CP-violating magnetic moments of atoms and molecules

Andrei Derevianko
Physics Department, University of Nevada, Reno
andrei@unr.edu

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Collaborators

UNR Theoretical Atomic Physics group with visitors, Basque restaurant, Apr 2006

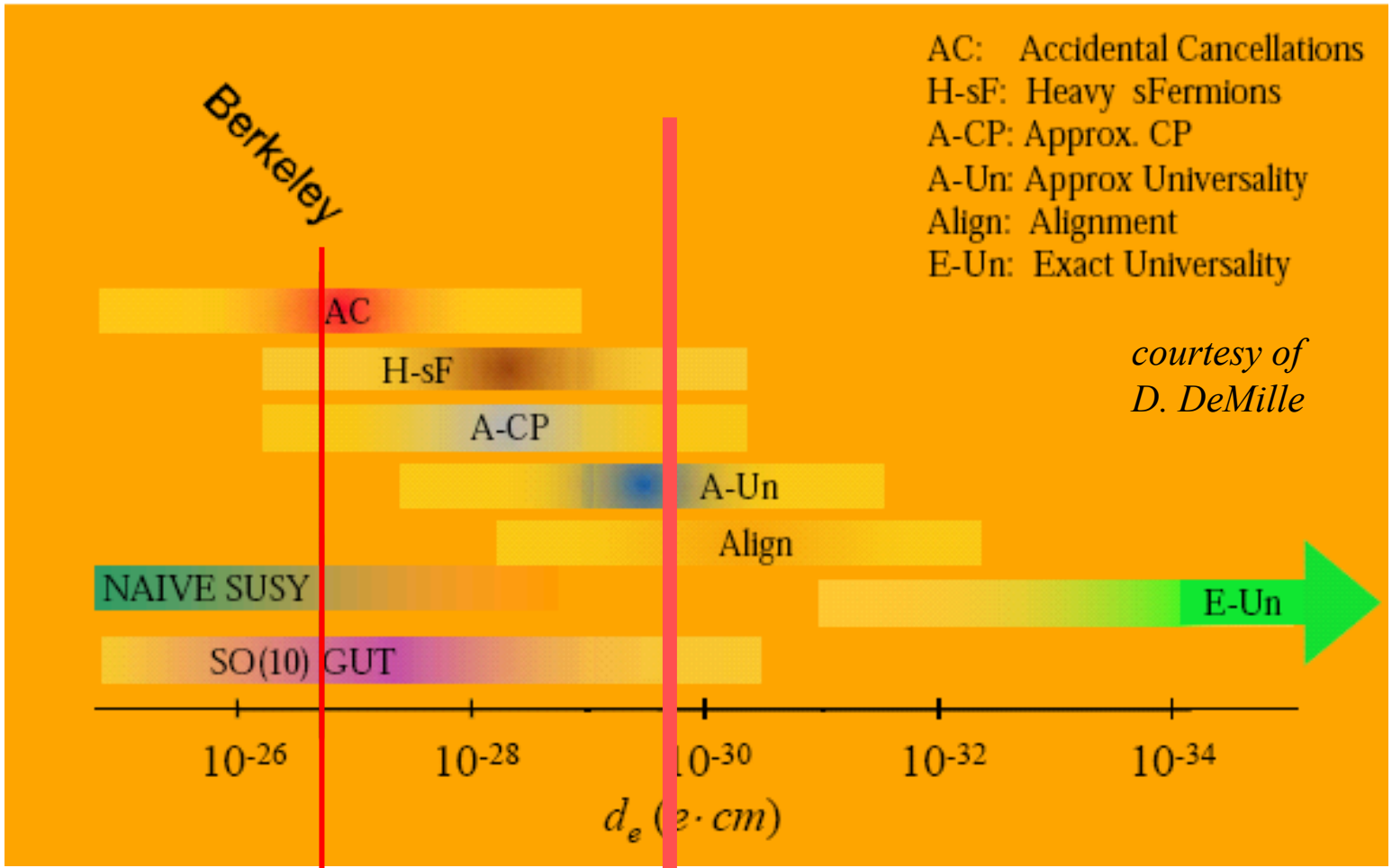
Outline

~~*CP* **E**DM~~ → ~~*CP* **M**DM~~

- *CP-violating atomic polarizability*

- *CP-violating molecular magnetic moments*
  - *Permanent ~~CP~~ **M**DM*
  - *Thermally-induced ~~CP~~ **M**DM*

