Atomic and Molecular EDMs

Field Theory Calculation of Electric Dipole Moments of Bound Systems

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EDMs13
February 15, 2013

Precision experiments on atoms complement direct high energy searches for new physics

- Example from astronomy: precision measurements of planetary orbits
- Careful perturbative calculations by LeVerrier and Adams accounting for planet-planet interactions led to discovery of Neptune in 1846
- Much more important calculation done 13 years later by LeVerrier on perihelion of Mercury gave important support to General Relativity
- Einstein's comment on the hard-working astronomers:

Letter to Arnold Sommerfeld, 1915:

- ‘The result of the perihelion motion of Mercury gives me great satisfaction. How helpful to us here is astronomy’ s pedantic accuracy, which I used to ridicule secretly!’

Famous 43 arc-second per century precession actually 585: LeVerrier could only account for 542: this kind of precision test requires carefully eliminating known effects. Will see that EDM tests are ‘cleaner’ .

Differentiate two kinds of precision test:

1) Mercury precession: after precise experiment (585), account for all known physics (542) to get new physics. Any error in either is a problem, will discuss four atomic examples.
2) Find an effect that no standard physics can mimic: edm leading example, though to get experimental precision (actually accuracy) a host of systematic effects must be controlled.

High accuracy measurements of magnetic moments

- Units of e-cm for electric dipole moment the same as for the Bohr magneton in gaussian units:

$$\mu_B = \frac{e\hbar}{2mc} = 1.93\ 10^{-11} e - cm$$

Two decades of work by Gabrielse and collaborators has led to the result (g-2)/2 = 0.001 159 652 180 73(28), 3 parts in 10^13, corresponding to 10^(-24) e cm.

The graveyard of countless theories of new particles coupling to the electron, as new one-loop corrections must be tiny

Much current interest in muon g-2 because of small discrepancy

- BNL E821 experiment found
- (g-2)/2=0.001 165 920 80(63)
- Standard model prediction (like Mercury example) requires high order QED along with difficult-to-handle hadronic effects, but 3 standard deviation difference from experiment may signal new physics
- Hadronic effects are increasing in importance in atomic physics as precision increases, limits tests of QED in some cases (particularly hyperfine splitting)
- Beginning to invert situation to use atoms as probes of nuclear structure

Another (probably coincidental) muon problem: spectrum of muonic hydrogen seems to indicate proton smaller than determined with other methods.

- Basic QED diagrams cross checked
- Proton polarization interesting but too small
- Higher moments investigated, but also small
- Renewed attention to electron scattering experiments
- Other muonic atoms (d, He) under investigation
- Problem still unsolved

T even atomic tests of electroweak physics (original neutral current)

- Parity nonconservation in cesium is included in the Particle Data Book as one of a set of tests of electroweak physics. Characterized by very low energy scales compared to other tests, running of coupling constants from 0 to 100 GeV working well (Jefferson lab Q_W will also provide a low energy test, as parity violating Moller scattering already does).

- Cesium experiment so accurate, and theory so advanced, that many have hesitated to start one of these difficult, long term projects in new systems. (Ba+, Fr, Tl all under consideration).

- New theoretical development indicates some corrections were missed, agreement with SM of cesium now slightly off.

Nonvanishing edms the original treatment of parity violation

- Norman Ramsey: teaching at Harvard (molecular beams), preparing lecture explaining that strong interactions conserve parity.
- Purcell attending lectures, Ramsey worried he would ask 'how do you know that?'. Decided he'd come up with an answer, and found it was not so obvious.
- First consideration: edm of neutron.
- (1950: 6 years before Lee and Yang, 14 before CP violation in kaons).

Schiff' s theorem and enhancement factors

- Early discussion of Salpeter showed that a nonrelativistic atom with electrons with nonvanishing edm' s would have a highly suppressed edm.
- Sandars later showed relativistic effects could lead to large enhancement factors, of order 100 for cesium.
- Field theory approach presently being explored, and new Lamb-shift like diagrams (the existence of which was pointed out by Sandars, Lindroth, and Lynn) will contribute.
- Present thallium bound: (Berkeley group)

$$d_e < 1.6 \times 10^{-27} e \text{ cm}$$

Thallium has 81 electrons: can one really calculate reliably the properties of such a complicated object?

