Max-Planck-Institut für Kernphysik

Status of theoretical calculations
Re n=5 $\rightarrow$ n=4 x-rays

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Outline

Dirac equation

- finite size effects & numerical solutions
- QED corrections
  - Uehling potential
  - Wichmann-Kroll + Källen-Sabry potentials
  - self energy
- interaction with atomic electrons

Hyperfine interactions

- electric quadrupole interaction
- quadrupole vacuum polarization
- higher order corrections & nuclear polarization

Re $n{=}5 \rightarrow n{=}4$ x-rays

Dirac equation for muonic atoms

- transition energies & probabilities of bound muon needed

- Dirac equation:
  $\left(c\,\boldsymbol{\alpha}\cdot\mathbf{p}+\beta\,m_\mu c^2+V(\mathbf{r})\right)|\psi\rangle = E\,|\psi\rangle$

- nuclear potential $V(\mathbf{r})$
  point like:

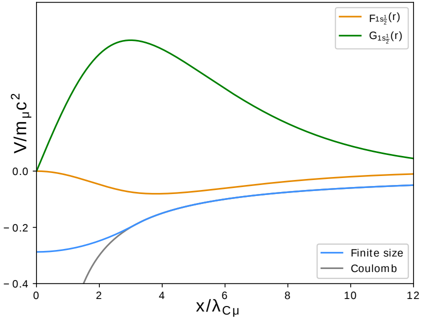
$$V_C(\mathbf{r}) = -\frac{Z\alpha}{r}$$

  finite size:

$$V(\mathbf{r}) = -Z\alpha\int \mathrm{d}^3\mathbf{r}'\,\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

- length scale - Bohr radius:

$$r_{B\mu} = \frac{\hbar}{m_\mu c Z\alpha}$$



Unperturbed muonic states

Dirac equation:

$$\left(c\,\boldsymbol{\alpha}\cdot\mathbf{p} + \beta\, m_\mu c^2 + V_0(r)\right)|n\kappa m\rangle = E_{n\kappa}\,|n\kappa m\rangle$$

spherically symmetric part of nuclear potential:

$$V_0(r_\mu) = -Z\alpha \int \mathrm{d}^3\mathbf{r}'\,\frac{\rho(\mathbf{r}')}{\max(\mathrm{r},\mathrm{r}')}$$

$\Downarrow$

$\rightarrow$ solution of radial Dirac eq. for $\langle r|n\kappa m\rangle = \frac{1}{r}\begin{pmatrix} G_{n\kappa}(r)\,\Omega_{\kappa m} \\ i\,F_{n\kappa}(r)\,\Omega_{-\kappa m}\end{pmatrix}$

$\Downarrow$

$\rightarrow$ solve with B-spline-based dual kinetic balance method.

V.M. Shabaev *et. al.*, Phys. Rev. Lett. **93**, 130405 (2004)

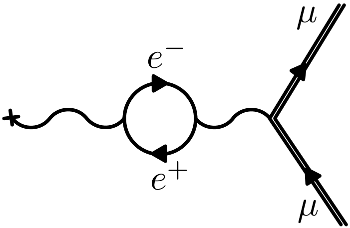
$\Downarrow$

$\rightarrow$ complete spectrum $E_{n\kappa}$

$+$ wave functions $G_{n\kappa}(r)$, $F_{n\kappa}(r)$ (numerically) available

Vacuum polarization order $\alpha(Z\alpha)$: Uehling potential

- correction to Coulomb potential at small distances
- electronic loop less surpressed (smaller mass)
- inclusion of Uehling potential: $V^{(0)}(r_\mu) \to V^{(0)}(r_\mu) + V_{\text{Uehl}}(r_\mu)$ in Dirac eq.



