Nuclear Schiff moment

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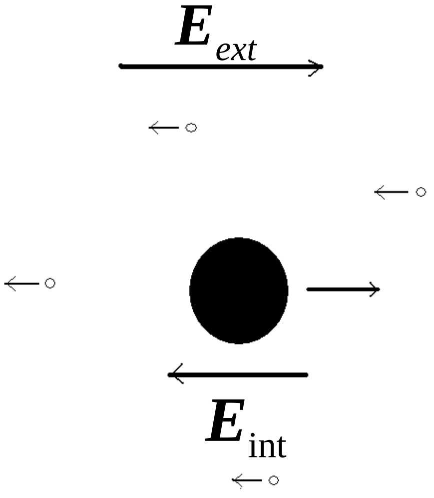
Schiff theorem

The energy of a neutral atom with a point like nucleus in an external electric field does not depend on a nuclear dipole moment.

This is true for electron dipole moment as well.

$$\boldsymbol{E}(0) = 0$$



Schiff moment operator (P- T-violating nuclear forces)

$$H_0 = \sum_a \frac{\boldsymbol{p}_a^2}{2m} - e\phi\left(\boldsymbol{r}_a\right) + \sum_{a \neq b} V\left(\boldsymbol{r}_a - \boldsymbol{r}_b\right) - \boldsymbol{d} \cdot \boldsymbol{E}_{ext} + e\sum_a \boldsymbol{r}_a E \cdot_{ext}$$

$$\langle [\boldsymbol{P}_e, H_0] \rangle = 0$$

$$\langle \sum_a e\nabla_a \phi\left(\boldsymbol{r}_a\right) \rangle - ZeE_{ext} = 0$$

In first order in a dipole moment and an external field we can add to the Hamiltonian the following expression:

$$-\frac{\vec{d}}{Z}\cdot\sum_a \vec{\nabla}_a \phi\left(\boldsymbol{r}_a\right)+\vec{d}\cdot\vec{E}_{ext}$$

One should remember that in this equation $\phi\left(\boldsymbol{r}\right)$ should be understood as a mean value over nuclear ground state, since

$$\left\langle d\cdot\nabla\phi\left(\boldsymbol{r}\right)\right\rangle_{nuc}\neq\left\langle d\right\rangle_{nuc}\cdot\left\langle\nabla\phi\left(\boldsymbol{r}\right)\right\rangle_{nuc}$$

We obtain $$H' = H_0-\frac{\vec{d}}{Z}\cdot\sum_a \vec{\nabla}_a \phi\left(\boldsymbol{r}_a\right)+\vec{d}\cdot\vec{E}_{ext}$$

$$H' = \sum_a\frac{\boldsymbol{p}_a^2}{2m}-e\tilde{\phi}\left(\boldsymbol{r}_a\right)+\sum_{a\neq b}V\left(\boldsymbol{r}_a-\boldsymbol{r}_b\right)+e\sum_a\boldsymbol{r}_a E_{ext}$$

where $$\tilde{\phi}(\boldsymbol{r}) = \int d^3 r' \frac{\rho_c(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + \frac{d\cdot\nabla}{Ze}\int d^3 r' \frac{\rho_c(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}$$

Expansion of $\rho_c(\boldsymbol{r})$

$$\rho_c(\boldsymbol{r}) = \sum_p e\delta(\boldsymbol{r}-\boldsymbol{r}_p) \approx Ze\delta(\boldsymbol{r}) - \sum_p e r_p^i \nabla^i \delta(\boldsymbol{r}) + \frac{1}{2}\sum_p e r_p^i r_p^j \nabla^i \nabla^j \delta(\boldsymbol{r})$$
$$-\frac{1}{6}\sum_p e r_p^i r_p^j r_p^k \nabla^i \nabla^j \nabla^k \delta(\boldsymbol{r}) + \ldots$$

$$\nabla^i\nabla^j\nabla^k - \frac{1}{5}(\delta_{ij}\nabla^k + \delta_{jk}\nabla^i + \delta_{ik}\nabla^j)\Delta + \frac{1}{5}(\delta_{ij}\nabla^k + \delta_{jk}\nabla^i + \delta_{ik}\nabla^j)\Delta$$

Dipole component

$$4\pi S^i \nabla^i \delta(\boldsymbol{r})$$ where

$$S^i = \frac{1}{10}\sum_p e\langle r_p^2 r^i\rangle - \frac{1}{6}\sum_p e\langle r^i\rangle\langle r_c\rangle - \frac{1}{15}\frac{\langle Q_{ij}\rangle}{Z}\sum_p e\langle r_p^j\rangle$$

$$\hat{S}^i = \frac{1}{10}\left(\sum_p e r_p^2 r^i - \frac{5}{3}\sum_p e r^i \langle r_c^2\rangle - \frac{2}{3}\frac{\langle Q_{ij}\rangle}{Ze}\sum_p e r_p^j\right)$$

The form of the above equation for the schiff moment is unique.
The coefficient 5/3 is fixed by condition of absence of the ghost dipole mode which corresponds to displacement of the nucleus as a whole.