- A: Very high accuracy is not needed for discovery phase of edm experiments: a factor of 2 is adequate.
- B: This level of accuracy is easily reached by a ‘cartoon’ of the atom if the electronic structure is not too complicated

Furry and Extended Furry Representation QED

- External Field Approximation: extra term in QED Hamiltonian

$$H_0 = \int d^3x \bar{\psi}(x)[\vec{\alpha} \cdot \vec{p} + \beta m - \frac{Z(|\vec{x}|)\alpha}{|\vec{x}|}]\psi(\vec{x})$$

$$\begin{aligned} H_I &= -e \int d^3x \bar{\psi}(x) \vec{\gamma} \cdot \vec{A}(x) \psi(x) \\ &+ \frac{\alpha}{2} \int \frac{d^3x d^3y}{|\vec{x} - \vec{y}|} \psi^\dagger(x)\psi(x)\psi^\dagger(y)\psi(y) \end{aligned}$$

Extended Furry Representation:

Redefine lowest order Hamiltonian to incorporate screening:

$$
\begin{aligned}
H_0 &= \int d^3x\psi^\dagger(x)[\vec{\alpha}\cdot\vec{p}+\beta m]\psi(x) \\
&+ \int d^3x\psi^\dagger(x)[U(|\vec{x}|) - \frac{Z(|\vec{x}|)\alpha}{|\vec{x}|}]\psi(x)
\end{aligned}
$$

and redefine

$$
H_I = H_I - \int d^3x\psi^\dagger(x)U(|\vec{x}|)\psi(x)
$$

Model Potential U:

Basic idea: at small distances electron sees full nuclear charge, but at large distances, for a neutral atom, electron sees unit charge. Illustrate for cesium:

$$U(r) = \frac{54\alpha}{r}[1 - \frac{e^{-\gamma r}}{(1+tr)^2}]$$

Choosing $$\gamma = 0.2445, t = 2.0453$$

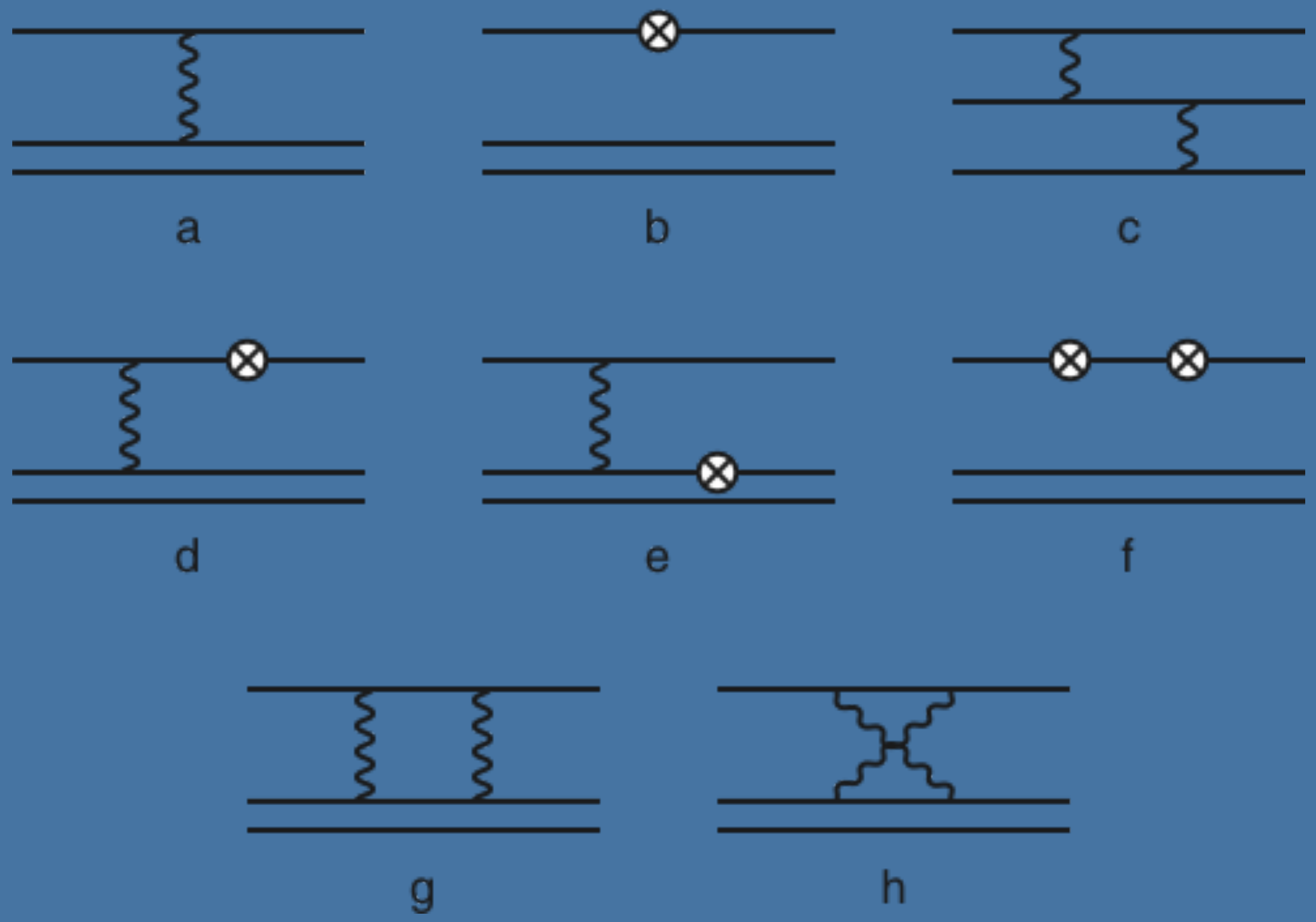
and then solving the Dirac equation with this extra potential gives a 'snapshot' of the atom that gives 10-20 percent accurate predictions for energies and matrix elements.