electron EDM and supersymmetry

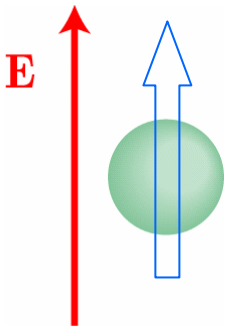


Present limit

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

Our proposal

CP-violating polarizability



$$\vec{\mathbf{D}} = \alpha \vec{\mathbf{E}}$$

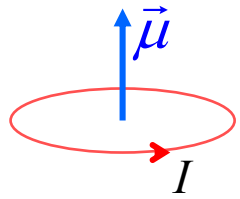
$$\vec{\mu}\ ? = ?\, \beta \vec{\mathbf{E}}$$

$\beta \neq 0$ implies P and T violation (or CP-violation)

T-reversal:

$$\vec{\mu} \xrightarrow{T} -\vec{\mu}$$

$$\vec{\mathbf{E}} \xrightarrow{T} +\vec{\mathbf{E}}$$

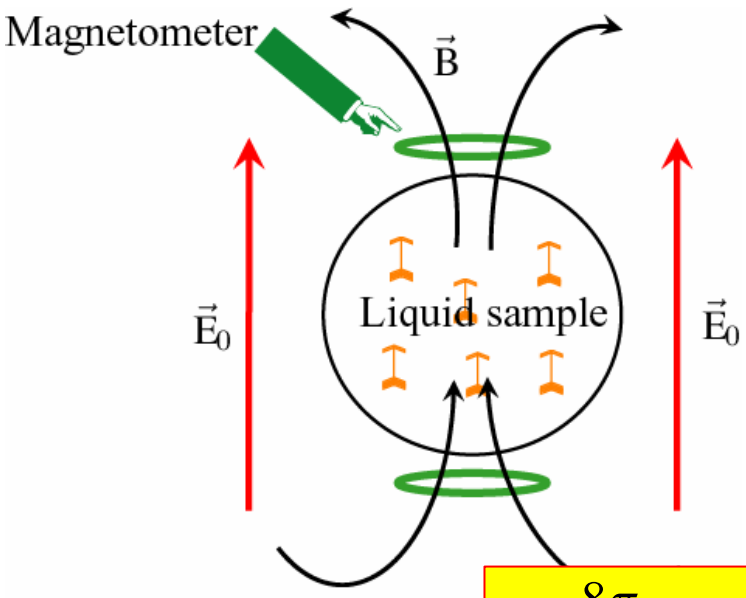


$$\vec{\mu}^{\mathrm{CP}} = \beta^{\mathrm{CP}}\, \vec{\mathbf{E}}$$

Baryshevskii 2004

I will relate this to eEDM

Measuring β^{CP}



$$B = \frac{8\pi}{3} n \beta^{CP} E_0$$

Signal $\propto$ number density and E-field

$\Rightarrow$ Liquid Xe: high number density
high E-field breakdown strength

M. Romalis (Princeton)

β^{CP} (LXe) = ? $\times$ d_e

electron EDM and β^{CP}

Coupling

$$V^{\mathrm{CP}} = -\vec{d}\cdot\vec{E} = -d_e\vec{\sigma}\cdot\vec{E}$$

$$\approx d_e\left(\frac{Z}{r^2}\right)\vec{\sigma}\cdot\hat{r}$$

The strongest E-field is near the nucleus

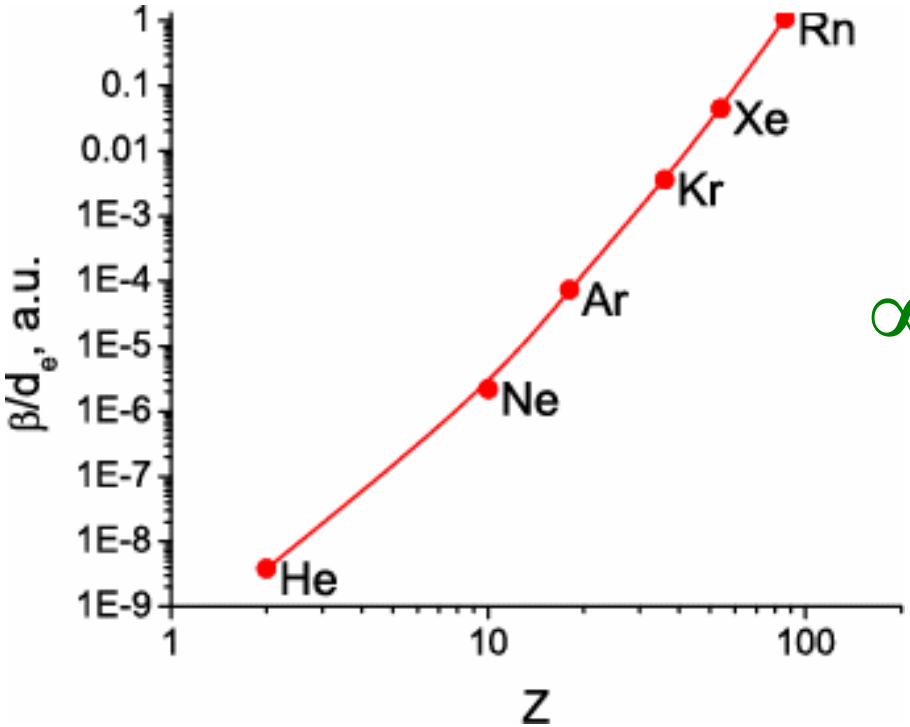
V^{CP} is a *pseudo*-scalar

$$\langle\mu\rangle = 2\sum_{i}^{\text{even}}\frac{\langle 0|\mu|i\rangle\langle i|-DE_{ext}|0\rangle}{\Delta E_{i0}}\overset{\text{odd}}{=}0$$

