\cdot\nabla -\frac{Ze^2}{r}+m_ec^2\alpha_0\right)\psi(\boldsymbol{r})=E\psi(\boldsymbol{r})$$

- In reality, nucleus has some finite mass mass shift
 ... and finite size field shift
- Mass shift has been discussed already in non-relativistic quantum mechanics.
- We have to introduce *reduced* mass: $m_e \rightarrow \frac{m_e M}{m_e + M}$
- This leads only to shift (not splitting!) of energy levels, moreover:

$$\frac{m_e}{M_p} \approx \frac{1}{1836} \qquad \longrightarrow \qquad \frac{m_e}{M_U} < 0.000003$$



Filed shift

• To estimate volume effect we will use the well known approximation and assume that nuclear charge is uniformly distributed within a sphere of radius:



• In this model, electrostatic potential due to the nucleus deviates from pure Coulomb one and is given by:

$$V(r) = \begin{cases} \frac{Ze^2}{2R} \left(\frac{r^2}{R^2} - 3\right) & r \le R \\ -\frac{Ze^2}{r} & r > R \end{cases}$$
$$\left(-i\hbar c \boldsymbol{\alpha} \cdot \nabla + V(r) + m_e c^2 \alpha_0\right) \psi(\boldsymbol{r}) = E \psi(\boldsymbol{r})$$



Filed shift

• Let us re-write Dirac equation as:

$$\left(-i\hbar c\boldsymbol{\alpha}\cdot\nabla-\frac{Ze^2}{r}+m_ec^2\alpha_0+V'(r)\right)\psi(\boldsymbol{r})=E\psi(\boldsymbol{r})$$

perturbation

• Where "perturbation term" is: $V'(r) = \begin{cases} \frac{Ze^2}{2R} \left(\frac{r^2}{R^2} + \frac{2R}{r} - 3 \right) & r \le R \\ 0 & r > R \end{cases}$

First-order energy shift: $\Delta E = \left\langle \psi_{n\kappa m} \left| V' \right| \psi_{n\kappa m} \right\rangle \propto \frac{Z^2 R^4}{n^3}$



How to measure the isotope shift?



Is the electron-nucleus interaction just an interaction of two point-like charges, one of which (nucleus) is infinitely heavy?



V(r) =

The difference in the transition frequency for two isotopes with masses M_A and $M_{A'}$ and (mean square) nuclear radii:

$$\nu_A - \nu_{A'} = K \frac{M_A - M_{A'}}{M_A M_{A'}} + F \delta \langle r^2 \rangle_{AA'}$$

Isotope shift in Ca⁺ ion

Recently, high-precision measurements have been performed at the QUEST institute to compare isotope shifts for the $S_{1/2} \rightarrow P_{1/2}$ and $S_{1/2} \rightarrow P_{3/2}$ transitions in Ca⁺ ion.

These transitions exhibit different behavior with respect to the field shift.

 $f = \frac{F_{D2}}{F_{D2}}$

Theoretical model	f
Hydrogenic	1.0051
Dirac-Fock	1.0010
Dirac-Fock + Core Pol.	1.0009
CCSD	1.0029
CCSD(T)	1.0048
MBPT	1.0011
CI+MBPT	1.0014(4)
Experimental value	1.0085(12)
	Theoretical model Hydrogenic Dirac-Fock Dirac-Fock + Core Pol. CCSD CCSD(T) MBPT CI+MBPT Experimental value

What is the reason for this big disagreement between experiment and theory? Many-electron or nuclear effects? QED?

Dielectronic recombinations

 One may consider process reversed to Auger decay: dielectronic recombination

Very important for spectroscopic purposes: dielectronic recombination is resonant capture process!

$$T_{kin} + E_b = E^{**}$$

One can vary kinetic energy of electrons (or ion beam) and to study DR cross sections (rates).

 Example: DR of initially lithium-like bismuth ions Bi⁸⁰⁺

Physica Scripta. T92, 191-194, 2001

Dielectronic recobination

• Dielectronic recombination (DR) is a resonant process in which a free electron is captured into an ion under the simultaneous excitation of bound electron(s), and where the multiply excited ion is stabilized afterwards by photon emission.

Isotope shift measurements with heavy ions

• DR spectroscopy may help us to resolve (hyper) fine structure of ionic levels.