Hartree-Fock potential somewhat complicated, but not needed and has disadvantage of being nonlocal. Calculations to be shown use a local potential similar to Hartree-Fock. Just a 'foot in the door'.

End result should not depend on U:

- Sodiumlike (11 electrons) Tungsten (Z=74):
- 3p1/2-3s transition measured to be 159.54(3) eV. Three different choices for U give lowest order results 150.51, 155.08, -1.30.
- Adding in one and two photon exchange diagrams gives 164.35, 164.55, 164.09
- ‘Discover’ 3 percent effect of 4.8 eV: Lamb shift (enhanced in highly charged ions)

Feynman diagrams corresponding to MBPT through 2'nd order



Expansion in powers of alpha, equivalent to sets of Feynman diagrams, central to success of QED

Desirable goal: extend this approach to all atoms and molecules, so instead of dealing with the many-body Hamiltonian and the alphabet soup of methods used to solve the Schrodinger equation one evaluates an agreed on set of diagrams. (Far in the future!)

[CC, CI, MBPT, HF, MCHF, …..]

Atomic electric dipole moments

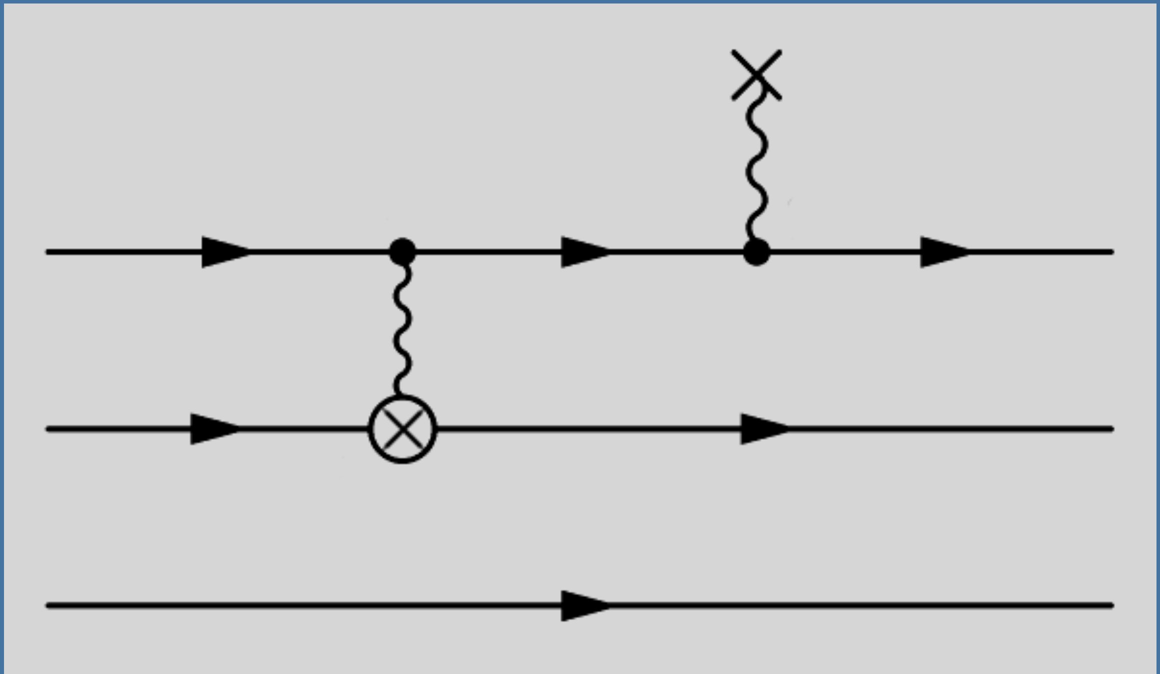
- Lagrangian for nonvanishing electron electric dipole moment similar to electron anomaly:

