Nuclear Structure V: Application to Time-Reversal Violation (and Atomic Electric Dipole Moments)

J. Engel

University of North Carolina

June 16, 2005

Outline

1. T Symmetry
   - T is Different
   - Observed T Violation
2. EDM's
   - Connection with T Violation
   - Shielding
3. Octupole Deformation
   - Why It Enhances Atomic EDM's
   - ^{225}Ra
4. Other Nuclei

Outline

The T Operator in QM is Different

.

- Not linear:

$$T[x,p]T^{-1} = -[x,p]$$

  so i is odd under T.

- Has no eigenstates in the conventional sense:

$$T|a\rangle = |a\rangle \quad \longrightarrow \quad T(\alpha|a\rangle) = \alpha^* T|a\rangle = \alpha^*|a\rangle \neq \alpha|a\rangle$$

  for α complex

- Typical physical states $|J,M\rangle$ not even close to eigenstates of T

As a result, T violation doesn't show up as "mixing of states with opposite T"

Is T Violated in the Real World?

Yup!

- Violation is seen in decay of K-mesons (direct) and B-mesons (through CP violation).
- And we strongly believe that T ($\equiv CP$) violation played an important role in the early universe, causing excess of matter over antimatter.

What is the Source of T-Violation?

K and B phenomena almost certainly due to a phase in the 3×3 CKM matrix, which converts (d, s, b) to "weak eigenstates" that couple to W and Z.

But this can't be responsible for "baryogenesis", which must arise outside the standard model, e.g. through

- supersymmetry
- heavy neutrinos
- Higgs sector ...

To confuse things more, there's the "strong CP problem."

We need to see T-violation outside mesonic systems to understand its sources. EDM's are not sensitive to CKM T violation, but are to other sources. They're already putting pressure on supersymmetry.

Outline

What Do EDM's Have to Do With T

Consider nondegenerate ground state $|g : J, M\rangle$. Symmetry under rotations $R_y(\pi) \Rightarrow$ for a vector operator like $\vec{d} \equiv \sum_i e_i \vec{r}_i$,

$$\langle g : J, M|\vec{d}|g : J, M\rangle = -\langle g : J, -M|\vec{d}|g : J, -M\rangle \ .$$

T takes M to $-M$, like $R_y(\pi)$. But $\vec{d}$ is *odd* under $R_y(\pi)$ and *even* under T, so for T conserved

$$\langle g : J, M|\vec{d}|g : J, M\rangle = +\langle g : J, -M|\vec{d}|g : J, -M\rangle \ .$$

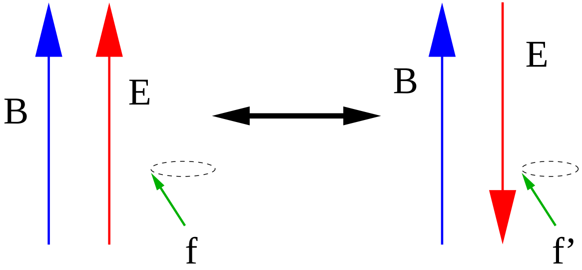
Together with the first equation, this implies

$$\langle \vec{d} \rangle = 0 \ .$$

If T is violated, argument fails because T can take $|g : JM\rangle$ to a *different* state with $J, -M$.

There are EDM Experiments on Neutrons, Atoms . . .

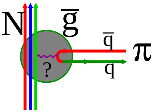
Basic principle:



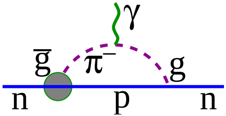
$$H = -\vec{\mu} \cdot \vec{B} - \vec{d} \cdot \vec{E}$$

and there is a change in precession frequency (linear in E) when $\vec{E}$ is flipped.

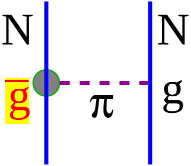
How Do Things Get EDM's?



- Underlying theory generates T-violating πNN vertex:
- A neutron gets a EDM from a diagram like this:



- A nucleus can get one from a nucleon EDM or through a T-violating nucleon-nucleon interaction, e.g.



$$H_T(12) \propto \bar{g}\, g \times \text{isopsin ops.} \times (\vec{\sigma}_1 - \vec{\sigma}_2) \cdot (\vec{\nabla}_1 - \vec{\nabla}_2) \frac{\exp(-m_\pi |\vec{r}_1 - \vec{r}_2|)}{|\vec{r}_1 - \vec{r}_2|}$$

- Finally, nuclear EDM induces atomic EDM.