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- Parity violation in heavy ions
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Unified electro-weak interaction

Standard Model of FUNDAMENTAL PARTICLES AND INTERACTIONS

FERMIONS Leptons spin = 1/2			matter constituents spin = 1/2, 3/2, 5/2,		
			Quarks spin = 1/2		
Flavor	Mass GeV/c ²	Electric charge	Flavor	Approx. Mass GeV/c ²	Electric
ve electron neutrino	<1×10 ⁻⁸	0	U up d down	0.003	2/3
v_{μ} muon neutrino	< 0.0002	0	C charm	1.3	2/3
μ muon	0.106	-1	S strange	0.1	-1/3
v_{τ} tau neutrino	<0.02	0	t top	175	2/3
au tau	1.7771	-1	b bottom	4.3	-1/3

of the biggest One successes of the Standard Model is the unification of the electromagnetic and the weak forces into the socalled electroweak force.

Note that electromagnetic interaction preserves spatial parity while weak interaction – not!

Unified electro-weak interaction

Parity violation (PV) is first time observed in famous Wu experiment (1956) on the betadecay of cobalt nuclei.

Further extensions of the Standard Model ?

Is our knowledge about the Standard Model (and, in particular, about its electroweak segment) complete?

New **experimental results** from the LHC collaborations might indicate the existence of new particles beyond the SM:

- Di-photon bump at 750 GeV ?
- Charged Higgs boson in H \rightarrow tb decay ?
- W' in high-mass di-boson resonances?

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Various **theoretical extensions** of the standard model suggest the existence of additional W' and Z' bosons which can modify the parameters of the electroweak interaction.

The neutral weak interaction currents which lead to the parity-violating effects in atomic systems attract special attention!

Weinberg angle

Besides high–energy LHC experiments, precision electroweak measurements in **atomic physics** attract currently much attention since they allow to explore low–energy regime! Weinberg angle is one of the key parameters of the electroweak theory.

It describes how the photon and neural boson Z are "produced" from original vector bosons:

 $\binom{\gamma}{Z^0} = \begin{pmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{pmatrix} \binom{B^0}{W^0}$

This formula, again, shows that the weak and electromagnetic interactions are representations of the same force.

Parity of atomic states (just a reminder!)

The parity operator commutes with the (non-relativistic) Hamiltonian of the hydrogen-like atom.

Therefore eigenfunctions of the Hamiltonian, i.e. atomic wavefunctions, have particular symmetry properties:

 $\psi_{nlm}(\mathbf{r}) = R_{nl}(\mathbf{r}) Y_{lm}(\theta, \varphi), \qquad \hat{P}\psi_{nlm}(\mathbf{r}) = \psi_{nlm}(-\mathbf{r}) = (-1)^l \psi_{nlm}(\mathbf{r})$

S-, D-, G- atomic states have positive parity, while P-, F-, Hhave negative parity.

This is all true if interaction inside an atom is purely electromagnetic....

Parity violating interactions

The effective Hamiltonian of the PV electron- $H_{PV} = \frac{G_F}{\sqrt{2}} \left(-\frac{Q_W}{2} \gamma_5 + \frac{\kappa}{I} \alpha \cdot I \right) \rho(\mathbf{r})$ nucleus interaction can be cast in the form: The nuclear-spin-dependent (NSD) part Dominant part is the nuclear-spinindependent (NSI) interaction that arises comes mainly from the electromagnetic due to exchange of neutral Z⁰ boson interaction with weakly interacting between nucleus and electrons. nucleons. W,Z^0 \oplus Weak charge $Q_{\mu\nu}$ characterizes NSI part: • NSD is characterized by the coupling constant k: $Q_W = Z(1 - 4\sin^2\theta_W) - N$ $|\kappa| \approx \frac{|Q_W|}{100}$

How we can observe the parity-violating interactions?

Atomic parity violation

Total angular momenta "selection rules":

- Nuclear spin independent interaction mixes only states with the same J's
- Nuclear spin dependent interaction can mix levels with different J's but same F's
- If the parity is broken due to the weak interaction this transition becomes possible!

PV experiments with neutral atoms

PV experiments with neutral atoms have provided us with valuable information on the weak interaction.

But! Analysis of these experiments is rather difficult task because of "manyelectron nature" of systems.