$$\langle\mu^{CP}\rangle = 2\sum_{ij}^{\text{even}}\frac{\langle 0|\mu|j\rangle\langle j|V^{CP}|i\rangle\langle i|-DE_{ext}|0\rangle}{(\Delta E_{i0})(\Delta E_{j0})}\overset{\text{odd}}{\overset{\text{odd}}{+\ldots\neq 0}}$$

Third order *ab initio* relativistic Hartree-Fock calculations…

Dirac-Hartree-Fock Results



Closed-shell atoms
Third-order calculations
ab initio relativistic

$\propto Z^5$

B. Ravaine, M. Kozlov and A. Derevianko, Phys. Rev. A **72**, *012101 (2005)*

Projected EDM sensitivity of LXe setup

$$d_e < \frac{B}{nE_0}\frac{3}{8\pi}\left(\frac{\beta^{CP}}{d_e}\right)^{-1}$$

$n \sim 10^{22}$ 1/cm^3

$E_{0,max} \sim 4\times10^5$ V/cm

$\beta^{CP}(\mathrm{LXe}) \approx 1.6\times10^{-2}\, d_e$ a.u.

Weakest measurable B-field

sensitivity $B_{min} \sim 3\times10^{-15}$ G Hz$^{-1/2}$ + 10 days of averaging *Lamoreaux (2004)*

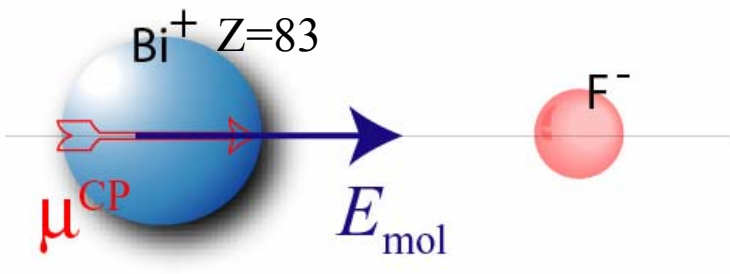
Projected $d_e(\beta^{CP},\mathrm{LXe}) < 6\times10^{-26}$ e cm

but

Present limit $d_e(\beta^{CP},\mathrm{Tl}) < 1.6\times10^{-27}$ e cm

Can we save the idea?

Permanent molecular CP-violating magnetic moment



Magnetic moment of diamagnetic molecules ($\Lambda=0$ $\Sigma=0$) is identically zero

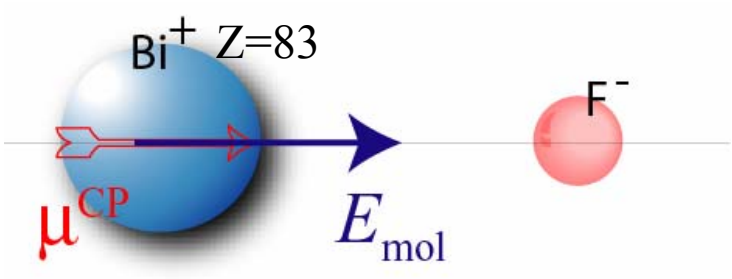
Yet, T and P violation lead to magnetic moments