Under small displacement the nuclear isoscalar density transforms as $\rho_0(\boldsymbol{r}+\boldsymbol{a})=\rho_0(\boldsymbol{r})+\boldsymbol{a}\frac{\partial\rho_0}{\partial\boldsymbol{r}}$

The transition density is: $\rho_{tr}(\boldsymbol{r})=\frac{\partial\rho_0}{\partial\boldsymbol{r}}$

The absence of the ghost mode means that the integral of the isoscalar part of the Schiff moment operator with this transition density must yield zero.

$$\int d^3r\, S_0^i(r)\frac{\partial\rho_0}{\partial r^i}=\int d^3r\,\frac{1}{10}\left(r^2r^i-\frac{5}{3}r^i\langle r_0^2\rangle-\frac{2}{3}\frac{Q_{ij}}{Z}r^j\right)\frac{\partial\rho_0}{\partial r^i}=0$$

P and T violating NN-interaction

$$W(\vec{r}_1-\vec{r}_2)=-\frac{g_\pi}{8\pi m_p}\left[(g_0\vec{\tau}_1\cdot\vec{\tau}_2+g_2(\vec{\tau}_1\cdot\vec{\tau}_2-3\tau_1^3\tau_2^3))(\vec{\sigma}_1-\vec{\sigma}_2)+g_1(\tau_1^3\vec{\sigma}_1-\tau_2^3\vec{\sigma}_2)\right]\cdot\vec{\nabla}_1\frac{\exp(-m_\pi r_{12})}{r_{12}}.$$

Opposite parity contribution to nuclear mean field

$$\delta U_{dir}(\vec{r})=\frac{g_\pi m_\pi^2}{\pi m_p}(\vec{\sigma}\cdot\vec{n})\tau^3\int_0^\infty r'^2 dr' b(r,r')\left[(g_0-2g_2)(\rho_p(r')-\rho_n(r'))+g_1(\rho_p(r')+\rho_n(r'))\right]$$

$$\frac{Z-N}{A}$$

Correction to a single particle orbit wave function $\delta\psi_\nu(r)$

$$\langle\nu|S|\nu\rangle=\langle\delta\psi_\nu|S|\psi_\nu\rangle+\langle\psi_\nu|S|\delta\psi_\nu\rangle$$

Core polarization

Response of the core particles to the strong residual interaction with the valence nucleon creates an additional contribution to the Schiff moment.

$$\langle \nu' | \tilde{S} | \nu \rangle = \langle \nu' | S^0 | \nu \rangle + \sum_{\mu' \mu} \langle \mu | \tilde{S} | \mu' \rangle \frac{n_\mu - n_{\mu'}}{\epsilon_\mu - \epsilon_{\mu'} + \omega} \langle \nu' \mu' | F + W | \mu \nu \rangle$$

$$|\mu\rangle \rightarrow \psi_\mu + \delta \psi_\mu$$

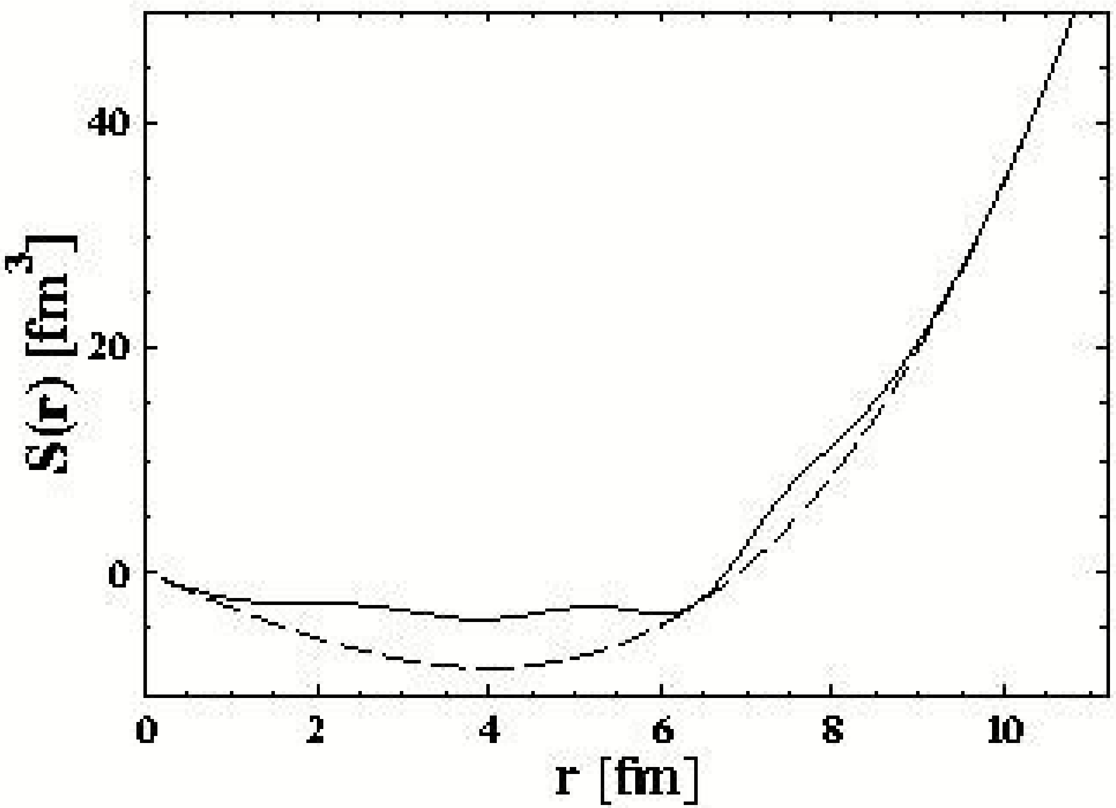
$$\langle \nu | \tilde{S} | \nu \rangle = \langle \delta \psi_\nu | \tilde{S} | \psi_\nu \rangle + \langle \psi_\nu | \tilde{S} | \delta \psi_\nu \rangle + \langle \psi_\nu | \delta S | \psi_\nu \rangle$$