$$\mathcal{L} = -\frac{i}{2} d_e \int d^3x \bar{\psi}(x) F^{\mu\nu} \sigma_{\mu\nu} \gamma_5 \psi(x)$$

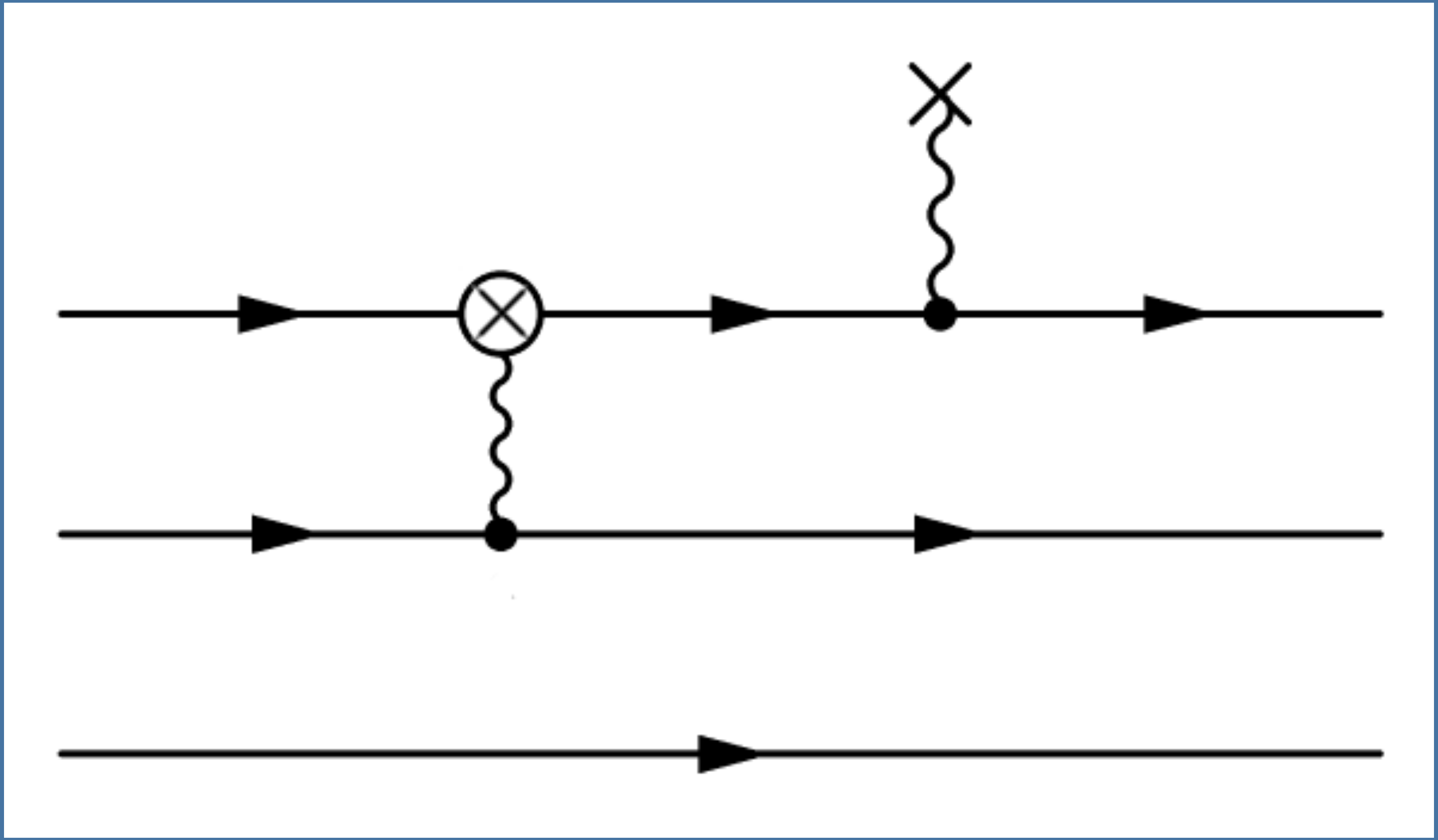
leads nonrelativistically to Hamiltonian

