Theory of electron EDM experiments with molecules

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Plan of the talk

Electric dipole moment of the electron in atoms
- Schiff theorem
- Atomic screening or atomic enhancement?

Heavy diatomic molecules
- Estimate of molecular enhancement
- Semi-empirical model
- Calculations of molecular effective field

eEDM experiments with molecules and solids
- Interference experiments
- Solid state magnetization experiments

Schiff theorem

Non-relativistic consideration of the electron in the stationary state immediately leads to the zero energy shift:

$$\delta\varepsilon = -\vec{d}_e \cdot \langle \vec{E} \rangle; \quad m\vec{a} = -e\vec{E}; \quad \langle \vec{a} \rangle = 0; \quad \Rightarrow \quad \boxed{\delta\varepsilon = 0}.$$

However, in the electron rest frame there is nonzero magnetic field and the force $\vec{F} \neq -e\vec{E}$. Therefore, generally $\langle \vec{E} \rangle \neq 0$. Relativistic Hamiltonian for the Dirac electron has the form:

$$H_d = -d_e \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix} \cdot \vec{\nabla}\phi,$$

where ϕ is atomic potential. We can rewrite H_d in a form that vanishes in non-relativistic limit and automatically satisfies Schiff theorem :

$$\boxed{H_d = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \cdot \vec{\nabla}\phi.}$$

Estimate of atomic energy shift due to eEDM [Sandars 1965, Flambaum 1976]

In the external electric field $\vec{E}$ the energy correction will be:

$$\delta\varepsilon = 2\frac{\langle 0|H_d|n\rangle\langle n|e\vec{r}\cdot\vec{E}|0\rangle}{\varepsilon_0 - \varepsilon_n}.$$

In atomic units $(\varepsilon_0 - \varepsilon_n) \sim \langle n|r|0\rangle \sim 1$ and

$$\delta\varepsilon \sim \langle H_d\rangle E = 2d_e E \left\langle \begin{pmatrix} 0 & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \cdot \vec{\nabla}\phi \right\rangle.$$

At large distances $\phi \sim 1$, but for $r \sim \frac{1}{Z}$, $\phi \sim \frac{Z}{r}$ and $\nabla\phi \sim Z^3$.
At large distances the small components of the Dirac orbitals $\sim \alpha$, while at short distances they are $\sim \alpha Z \times \psi(0) \sim \alpha Z^{3/2}$.
As a result, the above matrix element is given by the integral over the volume $V \sim Z^{-3}$.

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Estimate of atomic EDM
[Sandars 1965, Flambaum 1976]

The estimate of the atomic energy shift due to eEDM:

$$\delta\varepsilon \sim d_e E\,(\alpha Z)^2\,\psi^2(0)\,\left(\nabla\phi|_{r\sim 1/Z} V\right) \sim \alpha^2 Z^3 d_e E.$$

If we define atomic EDM so that:

$$\delta\varepsilon \equiv d_{\mathrm{at}} E,$$

we see that $d_{\mathrm{at}} = k_{\mathrm{at}} d_e \sim \alpha^2 Z^3 d_e$ and atomic enhancement factor

$$\boxed{k_{\mathrm{at}} \sim \alpha^2 Z^3.}$$

Calculations of atomic enhancement factors

- The estimate $k_{\rm at} \sim \alpha^2 Z^3$ showes that heavy atoms can work as amplifiers of eEDM. That was confirmed by accurate atomic calculations. For example, for Cs (Z=55), $k_{\rm Cs} \approx 120$ and for Tl (Z=81) $k_{\rm Tl} \approx -590$.
- Atomic enhancement factors are very sensitive to electron correlations. In particular, the Dirac-Fock calculation for Tl gives $k_{\rm Tl} = -1910$.
- Core-valence correlations usually increase the answer by 10 – 30%, while valence-valence correlations can work both ways.
- $k_{\rm at}$ depends on $|\psi_{\rm val}(0)|^2$ and becomes small when the angular momentum of the valence electron $j > \frac{1}{2}$. For this case correlations can even change the sign and the order of magnitude of the effect.

Summary for atoms

- Atomic EDM scales as $10\alpha^2 Z^3 \times d_e$ when valence electron has $j = \frac{1}{2}$ and is much smaller otherwise.
- The sign of d_{at} depends on the valence configuration.
- Atomic enhancement factor k_{at} is very sensitive to electron correlations, in particular for the case of $j > \frac{1}{2}$.
- Modern atomic theory allows reliable calculations of k_{at} for most heavy atoms of interest.