- Alternatively, we may explore APV effects as appear in few-electron ions!
- Few-electron ions may be perfect candidates for PV studies:
 - Relatively simple atomic systems
 - Large electron-nucleus overlap
 - Effect scales as Z⁵ (in contrast to Z³ in neutral systems)
 - Levels with opposite parities might be almost degenerated

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PV experiments with few-electron ions

A large number of parity-violation studies have been proposed in the recent years for ions in different charge states: from singly-ionized to hydrogen-like.

We will discuss today two (rather simple) cases of the parity violation in heliumlike ions:

- Two-photon ${}^{1}S_{0} \rightarrow {}^{3}P_{0}$ transition (NSI mixing)
- Hyperfine-induced ${}^{1}S_{0} \rightarrow {}^{3}S_{1}$ transition (NSP mixing)

Helium-like ions (just a reminder!)

- Helium-like ions are among the most promising candidates for the PV studies in high-Z domain.
- To identify the states of this two-electron system we will use spectroscopic notations in the "jj-coupling" scheme as:

$$n_1 l_{1j_1} n_2 l_{2j_2}^{2S+1} L_J$$

- For example, ground state: $1s^{2} S_0$.
- Can we find in helium-like ions almost degenerate levels with opposite parity?

Parity-violation in helium-like ions

F. Ferro, A. Artemyev, Th. Stöhlker, and A. S., Phys. Rev. A **81** (2010) 062503 F. Ferro, A. Artemyev, Th. Stöhlker, and A. S., Can. J. Phys. **89** (2011) 73

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Many-electron calculations: Basics

 High-precision analysis of helium energy levels is a rather complicated task. We discuss here (very roughly and over-simplified!) just few important steps.

TABLE I. Contributions to the energies of the $1s2s {}^{1}S_{0}$ and $1s2p {}^{3}P_{0}$ states in He-like 238 U ions, relative to the ionization threshold. All energies are in eV.

	$1s2s^1S_0$	$1s2p^3P_0$
Dirac energy (pointlike nucleus)	-34 215.481	-34215.4811
Nuclear size effects ^a	37.738	4.4133
Total zeroth-order energy	-34 177.743(27)	-34211.0678(56)
First-order correlation [30]	850.135	923.198
Second-order correlation	-6.5368	-5.6726
Higher-order correlation	-0.0005	-0.0174
Total electron correlations	843.598(1)	917.508(4)
One-electron QED correction [26]	49.547(75)	6.846(12)
Two-electron QED correction [17]	-3.8259(4)	-4.4740(3)
Higher-order QED correction [14]	-0.009(51)	0.002(73)
Nuclear polarization and recoil correction [27]	0.0890	0.0491
Total energy	-33 288.344(94)	-33 291.137(74)

^aA Fermi distribution for the nuclear charge with rms radius $\langle r^2 \rangle^{1/2} = 5.8569(33)$ fm [28] was adopted.

Parity-violation in helium-like ions

How to measure this mixing?

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Induced two-photon transitions

Simple idea is to induce direct transition between two states of interest. But... both states have zero total angular momentum.

One has to induce two-photon transition:

$$1s2p \, {}^{1}S_{0} + \gamma + \gamma \rightarrow 1s2s \, {}^{3}P_{0}$$

Simultaneous absorption (or emission) of two photons is one of the most known second-order QED processes.

Analysis of two-photon transitions can be traced back to the second-order perturbation theory:

$$M_{2\gamma} = \sum_{\nu} \frac{\langle \widetilde{\Psi}_{P} | \boldsymbol{\alpha} \boldsymbol{A}_{1} | \Psi_{\nu} \rangle \langle \Psi_{\nu} | \boldsymbol{\alpha} \boldsymbol{A}_{2} | \widetilde{\Psi}_{S} \rangle}{E_{\nu} - E_{S} + \hbar \omega}$$

2-photon absorption

Two-photon transitions: Theory

A. S., P. Indelicato, J. P. Santos, P. Amaro, and S. Fritzsche, Phys. Rev. A **84** (2011) 022511 S. Fritzsche, A.S., and A. Volotka, New J. Phys. **17** (2015) 103009