$$V_{\text{Uehl}}(r) = -\frac{2\alpha(\alpha Z)}{3\pi}\int_0^\infty \mathrm{d}\mathbf{r}'\rho(\mathbf{r}')\int_1^\infty \mathrm{dt}\left(1+\frac{1}{2\mathrm{t}^2}\right)$$
$$\times\frac{\sqrt{t^2-1}}{t^2}\,\frac{\exp(-2\mathrm{m_e}|\mathrm{r}-\mathrm{r}'|\mathrm{t})-\exp(-2\mathrm{m_e}(\mathrm{r}+\mathrm{r}')\mathrm{t})}{4m_e rt}$$

Fullerton, Rinker, PRA **13**, 1283 (1976)

Vacuum polarization order $\alpha(Z\alpha)^3$ and $\alpha^2(Z\alpha)$: Wichmann-Kroll and Källen-Sabry potential

Uehling potential is first order in α and $Z\alpha$

higher order vacuum polarization:

- increase interactions with nuclear potential $(Z\alpha)$
  $\rightarrow$ Next order: Wichmann-Kroll potential
- increase loops (α)
  $\rightarrow$ Next order: Källen-Sabry potential

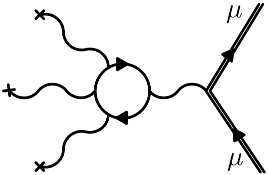
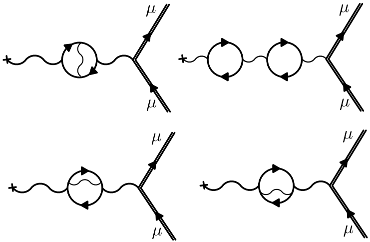


Diagram for $\alpha(Z\alpha)^3$ Wichmann-Kroll potential (point like)
Blomqvist, Nucl. Phys B **48**, 95 (1972)
Huang, Phys. Rev. A **14**, 1311 (1976)
Vogel, At. Dat. Nucl.Dat. Tab. **14**, 599 (1974)



Diagrams for $\alpha^2(Z\alpha)$ Källen-Sabry potential
P. Indelicato, Phys. Rev. A **87**, 022501 (2013)

Overview: QED corrections for ^{185}Re

QED corrections of different order in α and $Z\alpha$ for ^{185}Re:
(all energies in keV)

μ state	Dirac Eq.	$\alpha(Z\alpha)$	$\alpha^2(Z\alpha)$	$\alpha(Z\alpha)^3$	α SE
$1s1/2$	9323.87	60.79	0.50	-0.75	-2.90
$2s1/2$	3083.21	16.77	0.12	-0.25	-0.56
$2p1/2$	4031.20	26.42	0.21	-0.34	-0.32
$2p3/2$	3884.09	24.26	0.19	-0.31	-0.55
$3s1/2$	1418.64	7.72	0.06	-0.13	-0.20
$3d5/2$	1765.13	8.91	0.06	-0.13	-0.08

$\Rightarrow$ additional contributions:
- $\rightarrow$ muonic VP
- $\rightarrow$ mixed quadrupole VP
- $\rightarrow$ hadronic VP

Interaction with atomic electrons

Muonic binding energies depend on atomic electrons

$\Downarrow$

Screening potential:

$$V_e(\vec{r}_\mu) = -\alpha \int \mathrm{d}V \, \frac{\rho_e(\vec{r})}{|\vec{r}_\mu - \vec{r}|},$$

$$\rho_e(\vec{r}) = \sum_i \psi^\dagger_{e_i}(\vec{r}) \cdot \psi_{e_i}(\vec{r})$$

$\Downarrow$

Muon also screens one unit of nuclear charge:

- replace $Z \to Z - 1$ for electronic solutions
- 3-step calculation: muon - electron - muon

  P. Vogel, *Phys. Rev. A* **7**, 63 (1973)

$\Downarrow$

low lying muonic states: essentially H-like

Overview: electron screening

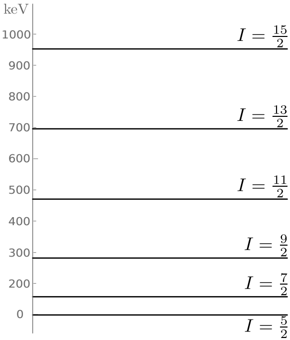
non-constant part for muonic ^{185}Re:
all energies in eV