A. Derevianko and M. Kozlov, Phys. Rev. A 72, 040101(R) (2005).

Polar molecules (BiF)

$$\mu^{CP} = \beta^{CP} E_0$$ increase the E-field

Huge internal molecular fields



$$E_{mol} \approx \frac{e}{R_e^2} \approx 4\times10^8 \frac{\mathrm{V}}{\mathrm{cm}}$$

$$\mu^{CP}(\mathrm{BiF}) < 10^{-17}\,\mu_B$$

Electron magnetic moment *g/2= 1.001 159 652 180 85 (76)*

Five orders of magnitude enhancement due to stronger fields and higher Z

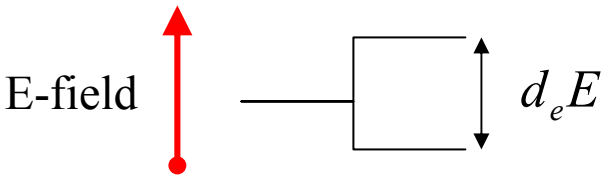
Thermally-induced molecular μ^{CP}

Gaining even more orders …

Kozlov & Derevianko Phys. Rev. Lett. **97**, *063001 (2006).*

Thermalized sample of spins in E-field

external E≠0, B=0



$$\frac{n_\uparrow}{n_\downarrow} \propto \exp\left[-\frac{d_e E}{kT}\right]$$

But

$$\vec{d} = d_e \vec{\sigma}$$

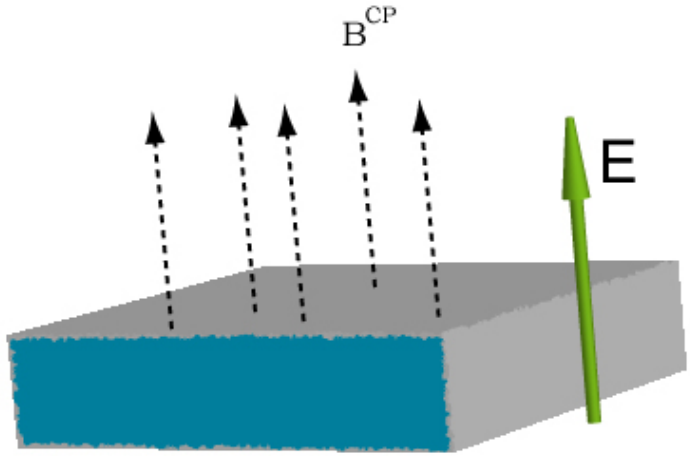
$$\vec{\mu}_e = -\mu_B \vec{\sigma} = -\mu_B \frac{\vec{d}}{d_e}$$

Misbalance in the spin up/down population => macroscopic magnetization=> ultraweak magnetic field

$$B^{CP} \propto n \quad \Longrightarrow \quad \text{work with solid state}$$

1. Shapiro idea 1968
2. Proof of principle experiment Vasiliev & Kolycheva 1978
3. Lamoreaux 2002: recent advances in magnetometry => competitive schemes

CP-violating magnetization



$$B^{CP} \propto \frac{2d_e E_{eff}}{kT} \propto E_{eff}$$

For solid-state samples

$$E_{eff} \approx E_{applied} \leq 10^5 \frac{\mathrm{V}}{\mathrm{cm}}$$

Can we increase E-field acting on eEDM?
How about molecules?

$$E_{eff} \approx 10^{11} \frac{\mathrm{V}}{\mathrm{cm}}$$

Potentially SIX orders of magnitude improvement

Kozlov & Derevianko Phys. Rev. Lett. ***97****, 063001 (2006).*

Thermally-induced molecular μ^{CP}

μ^{CP} per molecule is directed along the molecular axis

$$\left\langle \vec{\boldsymbol{\mu}}^{CP} \right\rangle = \mu_B \frac{d_e E_{eff}}{kT} \hat{\mathbf{n}}$$

For rotating molecules $\left\langle \hat{\mathbf{n}} \right\rangle = 0$

$$\left\langle \vec{\boldsymbol{\mu}}^{CP} \right\rangle = 0$$

We need to polarize the sample

$$\left\langle \hat{\mathbf{n}} \right\rangle \| \vec{\mathbf{E}}_{ext} \quad \Longrightarrow$$

$$\boxed{\left\langle \vec{\boldsymbol{\mu}}^{CP} \right\rangle \| \vec{\mathbf{E}}_{ext}}$$