Induced two-photon transitions

Induced two-photon transition rate:

$$\Gamma_{2\gamma} \propto I^2 \left| \sum_{\nu} \frac{\langle \widetilde{\Psi}_P | \boldsymbol{\alpha} \boldsymbol{A}_1 | \Psi_{\nu} \rangle \langle \Psi_{\nu} | \boldsymbol{\alpha} \boldsymbol{A}_2 | \widetilde{\Psi}_S \rangle}{E_{\nu} - E_S + \hbar \omega} \right|^2$$

Based on our many-body relativistic calculations we found that for helium-like uranium ion:

$$\Gamma_{2\gamma}(2E1) = I^2 \eta^2 (\boldsymbol{\epsilon}_1 \cdot \boldsymbol{\epsilon}_2)^2 \times 4.35 \cdot 10^{-20}$$
$$= I^2 (\boldsymbol{\epsilon}_1 \cdot \boldsymbol{\epsilon}_2)^2 \times 1.26 \cdot 10^{-33} \,\mathrm{s}^{-1}$$

Polarization vectors should be parallel!

 To "compete" with the spontaneous decay channel we have to induce two-photon E1E1 transition by <u>polarized light</u> with the intensity:

 $I \sim 10^{21} - 10^{22}$ W/cm²

PV experiments with few-electron ions

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Parity violating interactions

The effective Hamiltonian of the PV electron- $H_{PV} = \frac{G_F}{\sqrt{2}} \left(-\frac{Q_W}{2} \gamma_5 + \frac{\kappa}{I} \alpha \cdot I \right) \rho(\mathbf{r})$ nucleus interaction can be cast in the form: The nuclear-spin-dependent (NSD) part Dominant part is the nuclear-spinindependent (NSI) interaction that arises comes mainly from the electromagnetic due to exchange of neutral Z⁰ boson interaction with weakly interacting between nucleus and electrons. nucleons. W,Z^0 \oplus Weak charge $Q_{\mu\nu}$ characterizes NSI part: • NSD is characterized by the coupling constant k: $Q_W = Z(1 - 4\sin^2\theta_W) - N$ $|\kappa| \approx \frac{|Q_W|}{100}$

How we can observe the parity-violating interactions?

Nuclear spin-dependent PV effects

Nuclear spin-dependent PV Hamiltonian:

$$H_{PV,NSD} = \frac{G_F}{\sqrt{2}} \frac{\kappa}{I} \boldsymbol{\alpha} \cdot \boldsymbol{I} \rho(\boldsymbol{r})$$

Within the shell model, considering a single valence nucleon with orbital momentum / around a spherical core of constant density:

$$\kappa = \kappa_2 + \kappa_Q + \kappa_a$$

• The most important terms are anapole moment and $(V_e A_N)$ terms:

$$\kappa_{a} = \frac{K}{I+1} \cdot \frac{9}{10} g_{\nu} \mu_{\nu} \frac{\alpha}{m_{p} r_{0}} A^{2/3}$$
$$\kappa_{2} = \frac{1/2 - K}{I+1} \cdot C_{2\nu}$$

$$K = (I + 1/2)(-1)^{I+1/2-l}, \nu = P, N$$

Nuclear anapole moment

The effective one-body P-odd weak interaction between an unpaired nucleon and the nuclear core can then be obtained as:

$$\hat{W} = \frac{G}{2\sqrt{2}m_p} g[\boldsymbol{\sigma} \cdot \mathbf{p}\rho(r) + \rho(r)\boldsymbol{\sigma} \cdot \mathbf{p}]$$

where $\boldsymbol{\rho}$ is the density of core nucleons.

• Approximate analytical solution of the Hamiltonian $\widehat{H}=\widehat{H}_0+\widehat{W}$ is: $\psi={
m e}^{{
m i} hetam{\sigma}\cdot{
m r}}\psi_0$

The spin helix occurs due to the parity violating nucleon–nucleus interaction. The degree of spin rotation is proportional to the distance from the origin and the strength of the weak interaction.