μ-state	$n{=}1$ electrons	$n{=}1,2$ electrons
(constant)	4778	9361
$1s_{1/2}$	0	0
$2s_{1/2}$	-10.6	-12.4
$3s_{1/2}$	-40.2	-47.0
$4d_{3/2}$	-62.5	-73.2
$4d_{5/2}$	-64.0	-75.0
$4f_{5/2}$	-48.1	-56.4
$4f_{7/2}$	-49.0	-57.4
$5f_{5/2}$	-123.5	-144.6
$5f_{7/2}$	-124.8	-146.1
$5g_{7/2}$	-98.0	-114.8
$5g_{9/2}$	-98.8	-115.7

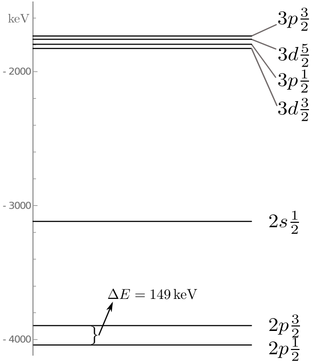
Hyperfine interactions

Additional nuclear structure effects: dynamical hyperfine structure

discrete nuclear states in $^{185}_{75}$Re:



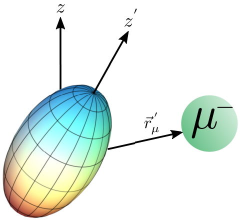
fine structure of bound muon in $^{185}_{75}$Re:



$\rightarrow$ Muonic fine structure and nuclear rotational states on similar scale

$\rightarrow$ Muonic transitions can excite nucleus!

Electric interaction between muon and nucleus



Muonic atom:

- muon as Dirac particle
- nucleus as symmetric rigid rotor
- electric interaction between nucleus and muon:

$$V(\mathbf{r}_\mu, \vartheta_N, \varphi_N) = -Z\alpha \int \mathrm{d}^3\mathbf{r}'_\mathrm{N} \, \frac{\rho(\mathbf{r}'_\mathrm{N})}{\left|\mathbf{r}'_\mu - \mathbf{r}'_\mathrm{N}\right|}$$

- expansion in multipole components

$$V(\mathbf{r}_\mu, \vartheta_N, \varphi_N) = V_0(r_\mu) + V_2(\mathbf{r}_\mu, \vartheta_N, \varphi_N) + \text{higher orders}$$

where $\quad V_0(r_\mu) = -Z\alpha \int \mathrm{d}^3\mathbf{r}'_\mathrm{N} \, \frac{\rho(\mathbf{r}'_\mathrm{N})}{\max(\mathrm{r}_\mu, \mathrm{r}_\mathrm{N})};$

$$V_2(\mathbf{r}_\mu, \vartheta_N, \varphi_N) = -Z\alpha \frac{4\pi}{5} \int dV_N' \; \rho(\vec{r}_\mu{}') \frac{r_<^2}{r_>^3} P_2(\cos\vartheta') \sum_{m=-2}^{2} \mathsf{Y}^*_{2m}(\beta, \alpha) \mathsf{Y}_{2m}(\vartheta_\mu, \varphi_\mu)$$

Dynamical hyperfine structure

- strong quadrupole interaction between $2p$ and $3d$ doublets
- nuclear excited rotational states on same scale
- diagonalise quadrupole interaction for every F value

$\rightarrow {}^{185}$Re with $I \in \{\frac{5}{2}, \frac{7}{2}, \frac{9}{2}\}$ + muonic $(2p\frac{1}{2}, 2p\frac{3}{2}) \rightarrow F \in \{1, ..., 6\}$

$F = 1$
- $2p^{3}/2$, $I = 5/2$

$F = 2$
- $2p^{1}/2$, $I = 5/2$
- $2p^{3}/2$, $I = 5/2$
- $2p^{3}/2$, $I = 7/2$

$F = 3$
- $2p^{1}/2$, $I = 5/2$
- $2p^{3}/2$, $I = 5/2$
- $2p^{1}/2$, $I = 7/2$
- $2p^{3}/2$, $I = 7/2$
- $2p^{3}/2$, $I = 9/2$