$$d_e \vec{\sigma} \cdot \vec{E}$$

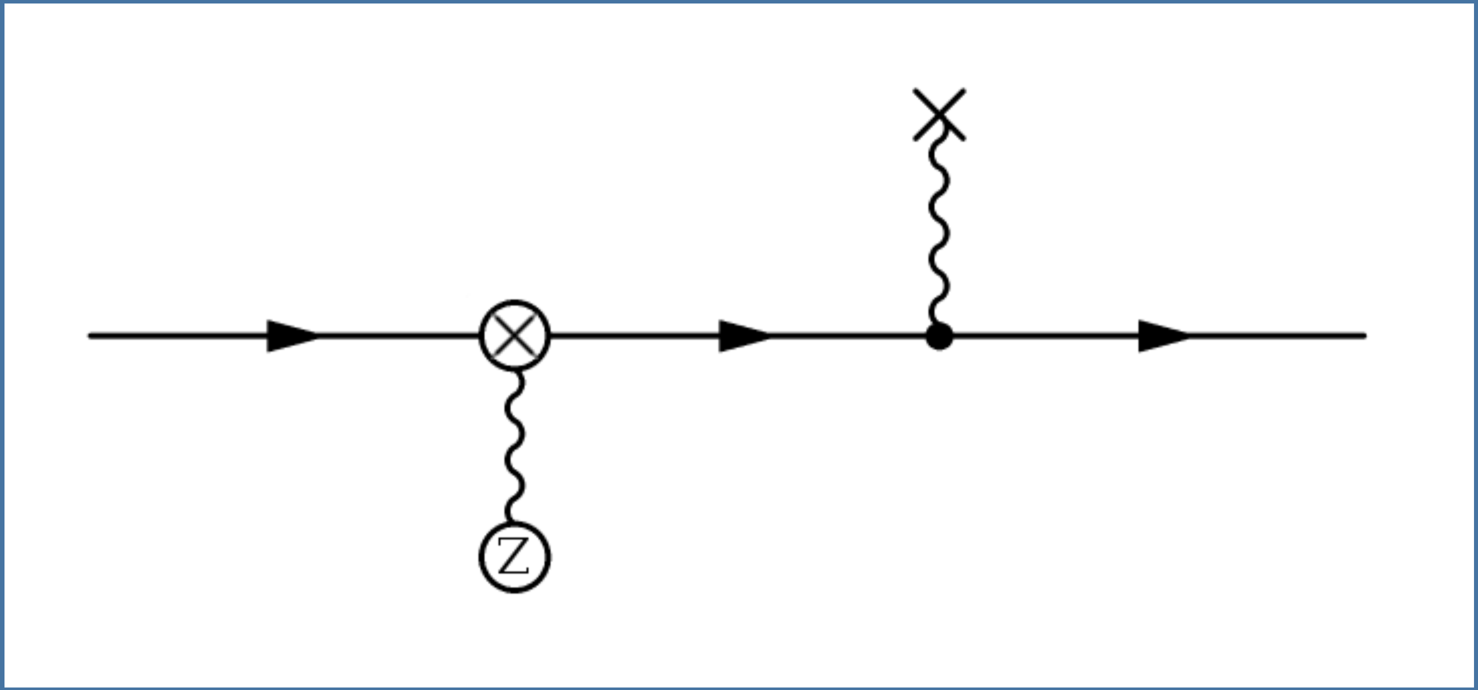
New Feynman rule (edm circled cross, external electric field other cross)