The goal of the atomic experiments discussed here is to constrain (or determine) the three $\bar{g}$'s.

Shielding by Electrons

Unfortunately for atomic experiments:

Theorem (Schiff)

The nuclear dipole moment causes the atomic electrons to rearrange themselves so that they develop a dipole moment opposite that of the nucleus. In the limit of nonrelativistic electrons and a point nucleus the electrons' dipole moment exactly cancels the nuclear moment, so that the net atomic dipole moment vanishes!

Skip proof

Shielding by Electrons

Proof

Consider atom with nonrelativistic constituents (with dipole moments $\vec{d}_k$) held together by electrostatic forces. The atom has a "bare" edm $\boxed{\vec{d} \equiv \sum_k \vec{d}_k}$ and a Hamiltonian

$$
\begin{aligned}
H = & \sum_k \frac{p_k^2}{2m_k} + \sum_k V(\vec{r}_k) & - \sum_k \vec{d}_k \cdot \vec{E}_k \\
= & \quad H_0 & + \sum_k (1/e_k) \vec{d}_k \cdot \vec{\nabla} V(\vec{r}_k) \\
= & \quad H_0 & + i \sum_k (1/e_k) \left[\vec{d}_k \cdot \vec{p}_k , H_0 \right]
\end{aligned}
$$

$\Uparrow$ K.E. + Coulomb $\qquad$ $\Uparrow$ dipole perturbation

Shielding by Electrons

The perturbing Hamiltonian

$$H_d = i \sum_k (1/e_k) \left[\vec{d}_k \cdot \vec{p}_k , H_0 \right]$$

shifts the ground state $|0\rangle$ to

$$\begin{aligned} |\tilde{0}\rangle &= |0\rangle + \sum_m \frac{|m\rangle\langle m|H_d|0\rangle}{E_0 - E_m} \\ &= |0\rangle + \sum_m \frac{|m\rangle\langle m| i \sum_k (1/e_k) \vec{d}_k \cdot \vec{p}_k |0\rangle (E_0 - E_m)}{E_0 - E_m} \\ &= \left(1 + i \sum_k (1/e_k) \vec{d}_k \cdot \vec{p}_k \right) |0\rangle \end{aligned}$$

Shielding by Electrons

The induced dipole moment $\vec{d}'$ is

$$
\begin{aligned}
\vec{d}' &= \langle\tilde{0}|\sum_j e_j \vec{r}_j|\tilde{0}\rangle \\
&= \langle 0|\left(1 - i\textstyle\sum_k (1/e_k)\vec{d}_k\cdot\vec{p}_k\right)\left(\textstyle\sum_j e_j\vec{r}_j\right) \\
&\qquad \times \left(1 + i\textstyle\sum_k (1/e_k)\vec{d}_k\cdot\vec{p}_k\right)|0\rangle \\
&= i\langle 0|\left[\textstyle\sum_j e_j\vec{r}_j, \sum_k (1/e_k)\vec{d}_k\cdot\vec{p}_k\right]|0\rangle \\
&= -\langle 0|\sum_k \vec{d}_k|0\rangle = -\sum_k \vec{d}_k \\
&= -\vec{d}
\end{aligned}
$$

So the net EDM is zero!

All is Not Lost, Though...

The nucleus has finite size. Shielding is not complete, and nuclear T violation can still induce atomic EDM $\vec{d}$.

Post-screening nucleus-electron interaction doesn't explicitly involve the nuclear EDM $\vec{D}$, but rather a related quantity:

The nuclear "Schiff moment"

$$\vec{S} \approx \sum_p e_p r_p^2 \vec{r}_p \ .$$

If, as you'd expect, $\langle \vec{S} \rangle \approx R_N^2 \langle \vec{D} \rangle$, then $\vec{d}$ is down from $\langle \vec{D} \rangle$ by

$$O\left(\frac{R_N^2}{R_A^2}\right) \approx 10^{-8} \ .$$

Ughh! Fortunately the large nuclear charge and relativistic wave functions offset this factor by $10Z^2 \approx 10^5$.

Overall suppression of $\langle \vec{D} \rangle$ is only about 10^{-3}.

Comparing Limits

Limit on the neutron EDM: $d_N < 6 \times 10^{-26}$ e cm
Limit on the ^{199}Hg EDM: $d < 2 \times 10^{-28}$ e cm

So neutron measurements still more sensitive, assuming d_N and D are comparable. But conclusion depends on cause of T violation; sometimes $D > d_N$ and ^{199}Hg provides better limits.