This link violates Time and Parity

Effective E-field in the molecules

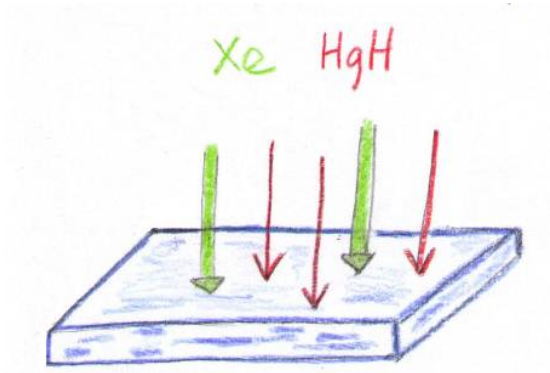
polar molecules
radicals (unpaired electron)
Heavy constituents $E_{eff} \sim Z^3$

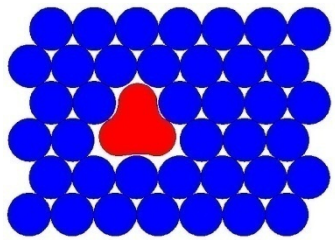
Molecule	$E_{\text{eff}}, V/cm$
BaF	8×10^9
YbF	3×10^{10}
HgH	8×10^{10}

Problem: How to make a solid out of highly reactive species?

Matrix isolation (manufacturing a designer solid)

Developed in 1950's. ESR spectroscopy, …



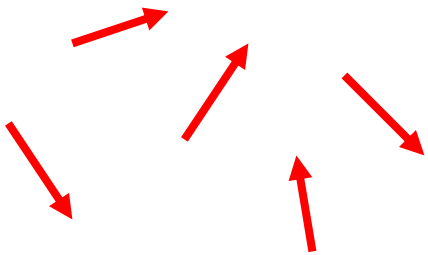


Cold substrate ~ 4 K
Hosts: Ne, Ar, Xe, SF_6, …

Matrix ratios as high as 1:100 => $n_{guests} \sim 10^{20}$ 1/cc

Samples are typically small ~ 1mm thickness x 1cm^2 area

Upper limit on the number density



Dipole-Dipole interaction b/w the molecules
Possible phase transitions
To avoid alignment

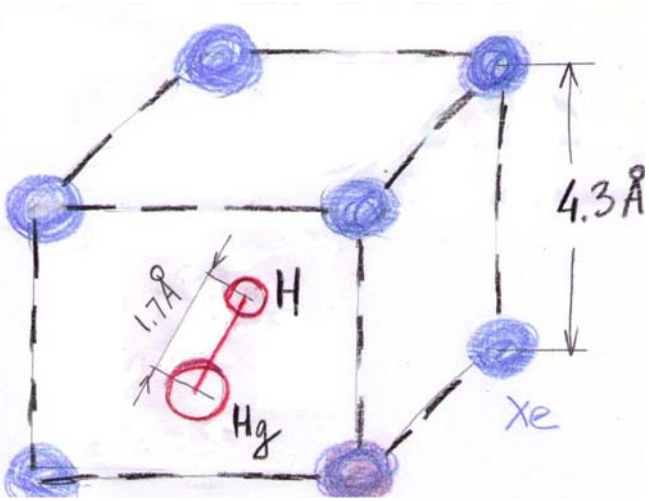
$$V_{DD} < kT$$

$$n_{\max} \approx \frac{kT}{D^2}$$

Molecule	$D(D)$	$n_{\max}, 1/\mathrm{cm}^3$
BaF	3.17	3×10^{18}
YbF	3.91	2×10^{18}
HgH	0.47	2×10^{20}

Corresponding matrix ratio ~ 1:100

Molecule in a matrix cage



To the first approximation molecules are "free"
HFS constants for trapped and free molecules differ by a few %

$$H \approx -D \cdot E^{*} + 2 d_e E_{eff} \Omega$$

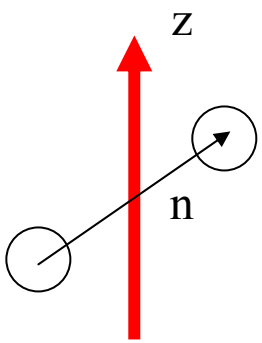
$$E^{*} = E_{ext} / \varepsilon$$

For our densities ε=2 => $E=E_{ext}/2$

$$\left\langle \mu^{CP} \right\rangle = \mu_B \frac{d_e E_{eff}}{kT} \left\langle n_z \right\rangle$$