Valence electron edm effect



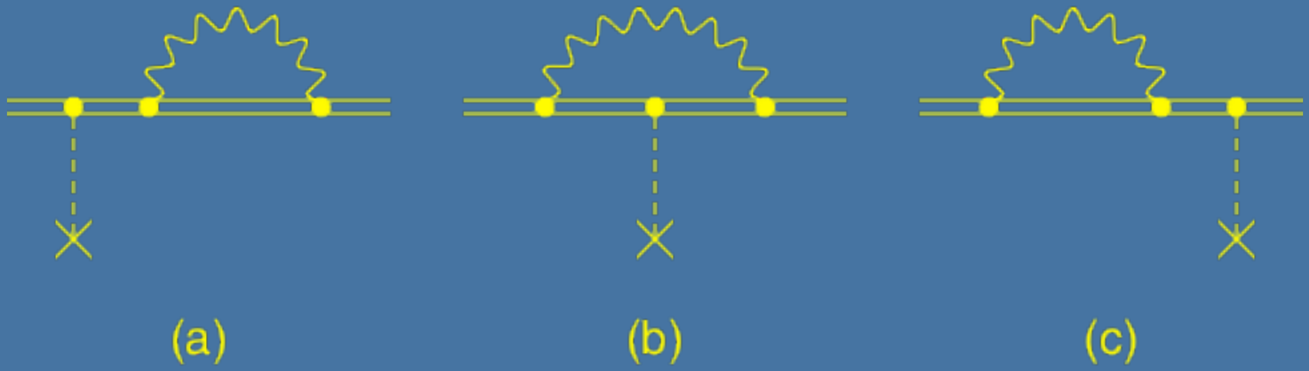
Interaction of nucleus with electron edm



Large enhancement factors result for cesium and thallium

- Cesium R=130, Thallium R=-685: latter adds almost three extra digits to bound on electron edm.
- Feynman diagram breakup for thallium:
- -219 valence, -573 nucleus (-793 sum)
- Schiff theorem for lithium: terms of order 8 cancel to 0.004
- Advantage of field theory approach: can evaluate same diagrams in the neutron: result shows no enhancement factor present.

Feynman diagrams for radiative corrections to one-potential perturbations



$$E_b = -4\pi i\alpha \int d^3x d^3y d^3z \int \frac{d^n k}{(2\pi)^n} \frac{e^{i\vec{k}\cdot(\vec{x}-\vec{z})}}{k^2}$$
$$\cdot \quad \bar{\psi}_v(\vec{x})\gamma_\mu S_F(\vec{x},\vec{y};E-k_0)V(\vec{y})S_F(\vec{y},\vec{z},\epsilon_v-k_0)\psi_v(\vec{z})$$

Dirac Coulomb propagator S_F handled with either basis set techniques or differential equation methods: complications arise with reference state singularities.

Future applications:

- New edm diagrams similar to the Lamb shift can be studied.
- Two photon effects should improve accuracy.
- Extend methods of bound state field theory used in atomic physics to the proton and neutron: presently studying muonic hydrogen with this approach, but in general an alternative to dispersion theory calculations
- Possible extension to molecules challenging.

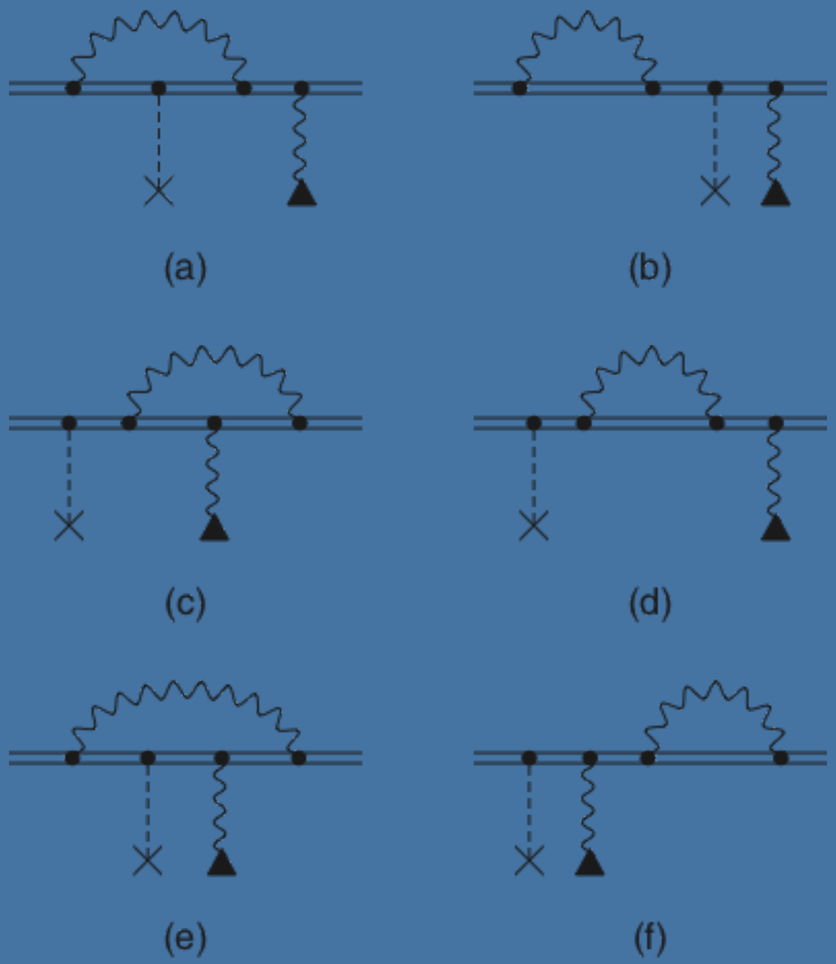
1968 Sandars calculation (show 1986 JS and coworkers calculation, note 2007 Ramsey-Musolf et. al. paper)