$F = 4$
- $2p^{1}/2$, $I = 7/2$
- $2p^{3}/2$, $I = 5/2$
- $2p^{1}/2$, $I = 9/2$
- $2p^{3}/2$, $I = 7/2$
- $2p^{3}/2$, $I = 9/2$

$F = 5$
- $2p^{1}/2$, $I = 9/2$
- $2p^{3}/2$, $I = 9/2$
- $2p^{3}/2$, $I = 7/2$

$F = 6$
- $2p^{3}/2$, $I = 9/2$

Uehling-quadrupole interaction

- Uehling potential for deformed charge distribution:

$$V_{\text{uehl}}(\mathbf{r}_\mu) = -Z\alpha\frac{2\alpha}{3\pi}\int \mathrm{d}^3\mathbf{r}_\mathrm{N}\,\rho(\mathbf{r}_\mathrm{N})\frac{\mathrm{K}_1(2\mathrm{m}_\mathrm{e}|\mathbf{r}_\mu - \mathbf{r}_\mathrm{N}|)}{|\mathbf{r}_\mu - \mathbf{r}_\mathrm{N}|},$$

where

$$K_n(x) = \int_1^\infty \mathrm{d}t\,\mathrm{e}^{-xt}\left(\frac{1}{t^3} + \frac{1}{2t^5}\right)\sqrt{t^2-1}\,t^n.$$

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- analogous to classical electrodynamics:

$$\frac{1}{|\mathbf{r}_\mu - \mathbf{r}_N|} = \sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}\sum_{m=-l}^{l}\mathrm{C}^*_{\mathrm{lm}}(\vartheta_\mathrm{N},\varphi_\mathrm{N})\mathrm{C}_{\mathrm{lm}}(\vartheta_\mu,\varphi_\mu),$$

$$\frac{K_1(2m_e|\mathbf{r}_\mu - \mathbf{r}_N|)}{|\mathbf{r}_\mu - \mathbf{r}_N|} = \sum_{l=0}^{\infty}c_l(r_\mu, r_N)\sum_{m=-l}^{l}\mathrm{C}^*_{\mathrm{lm}}(\vartheta_\mathrm{N},\varphi_\mathrm{N})\mathrm{C}_{\mathrm{lm}}(\vartheta_\mu,\varphi_\mu)$$

- $l=2$ term: Uehling correction to quadrupole interaction (arXiv:1809.06623)
  ^{185}Re: ≤ 410 eV
  ^{235}U: ≤ 910 eV

Nuclear polarization correction

after diagonalization of finestructure doublet and nuclear rotational band:
residual corrections of energy levels by

1. muonic states except finestructure doublet
2. nuclear states except ground state rotational band

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1. 2nd order perturbation theory, considering quadrupole interaction:

$$\Delta E = \sum_{\beta \notin M} \frac{\langle F\alpha|\mathrm{H_Q}|\mathrm{F}\beta\rangle^2}{E_{F\alpha} - E_{F\beta}}$$

$^{185}_{75}$Re	ΔE/keV
$(1s\frac{1}{2})$ states	≤ 3.2 keV
$(2p\frac{1}{2}, 2p\frac{3}{2})$ states	≤ 2.5 keV
$(3d\frac{3}{2}, 3d\frac{5}{2})$ states	≤ 0.2 keV

(arXiv:1809.06623)

Nuclear polarization correction

after diagonalization of finestructure doublet and nuclear rotational band: residual corrections of energy levels by

1. muonic states except finestructure doublet
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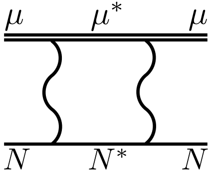
2. nuclear polarization corrections