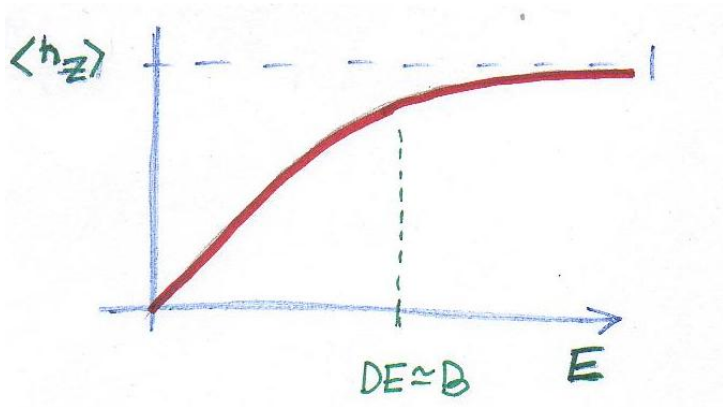
$\left\langle n_z \right\rangle (E^{*}) \le 1$ degree of polarization

Degree of polarization



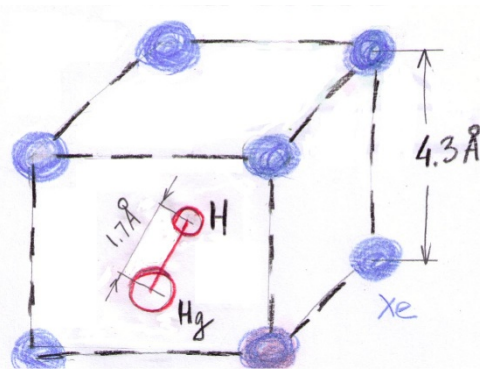
For rotating molecules $\langle n_z \rangle = 0$

External E-field couples to the molecular dipole moment



In a thermal sample DE/kT ~ 1 @ E ~ 10^5 V/cm

Breakdown strength for LXe 4 x 10^5 V/cm



Molecular axis evolves in a complex multi-valley potential
-hindered rotations
-librations
-Some evidence of rotations for HXeBr and Hydrates
-molecules are small (1.7 A vs 4.3 A)

Permanent vs thermally-induced μ^{CP}

$$\left\langle \mu^{CP} \right\rangle = \mu_B \frac{d_e E_{eff}}{kT} \left\langle n_z \right\rangle$$

For the present limit on eEDM

$$\left\langle \mu^{CP}\left(\mathrm{HgH}\right) \right\rangle < 1.4 \times 10^{-12} \left\langle n_z \right\rangle \mu_B$$

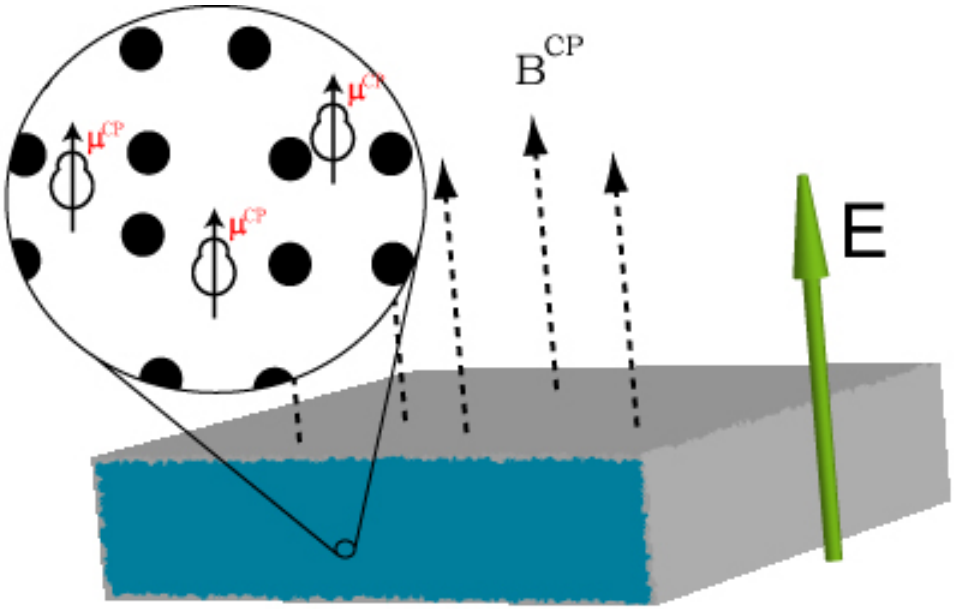
The largest permanent μ^{CP}

$$\mu^{CP}\left(\mathrm{BiF}\right) < 3 \times 10^{-17} \left\langle n_z \right\rangle \mu_B$$