Estimate of molecular enhancement factor

- Internal electric field in the polar molecule $E_{\mathrm{mol}} \sim \frac{e}{R_o^2} \sim 10^9\ \mathrm{V/cm}$, which is 4 – 5 orders of magnitude larger than typical laboratory field in EDM experiment. This field is directed along the molecular axis and is averaged by rotation of the molecule.
- In the external electric field E_{lab} molecular axis is polarized in the direction of the field. For $\Sigma_{1/2}$-molecule in the rotational level J the complete polarization requires the field $D_{\mathrm{mol}} E_{\mathrm{lab}} \approx 2BJ$, i.e. $E_{\mathrm{lab}} \sim 10^4\ \mathrm{V/cm}$. For molecules with Ω-doubling a much smaller field may be sufficient.
- Typical molecular enhancement factor

$$\boxed{k_{\mathrm{mol}} \sim k_{\mathrm{at}} \times \frac{E_{\mathrm{mol}}}{E_{\mathrm{lab}}} \sim 10^4 k_{\mathrm{at}}.}$$

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For a molecule with heavy atom the matrix element of operator H_d depends on the short distances $r \sim 1/Z$.

At such distances:

- Valence electrons are relativistic and move in unscreened (spherically symmetric) Coulomb potential of the heavy nucleus.
- Electronic wave function can be expanded in partial waves. These partial waves rapidly decrease with the angular momentum j because of the centrifugal barrier.
- Each partial wave is hydrogenic and has simple analytical form.
- Normalization coefficients for partial waves are defined by matching with the wave function at large distances where the wave function depends on the details of the molecular field.

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Semi-empirical molecular wave function

For the molecule with one unpaired electron we can write:

$$|\Lambda,\Omega\rangle = |\lambda=\Lambda,\omega=\Omega\rangle_{\text{unpaired}}|\Lambda_c=0,\Omega_c=0\rangle_{\text{coupled}}$$

In the vicinity of the heavy nucleus wave function can be expanded in spherical waves

$$\begin{aligned} |\lambda,\omega\rangle &= \sum_{\kappa} C_\kappa |l,j,\omega\rangle, \\ \kappa &= (l-j)(2j+1) \end{aligned}$$

Here $|l,j,\omega\rangle$ are normalized four-component spherical waves:

$$|l,j,\omega\rangle = \begin{pmatrix} f_\kappa Y^{l}_{j,\omega} \\ i g_\kappa Y^{2j-l}_{j,\omega} \end{pmatrix}$$

f_κ and g_κ are radial functions and $Y^{l}_{j,\omega}$ is the spherical spinor.

At the small distances solutions of the Dirac equation are:

$$\begin{aligned}
\begin{pmatrix} f_\kappa \\ g_\kappa \end{pmatrix} &= \frac{\kappa/|\kappa|}{Z^{1/2}r}\begin{pmatrix} (\gamma+\kappa)J_{2\gamma}(x) - \frac{x}{2}J_{2\gamma-1}(x) \\ \alpha Z J_{2\gamma}(x) \end{pmatrix} \\
x &= \sqrt{8Zr} \\
\gamma &= \sqrt{\kappa^2 - \alpha^2 Z^2}
\end{aligned}$$

Interaction of eEDM d_e with the molecular electric field Z/r^2 is given by the matrix element:

$$\langle \lambda, \omega | H_d | \lambda, \omega \rangle = W_d d_e \omega,$$

where parameter W_d defines effective electric field felt by the unpaired electron in the molecule, $E_{\mathrm{eff}} \equiv \frac{1}{2} W_d$.

At short distances molecular potential field corresponds to the unscreened field of the nucleus and we can calculate W_d explicitly:

$$W_d = 8\sum_i C_{-i}C_i \int_0^\infty g_{-i}g_i \frac{d\phi}{dr} r^2 dr$$

$$= 16\alpha^2 Z^3 \left(\frac{C_{-1}C_1}{\gamma_{1/2}(4\gamma_{1/2}^2 - 1)} + \frac{C_{-2}C_2}{\gamma_{3/2}(4\gamma_{3/2}^2 - 1)} + \ldots \right)$$

Coefficients in this expansion rapidly decrease with κ!