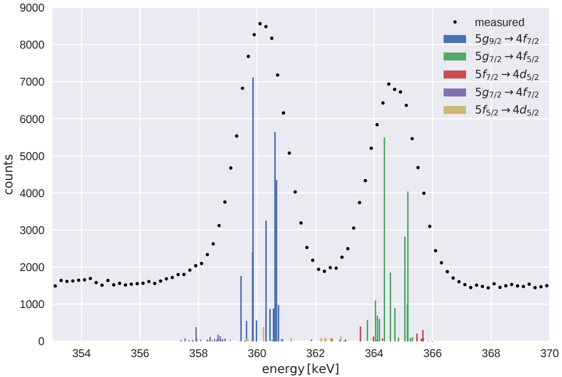


→advanced nuclear model or nuclear data needed!

Fitting of Re $n=5 \to n=4$ x-rays

- theoretical prediction of Q-dependence for $(5g, 5f) \to (4f, 4d)$
- including finite size, vacuum polarization, self energy, electric quadrupole, magnetic dipole, recoil
- quadratic fit of energies and intensities

$$\Delta E^{if}(Q) = \Delta E_0^{if} + \Delta E_1^{if} Q + \Delta E_2^{if} Q^2,$$
$$I^{if}(Q) = I_0^{if} + I_1^{if} Q + I_2^{if} Q^2.$$



Summary

- ab initio approach for given charge distribution

  including:
  - QED (Uehling + higher order)
  - electron screening
  - electric quadrupole interaction
  - magnetic dipole interaction
  - dynamical hyperfine structure

- quadratic fit for Q-dependence of Re $n{=}5 \to n{=}4$ x-rays

- outlook:
  - Nuclear polarization corrections needed for low-lying states

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Thank you for your attention!

Backup

Comparison with experimental spectra

- experimentally accessible: transition energies between states
- in principle large number of transitions
- consider observed intensity of lines
  $I_{\alpha\to\beta} = P_\alpha T_{\alpha\to\beta}$
  P_α: population of state α
  $T_{\alpha\to\beta}$: transition probability from α to β

transition probabilities

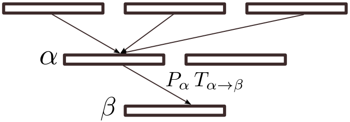
- selection rules - E1 transition dominant

For state $|FM\alpha\rangle = \sum_i a_i^{(\alpha)} |FM(n\kappa)_i(IK)_i\rangle$:

$$T_{\alpha\to\beta} = \sum_{M_1,M_2,M} \left\langle F_1M_1\alpha|\hat{T}_{JM}|F_2M_2\beta\right\rangle^2 \tag{1}$$

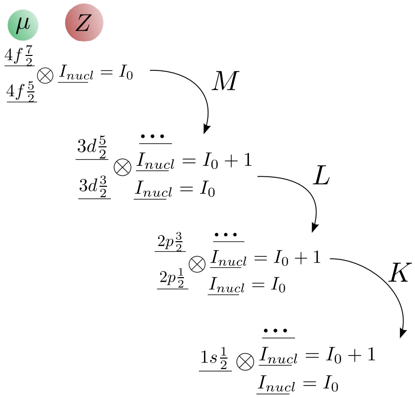
population

- depends on previous transitions
- demands cascade calculations



Comparison with experimental spectra

- muon capture
  if $r_{n_\mu, B\mu} = r_{B\,e}$
  $\rightarrow n_\mu = \sqrt{m_\mu / m_e} \approx 14$
- no control of population
  assumption:
  initially statistical populated
  $\sim 2F + 1$
- cascade towards muonic
  ground state



main cascade: $4f \rightarrow 3d \rightarrow 2p \rightarrow 1s$
$\rightarrow$ S. Devons et al., Muonic atoms, in Adv. in Nucl. Phys.: Vol. 2
$\rightarrow$ electric dipole transitions with $(n, l = n-1) \rightarrow (n-1, l = n-2)$

$\rightarrow$ calculation of corresponding model spaces
and transition probabilities.

Preliminary results for ^{185}Re $2p$-$1s$ x rays