And in certain *other* atoms:

$$\langle \vec{S} \rangle >> R_N^2 \langle \vec{D} \rangle$$

making them much better places to look.

Why?

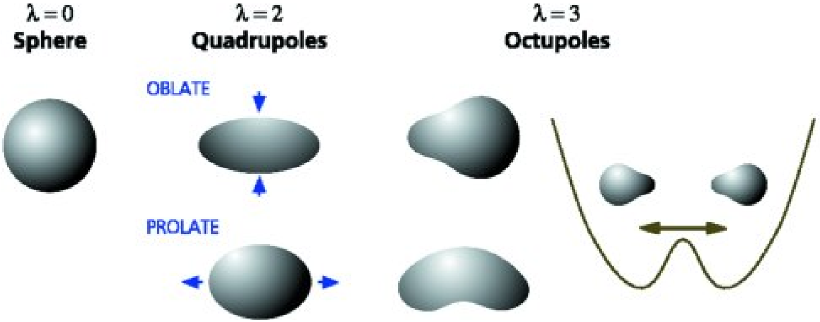
Collective nuclear effects

(i.e. funny shape deformation)

Outline

1. T Symmetry
   - T is Different
   - Observed T Violation
2. EDM's
   - Connection with T Violation
   - Shielding
3. Octupole Deformation
   - Why It Enhances Atomic EDM's
   - ^{225}Ra
4. Other Nuclei

Nuclear Deformation



Analogy: Collective Quadrupole Moments

$$|\Psi_{JM}\rangle \propto D^{J*}_{MK}(\theta,\phi)|\chi^{\text{intr.}}_K\rangle \ ,$$

where K is the projection of $\vec{J}$ on the symmetry axis. The intrinsic states are deformed.

When $K = 0$, the quadrupole operator can be written as

$$Q_\mu = D^2_{\mu 0} Q^{\text{intr.}}_0$$

so that matrix elements within a rotational band look like:

$$\langle \Psi_{JM}|Q_\mu|\Psi_{J'M'}\rangle = \left(\int \text{three } D\text{−functions}\right) \times \langle \chi^{\text{intr.}}|Q^{\text{intr.}}_0|\chi^{\text{intr.}}\rangle$$

So the quadrupole moment and $E2$ transition rates are proportional to the intrinsic quadrupole moment, which can be large/collective.

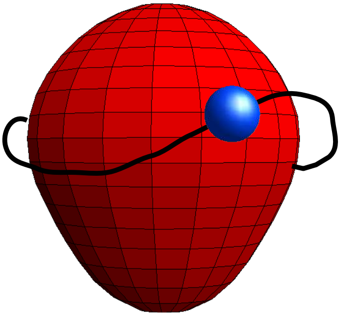
Now What About Schiff Moments?

Need a T-violating nuclear interaction H_T to get one. Treating H_T as perturbation:

$$\langle \vec{S} \rangle = \sum_m \frac{\langle 0 | \vec{S} | m \rangle \langle m | H_T | 0 \rangle}{E_0 - E_m} + c.c.$$

where $|0\rangle$ is the unperturbed nuclear ground state.

$\langle \vec{S} \rangle$ will not be enhanced if nucleus is only quadrupole deformed. Need octupole deformation too.



Then, two collective effects help you out:

1. Parity doubling
2. Large and robust intrinsic Schiff moments

Point 1: Parity Doublets

When the intrinsic state is asymmetric, it breaks parity (spontaneously) because $|\bigcirc\!\circ\rangle$ and $|\circ\!\bigcirc\rangle$ are degenerate, with

$$P|\bigcirc\!\circ\rangle = |\circ\!\bigcirc\rangle \; .$$

Physical states must have good parity:

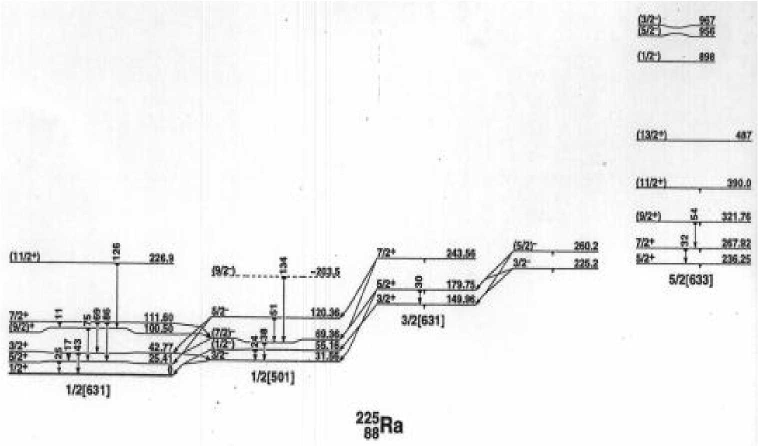
$$|\chi^{\text{intr.}}(\pm)\rangle = 1/\sqrt{2}\,(|\bigcirc\!\circ\rangle \pm |\circ\!\bigcirc\rangle)$$

These will be nearly degenerate if the deformation is rigid. So our expression for the Schiff moment becomes

$$\langle \vec{S} \rangle \approx \frac{\langle 0|\vec{S}|\bar{0}\rangle \langle \bar{0}|H_T|0\rangle}{E_0 - E_{\bar{0}}} + c.c.$$

where $|0\rangle$ and $|\bar{0}\rangle$ form a parity doublet.

Spectrum of ^{225}Ra



Point 2: Large Intrinsic Schiff Moment

$$\langle 0|\vec{S}|\bar{0}\rangle \propto \langle \bigcirc\!\!\circ|\vec{S}^{\mathrm{intr.}}|\bigcirc\!\!\circ\rangle \equiv \langle \vec{S}^{\mathrm{intr.}}\rangle$$

just like in quadrupole transitions, so that

$$\langle \vec{S}\rangle \approx -2/3\,\frac{\langle \vec{S}^{\mathrm{intr.}}\rangle\langle H_T\rangle}{E_0 - E_{\bar{0}}}$$

and furthermore

$$\langle \vec{S}^{\mathrm{intr.}}\rangle > R_N^2\langle \vec{D}^{\mathrm{intr.}}\rangle\ .$$

Dipole moments in these nuclei are collective also, but subject to a cancellation: they vanish in the limit $\rho_{\mathrm{neutron}} = \rho_{\mathrm{proton}}$.

Net result: $\langle \vec{S}\rangle$ is enhanced in an octupole-deformed nucleus like ^{225}Ra by 2 or 3 orders of magnitude over ^{199}Hg, according to collective-model estimates.

Skip ^{225}Ra calculation

2 **or** 3 orders? The Issue of H_T

An order of magnitude uncertainty can deter experimentalists. Why is it there and can it be reduced?

The matrix element of H_T depends on spin, and so is very sensitive to the state of the valence particles. For heavy pions:

$$\langle H_T \rangle \sim a\langle \vec{\sigma}_n \cdot \vec{\nabla}\rho_n \rangle + b\langle \vec{\sigma}_n \cdot \vec{\nabla}\rho_p \rangle + \ldots$$

In simple collective models one valence nucleon carries all the spin. But in reality the valence nucleon can polarize the core. (This quenches magnetic moments and E1 transitions.)

To treat delicate spin-dependent Hamiltonian accurately, need a good *self-consistent* mean-field wave function with which to start. Much of core polarization is then automatically accounted for.

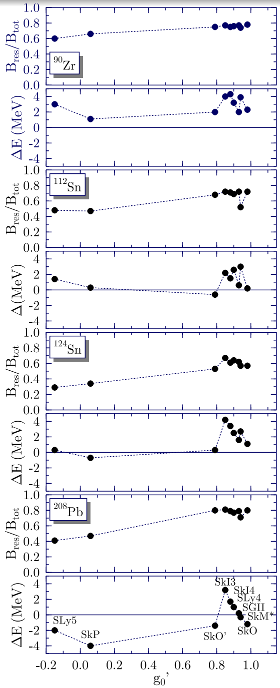
Calculation in ^{225}Ra

P- and *T*-Breaking Odd-*A* Hartree-Fock

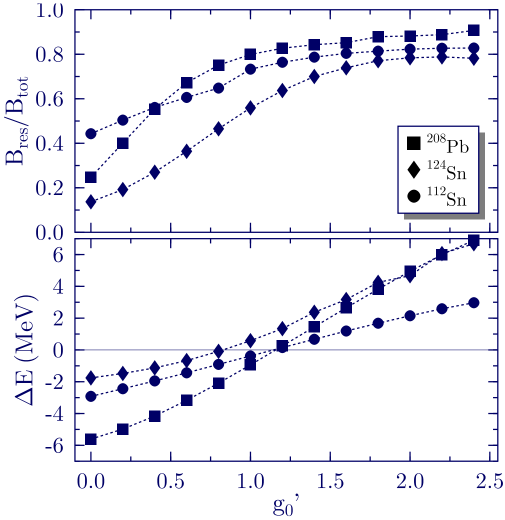
- We break all possible symmetries.
- Core polarization of all kinds automatically included.
- For the effective *NN* interaction we used a Skyrme force — SkO′ — specially fitted to spin excitations (Gamow-Teller resonances)
- All this is accomplished with the program `HFODD` (Dobaczewski et al).