For low T

$$\left\langle \mu^{CP} \right\rangle \ll \mu^{CP}$$

Schematics & sensitivity



$$B^{CP} = 4\pi\gamma\, n\, \mu^{CP}$$

- Weakest measurable B-field
- Signal-to-noise ratio

Weakest measurable B-field

Demonstrated (atomic magnetometer, Princeton) 5.4×10^{-12} G/$\sqrt{\text{Hz}}$

Projected (SQUID, Lamoreaux) 3×10^{-15} G/$\sqrt{\text{Hz}}$

The present limit on eEDM can be recovered within

$$t_{\text{demostrated}} = 5\times10^{-2} \quad \text{sec}$$
$$t_{\text{projected}} = 10^{-8} \quad \text{sec}$$

For *t*=1week the limit on eEDM can be improved by factors

$$3\times10^{3} \quad (\text{demostrated})$$
$$6\times10^{6} \quad (\text{projected})$$

@ T=4K
Dillution fridge T->mK

Assumptions: $\gamma=1$, $\langle n_z\rangle\sim1$

Signal-to-noise

Radicals have traditional magnetic moments $\mu_{mol} = 2\mu_B \Omega n_z$

Random magnetization of the sample => B-field noise
Noise is not correlated with E_{ext}

$$\frac{S}{N} = 3\frac{\langle \mu^{CP} \rangle}{\mu_B}\sqrt{N\frac{t}{\tau}}$$

integration time

correlation time

number of molecules

$$\tau \sim \frac{h}{D^2 n}$$

dipolar interactions
(Strong spin-axis coupling)

Budker, Lamoreaux, Sushkov & Sushkov PRA (2006)

S/N numerical estimate

$V=10^{-3}$ cm^3 matrix ratio 1:100

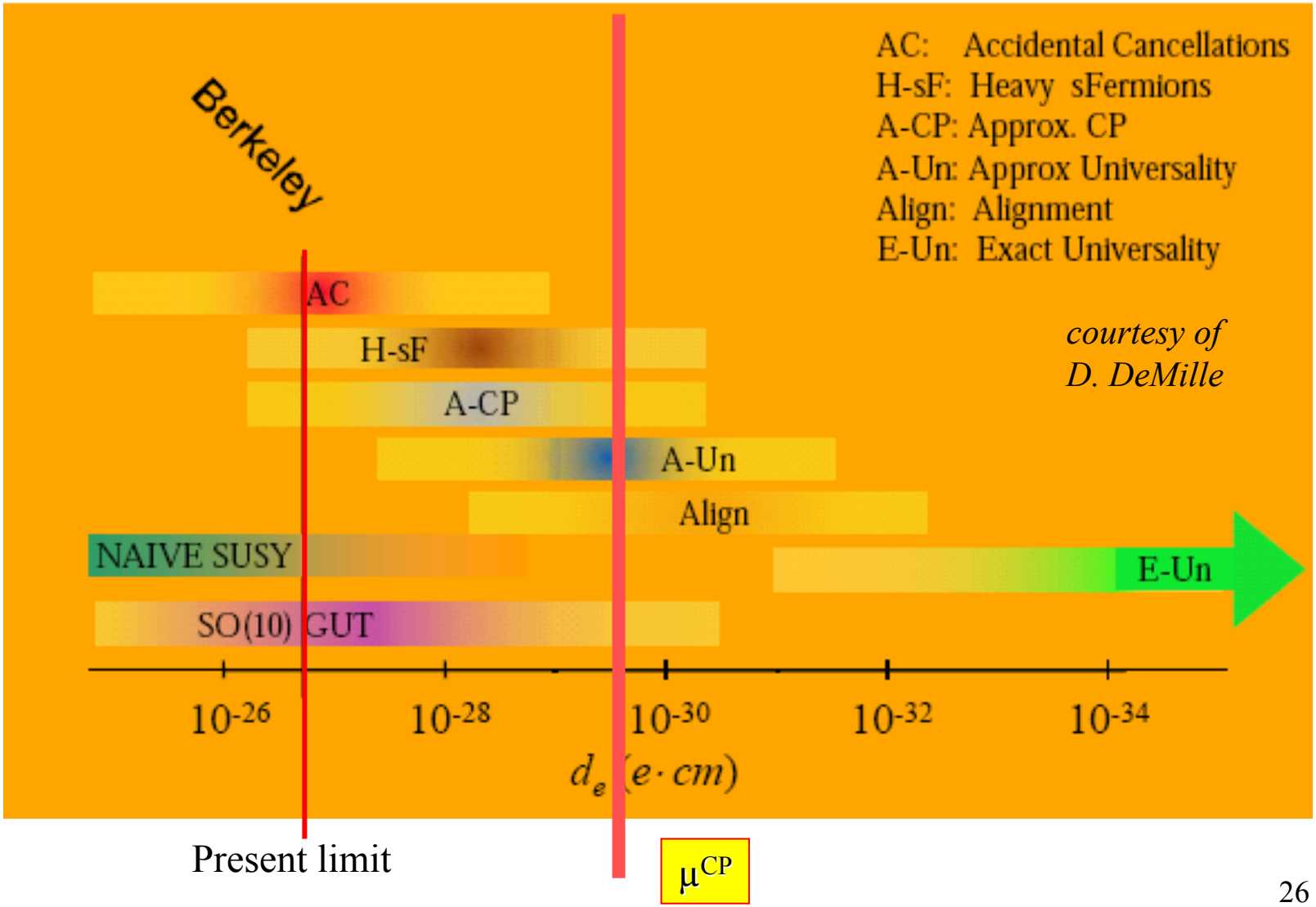
S/N =1 + present limit on eEDM => $t = 10^{-5}$ sec