For $\Sigma_{1/2}$-molecules we can leave only the first term of partial wave expansion:

$$W_d \approx \frac{16\alpha^2 Z^3}{\gamma_{1/2}(4\gamma_{1/2}^2 - 1)} C_{-1} C_1 .$$

Is it possible to determine coefficients C_{-1} and C_1?

- We need accurate relativistic wave function in the core region. Such ab initio calculations are very difficult!
- We can try to find molecular observables which depend on these parameters and can be measured.

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Hyperfine structure

Magnetic hyperfine structure (HFS) of diatomic molecule:

- Like eEDM interaction depends on the spin density.
- Magnetic field of the nucleus decreases as $1/r^3$ and matrix element depends on the wave function at short distances.
- Hyperfine structure of diatomic molecule is given by the axial tensor $\hat{A}$, which depends on two parameters: isotropic constant (A) and dipole constant (A_d).
- Partial wave expansions for A and for A_d converge rapidly.

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Semi-empirical equations for YbF molecule

Hyperfine constants for YbF molecule were measured in a rare-gas matrix [Van Zee et al, 1977]:

$$\left\{\begin{array}{lcr} A & = & 7617\ \mathrm{MHz},\\ A_d & = & 102\ \mathrm{MHz}.\end{array}\right.$$

That leads to the following equations for coefficients C_κ:

$$\left\{\begin{array}{lcr} 31170C_{-1}^2 - 1330C_1^2 - 50C_2^2 + \ldots & = & 7617,\\ 5510C_1^2 + 379C_2^2 + \ldots & = & 102.\end{array}\right.$$

Truncating expansions at C_1 we get:

$$\left\{\begin{array}{lcl} C_{-1}^2 & = & 0.24,\\ C_1^2 & = & 0.019.\end{array}\right. \Rightarrow |C_{-1}C_1| = 0.067 \Rightarrow E_{\mathrm{eff}} = 3 \times 10^{10}\ \mathrm{V/cm}$$

Calculations of effective field for YbF molecule

Method	E_{eff} (10^9 V/cm)	Reference
Semi-empirical (SE)	-31	Kozlov & Ezhov 1994
Eff. Core Potential (ECP)	-19	Titov et al 1996
SE with f-hole correction	-26	Kozlov 1997
HFD + Core Polarization	-13×2	Quiney et al 1998
Unrestricted HFD	-25	Parpia 1998
ECP+Effective operators	-25	Mosyagin et al 1998
HFD+CI	-22	Noyak & Chaudhuri 06

$$\boxed{E_{\mathrm{eff}}(\mathrm{YbF}) = -(25 \pm 3) \times 10^9\ \mathrm{V/cm}}$$

Calculations of effective field in diatomics

Molecule	State	$E_{\text{eff}}\ \left(10^9\,\frac{\text{V}}{\text{cm}}\right)$	Reference
BaF	$\Sigma_{1/2}$	-7.8 ± 0.5	Kozlov 1985
		-7.5	Kozlov et al 1997
		-7.3	Noyak & Chaudhuri 06
HgF	$\Sigma_{1/2}$	-97	Kozlov 1985
		-99	Dmitriev et al 1992
PbF	$\Pi_{1/2}$	$+29$	Dmitriev et al 1992
PbO	Π_1^*	-50	Kozlov & DeMille 02
		-24	Petrov et al 04
HI^+	$\Pi_{3/2}$	-4	Ravine et al 04
		$+3.5$	Isaev et al 05

eEDM enhancement in molecules

- There is general qualitative understanding of the d_e enhancement in diatomic molecules.
- Radicals with with one unpaired electron in $^2\Sigma_{1/2}$-state are best studied. For given Z they have largest effective field E_eff. There is good agreement between different semi-empirical and *ab initio* calculations and E_eff is known with approximately 10% accuracy.
- For other molecules E_eff is usually smaller and semi-empirical methods are much less reliable. *Ab initio* methods can still be used. Test calculations of HFS and other observables are very important.
- For $\Pi_{3/2}$-molecules the effective field on the valence electron is strongly suppressed. Correlation corrections become crucial and calculations are very difficult.

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Ongoing and planned eEDM experiments

- Spectroscopic experiments with molecules

At present experiment on YbF is going in London and on PbO in Yale.