- In an atom, electric fields from nucleus and other electrons shield effect of edm nonrelativistically (Schiff theorem), but enhance it for heavy atoms. Need to go to second order perturbation theory, with

$$H_I = \sum_i (-eE_{\rm ex} z_i +$$

$$d_e \gamma_0 \Sigma_i \cdot (E_{\rm ex} \hat{z}_i - \frac{1}{e} \nabla_i V))$$

Feynman diagrams for radiative corrections to PNC



$$\begin{aligned}\gamma_0 \vec{\Sigma} \cdot \vec{\nabla} V &= i[\gamma_0 \vec{\Sigma} \cdot \vec{p}, V] \\ &= i[\gamma_0 \vec{\Sigma} \cdot \vec{p}, H_0] - i[\gamma_0 \vec{\Sigma} \cdot \vec{p}, \sum_i (\vec{\alpha}_i \cdot \vec{p}_i + m\beta_i)]\end{aligned}$$

First term leads to cancellation of first order effect (Shiff' s theorem): second becomes

$$-2i\gamma_0\gamma_5\vec{p}^{\,2}$$

Now have a one-body operator to work with: still need to evaluate

$$-2id_e E_{\text{ex}} \sum_m \frac{\langle 0|z|m\rangle\langle m|\gamma_0\gamma_5\vec{p}^{\,2}|0\rangle + \langle 0|\gamma_0\gamma_5\vec{p}^{\,2}|m\rangle\langle m|z|0\rangle}{E_0 - E_m}$$

Summation over m carried out with finite basis set techniques. For cesium, enhancement factor of 158, 90 percent from 5p ½ state: first order MBPT corrections are large, giving a total of 80: more sophisticated calculations give 113. Same calculation for lithium gives 0.005, again, Shiff theorem in action.

Gell-Mann Low formalism

Use S-matrix methods, but modify Hamiltonian,

$$H_I \to \lambda e^{-\epsilon|t|} H_I$$

$$\Delta E = \frac{i\epsilon}{2} \frac{\partial}{\partial \lambda} \ln \langle \psi_0 | S_{\epsilon,\lambda} | \psi_0 \rangle$$

Standard Feynman diagram techniques can now be employed

V includes energy of interaction with nucleus and electron-electron repulsion: useful trick is to write

$$V = H_0 - \sum_i (\vec{\alpha}_i \cdot \vec{p}_i + m\beta_i)$$

Isolate terms linear in $d_e E_{\rm ex}$

from first and second order perturbation theory, with

$$\Delta E_1 = d_e E_{\rm ex} \langle 0 | \gamma_0 \Sigma_3 | 0 \rangle$$

$$\begin{aligned} \Delta E_2 &= d_e E_{\rm ex} \sum_m \frac{\langle 0 | z | m \rangle \langle m | \gamma_0 \vec{\Sigma} \cdot \vec{\nabla} V | 0 \rangle}{E_0 - E_m} \\ &+ d_e E_{\rm ex} \sum_m \frac{\langle 0 | \gamma_0 \vec{\Sigma} \cdot \vec{\nabla} V | m \rangle \langle m | z | 0 \rangle}{E_0 - E_m} \end{aligned}$$

Standard model electron edm is extremely small, so any detection is new physics.

- Generic supersymmetry already predicts edm’s ruled out by experiment, but turning on of the LHC may discover supersymmetric particles, in which case atomic physics will provide useful constraints for model builders.
- Berkeley proposal (Gould, Munger) to improve cesium edm by two orders of magnitude would lead to very strong constraints.