If t= *1week*, the present limit can be improved by 2×10^5

These estimates are consistent with the B-field estimates

For permanent μ^{CP} we deal with diamagnetic molecules => noise is strongly suppressed

electron EDM and supersymmetry



Artificial vacuum footnote

"ARTIFICIAL VACUUM" FOR *T*-VIOLATION EXPERIMENT

Craig PRYOR
Department of Physics, University of California, Santa Barbara, CA 93106, USA

and

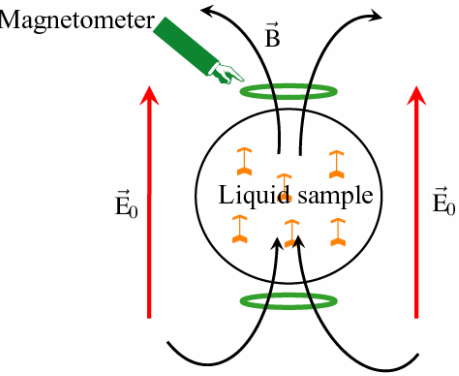
Frank WILCZEK
Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA

Received 14 October 1986

We point out the possible use of matrix isolation spectroscopy in experimental tests of fundamental physics. As a concrete example we show how this technique might be applied to measuring the *T*-violation electron electric dipole moment d_e. We estimate that a dipole moment could be detected down to $d_e \sim 6 \times 10^{-25} e$ cm, in comparison to the current limit of $d_e < 10^{-24} e$ cm.

Phys. Lett B **194,** 137 (1987)

matrix isolated Cs atoms

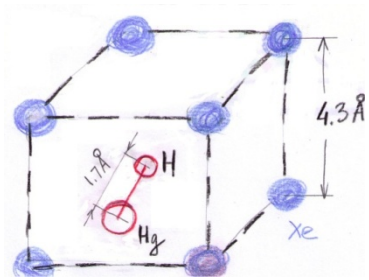


Summary

⇨ Concepts of β^{CP} and μ^{CP}

$$\vec{\mu}^{CP} = \beta^{CP}\vec{\mathbf{E}} \qquad \vec{D}^{CP} = \beta^{CP}\vec{\mathbf{B}}$$

$$H = -\beta^{CP}\vec{\mathbf{E}}\cdot\vec{\mathbf{B}}$$



⇨ Permanent molecular μ^{CP} (closed-shell μ=0)

⇨ Thermally-induced μ^{CP} – promising technique

⇨ ? Other techniques?

⇨ Systematics?