Nuclear anapole moment

It was shown that within the nuclear shell model:

$$\kappa_{a} = \frac{K}{I+1} \cdot \frac{9}{10} g_{\nu} \mu_{\nu} \frac{\alpha}{m_{p}r_{0}} A^{2/3}$$
Parameter describing hadronic PV interaction between valence nucleon and nuclear core a valence nucleon

• The PV NN interaction is typically parameterized using the meson-exchange picture of Desplanques, Donoghue, and Holstein (DDH) which describes the constants g_{ν} in terms of the following combination of meson–nucleon parity non-conserving interaction constants:

$$g_{p} = 2.0 \times 10^{5} W_{\rho} \left[176 \frac{W_{\pi}}{W_{\rho}} f_{\pi} - 19.5 h_{\rho}^{0} - 4.7 h_{\rho}^{1} + 1.3 h_{\rho}^{2} - 11.3 (h_{\omega}^{0} + h_{\omega}^{1}) \right]$$
$$g_{n} = 2.0 \times 10^{5} W_{\rho} \left[-118 \frac{W_{\pi}}{W_{\rho}} f_{\pi} - 18.9 h_{\rho}^{0} + 8.4 h_{\rho}^{1} - 1.3 h_{\rho}^{2} - 12.8 (h_{\omega}^{0} - h_{\omega}^{1}) \right]$$

Cs experiment: DDH "h nd effective coupling constants (g) at DDH values for the meson-nucleon coupling $f_{\pi} = [7 \pm 2] \times 10^{-7}$ h_{ω}^{0} h^1_{ω} h_{ρ}^{1} h_{ρ}^2 fπ ho g_{pn} g_{np} $g_{pp} = g_{nn}$ g_p g_n -11.4-0.19-9.5-1.9-1.16.5 -2.21.5 4.5 0.2

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Parity-violation in helium-like ions

Owing to the (spin-dependent) part of PV Hamiltonian, the $2^{1}S_{0}$ atomic state in He-like ions with nuclear spin $I \neq 0$ can be described as:

$$|1s \ 2s \ {}^{1}S_{0}, F = I\rangle + i\eta |1s \ 2p \ {}^{3}P_{1}, F = I\rangle$$

Mixing coefficient (for ⁷⁷Se) is $\eta \propto 10^{-9}$.

Towards analysis of nuclear PV effects

Novel schemes for studying the nuclear-spindependent part of the atomic parity violation have been also proposed.

Probability of the induced $1s2s {}^{1}S_{0} \rightarrow 1s 2s {}^{3}S_{1}$ transition in He-like ions: $\Gamma_{\lambda}(M1 + E1) = (2I + 1) \cdot \Gamma_{M1} \cdot (1 + \lambda A)$ parity-preserving rate (M1)

Asymmetry coefficient $A = (\Gamma_+ - \Gamma_-)/(\Gamma_+ + \Gamma_-)$ is directly related to the nuclear-spin dependent mixing parameter: $A \propto \eta/(2I + 1)$

For medium-Z ions the asymmetry reaches $A \propto 10^{-7}$!

Nuclear PV effects: Estimates

- Based on the predictions of the Standard Model we have estimated the size of the expected asymmetry for several isotopes.
- Stable isotope of ⁷⁷Se seems to be most convenient for the study.

Ion	$t_{1/2}$	Ι	μ	$10^{-7} \mathcal{A}$
⁷⁰ ₃₃ As	53 min	4	2.106 100	0.801 74
⁷¹ ₃₃ As	65.3 h	5/2	1.673 500	1.25177
⁷² ₃₃ As	26 h	2	-2.156600	1.278 89
⁷⁴ ₃₃ As	17.78 d	2	-1.597000	1.335 09
⁷⁵ ₃₃ As	stable	3/2	1.439 475	2.08691
⁷⁶ ₃₃ As	26.3 h	2	-0.906000	1.403 86
⁷³ ₃₄ Se	7.1 h	9/2	0.8700 000	0.623 39
⁷⁵ ₃₄ Se	118.5 d	5/2	0.6700 000	1.08438
⁷⁷ ₃₄ Se	stable	1/2	0.535 0422	4.663 09
⁷⁹ Se	65000 yr	7/2	-1.0180000	0.78713

- To induce M1+E1 (PV) transition in He-like Se we need to apply circularly polarized light of:
 - energy 43.85 eV (extreme ultraviolet)
 - intensity $I \propto 10^{12} 10^{13} \text{ W/cm}^2$ (to "compete" with the spontaneous E1E1 decay)

F. Ferro, A. S., and Th. Stöhlker, Phys. Rev. A 83 (2011) 052518

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