Existing Forces and GT Resonances

Quality of forces in GT channel more or less random.

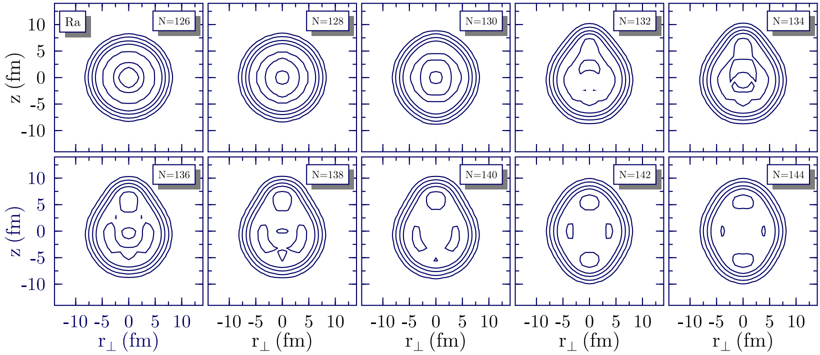


Fitting the Spin-Dependent Parameters

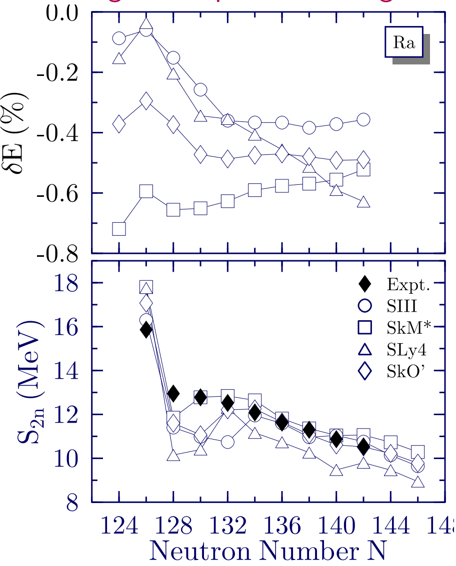


Results of the Calculation

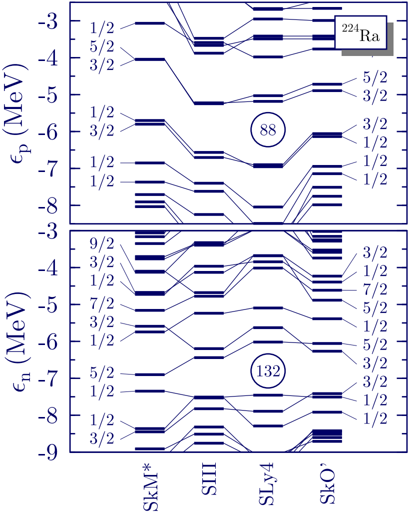
Density distributions of the Radium isotopes

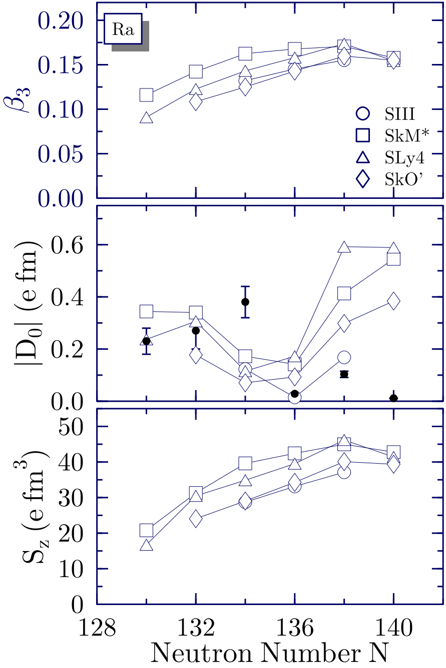


Binding and Separation Energies



Single-Particle Energies





Octupole, Dipole, Schiff Stuff

Resuts for Schiff Moment

We can write $\langle S_z \rangle$ as

$$\langle S_z \rangle = a_0 \ \bar{g}_0 + a_1 \ \bar{g}_1 + a_2 \ \bar{g}_2 \ ,$$

where the a's are what we calculate.