Form of Dirac wave functions:

$$\psi_v(\vec{r}) = \frac{1}{r}\begin{pmatrix} ig_v(r)\chi_{\kappa\nu}(\hat{r}) \\ f_v(r)\chi_{-\kappa\nu}(\hat{r}) \end{pmatrix}$$

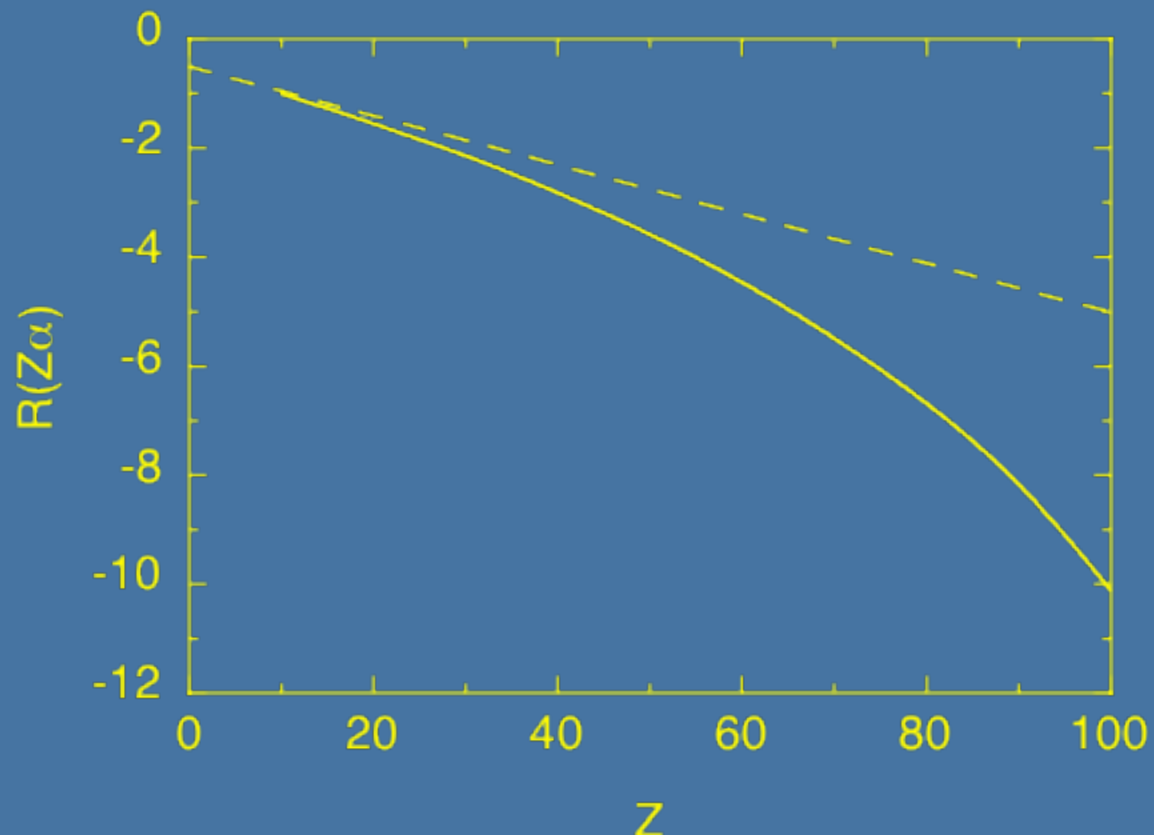
Basic building block of MBPT: 1 Coulomb photon exchange

$$g_{ijkl} = \alpha \int \frac{d^3x d^3y}{|\vec{x}-\vec{y}|} \psi_i^\dagger(\vec{x})\psi_k(\vec{x})\psi_j^\dagger(\vec{y})\psi_l(\vec{y})$$

Order of magnitude of g is a.u., same as energy

(For highly charged ions, g is Z a.u, energies are Z^2 a.u.)

Binding correction changes to -1/2 for radiative corrections to PNC from electron-Z vertex



This is hydrogenic: extension to cesium carried out by Pachucki, Shabaev, and Yerokhin gives similar answers and changes Marciano-Sirlin calculation.

Relation of PNC and edm calculations

- Sandar's manipulation gives 1-body form for edm operator: PNC automatically of this form, arising from exchange of a Z boson between the nucleus and an atomic electron (External electric field now time varying to allow 6s to 7s transition)

$$h_w = 2i\frac{d_e}{e}\gamma_0\gamma_5\vec{p}^2 \rightarrow h_w = -\frac{G_F}{\sqrt{8}}\gamma_5\rho(\vec{r})$$

Lowest order calculations similar and give qualitative agreement with cesium PNC