Experiment on PbF is planned in Oklahoma.

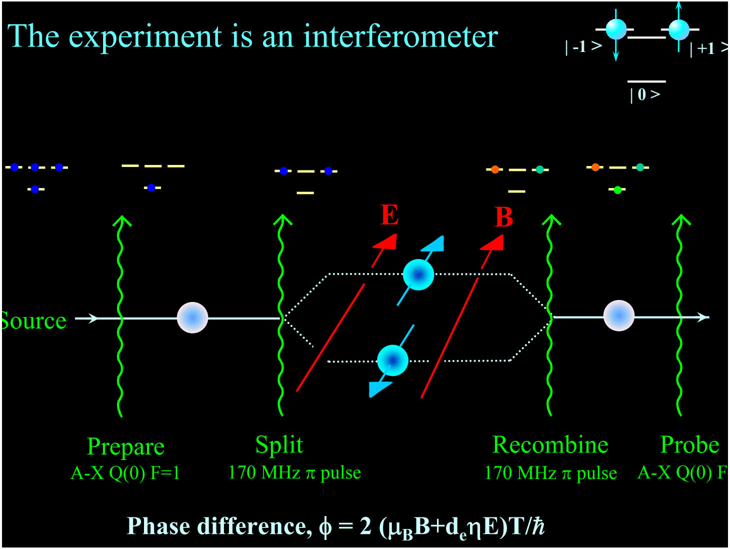
Experiment with trapped molecular ions is planned in Boulder.

- Shapiro-type experiments with solids

In Amherst electric polarization in magnetic field is observed in Gadolinium-Iron Garnet.

In Los Alamos magnetization in electric field is observed in Gadolinium-Gallium Garnet.

Molecular beam experiment [Ben Sauer, UCN-2005]



The experiment is an interferometer

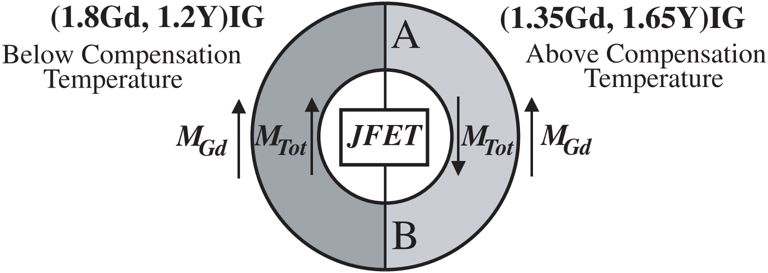
Phase difference, $\phi = 2\,(\mu_B B + d_e \eta E)T/\hbar$

Solid state EDM experiments

- In 1968 Shapiro suggested to look for magnetization of a paramagnetic substance with unpaired electrons in the external electric field. Enhancement factor here is roughly $k_{\mathrm{at}}/\varepsilon$.
- Magnetic flux is proportional to the spin density and the surface area. Thus, it is advantageous to do experiment with macroscopic solid sample. Such experiment was done in 1978 by Vasil'ev & Kolicheva.
- In 2001 Lamoreaux showed that advances in magnetometry and new materials, such as gadolinium garnets, allow to raise current sensitivity to eEDM by several orders of magnitude.

eEDM experiment with Gadolinium-Iron Garnet (GdIG)

[Heidenreich *et al.* PRL, **95**, 253004 (2005)]



Shapiro-type experiment with diatomic radicals in a noble gas matrix

- One can look for magnetization in the electric field of a sample of diatomic radicals frozen in a noble gas matrix.
- Here we can have 5 orders of magnitude gain in the enhancement factor.
- The number of spins will be $4 \div 6$ orders of magnitude smaller.
- $\Rightarrow$ The net gain $10^2 \div 10^3$ in S/N compared to solid state experiment. [Kozlov & Derevianko, PRL 97 063001 (2006)].

Some ongoing & planned experiments

Group	Object	Method		Result (e cm)
IC London	YbF	beam	spectroscopy	10^{-27}/day
Yale	PbO	cell	spectroscopy	testing
Oklahoma	PbF	trap	spectroscopy	design
JILA	HfH^+	trap	spectroscopy	design
Amherst	Gd^{3+}	GdIG	voltage	10^{-24}
Los Alamos	Gd^{3+}	GdGG	magnetometery	10^{-23}
	HgH	matrix	magnetometery	proposal