With SkO$'$:

	a_0	a_1	a_2
zero-range (direct only)	-5.1	10.4	-10.1
finite-range (direct only)	-1.9	6.3	-3.8
finite-range + src (direct only)	-1.7	6.0	-3.5
finite-range + src (direct + exchange)	**-1.5**	**6.0**	**-4.0**

What It All Means

For ^{225}Ra, get

$$\langle S_z \rangle_{\mathrm{Ra}} = -1.5\ g\bar{g}_0\ + 6.0\ g\bar{g}_1\ - 4.0\ g\bar{g}_2\ \ (\mathrm{e\ fm}^3)$$

The best calculation in ^{199}Hg (RPA polarization of a spherical even-even core) by Dmitriev and Sen'kov gives

$$\langle S_z \rangle_{\mathrm{Hg}} = 0.0004\ g\bar{g}_0\ + 0.06\ g\bar{g}_1\ + 0.009\ g\bar{g}_2\ \ (\mathrm{e\ fm}^3)$$

If the three $\bar{g}$'s are comparable, the Schiff moment in Ra is larger by over 100, on average.

Dzuba et al. [PRA66, 012111 (2002)] find further enhancement of the Ra EDM by a factor of 3 in the atomic physics.

Looks good for the Ra experiment!

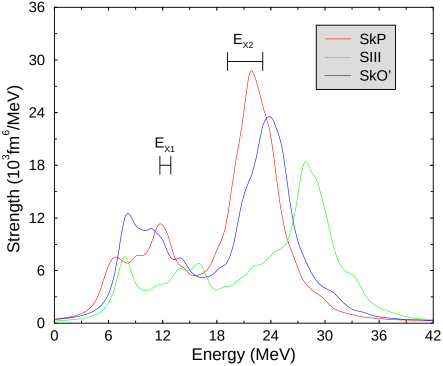
Outline

^{199}Hg

Obviously important. Calculations exist but but have problems.

Just completed Skyrme-QRPA calculation

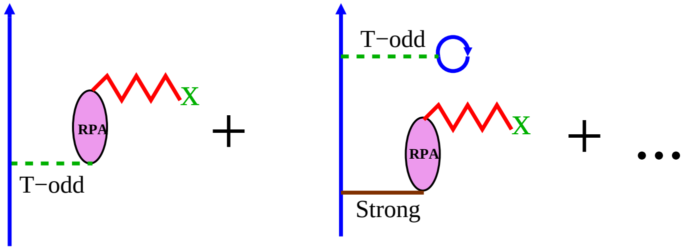
In ^{199}Hg, there is no parity doublet. Lots of states contribute to sum. But the isoscalar Schiff (= isoscalar $E1$) strength distribution is actually measured in some nuclei (like ^{208}Pb).



The ^{199}Hg Schiff Moment

Calculation by J.H. de Jesus

1. Obtained ground and excited states of ^{198}Hg "core" in spherical HFB+QRPA.
2. Included effects of core polarization on $\langle\vec{S}\rangle$ in ^{199}Hg.



Results

Early result of Flambaum et al

$$\langle S_z \rangle_{\mathrm{Hg}} = 0.09\ g\bar{g}_0\ + 0.09\ g\bar{g}_1\ + 0.2\ g\bar{g}_2\ \ (\mathrm{e\ fm}^3)$$

Dmitriev and Sen'kov: Landau-Migdal RPA

$$\langle S_z \rangle_{\mathrm{Hg}} = \boxed{0.0004}\ g\bar{g}_0\ + 0.06\ g\bar{g}_1\ + 0.009\ g\bar{g}_2\ \ (\mathrm{e\ fm}^3)$$

Small isoscalar coefficient would mean that Hg no longer sets best limit on $\bar{\theta}_{QCD}$.

Our result with SkO'

$$\langle S_z \rangle_{\mathrm{Hg}} = 0.006\ g\bar{g}_0\ + 0.07\ g\bar{g}_1\ + 0.009\ g\bar{g}_2\ \ (\mathrm{e\ fm}^3)$$

Results with other Skyrme interactions are the same to within factors of 2 or 3. Finally...

It's possible to improve these calculations, but not easy!

THE END