Elimination of the ghost mode contribution

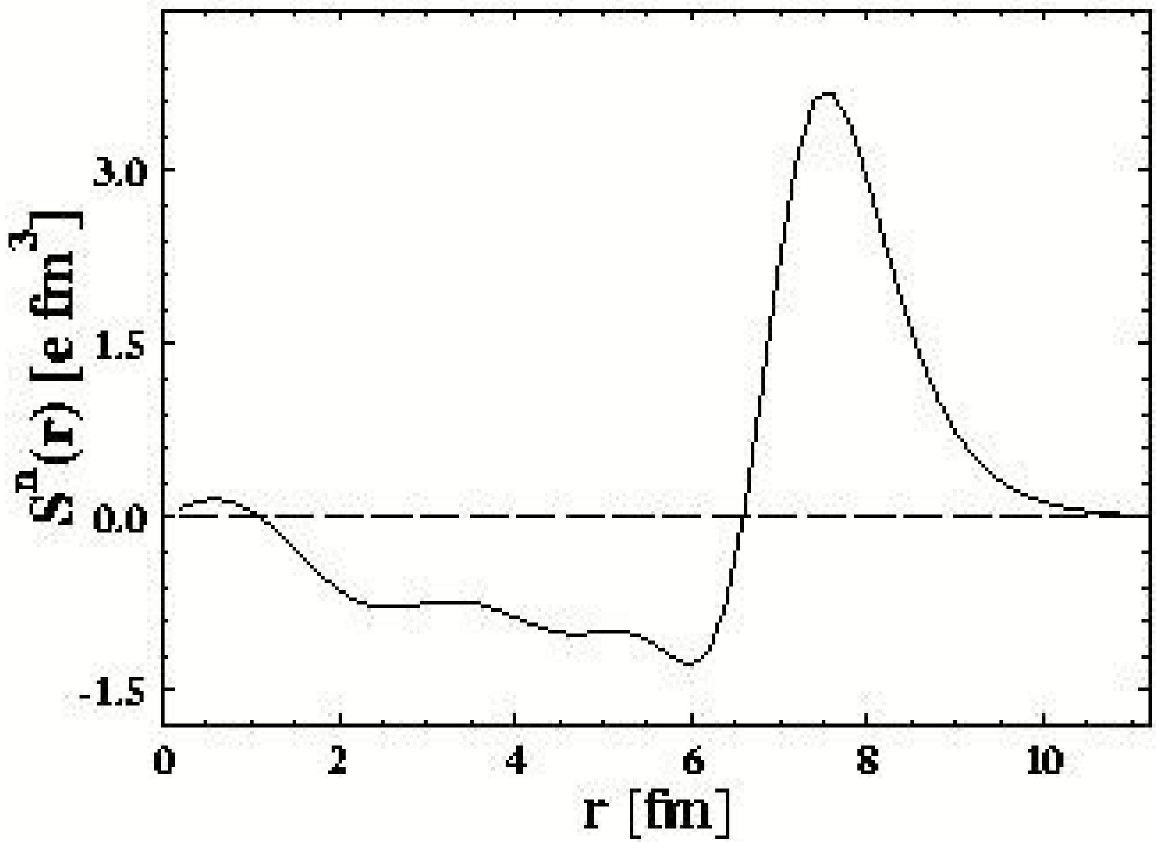
$$S(r|\omega)=\frac{a(r)}{\omega^2-\omega_0^2}+b(r|\omega=0)+O(\frac{\omega^2}{E_{ex}^2})$$

$$J_n(r)=\oint \omega^n S(r|\omega)\,d\omega \qquad \omega_0 \ll |\omega| \ll E_{ex}$$

$$b(r|\omega=0)=J_{-1}(r) \qquad \omega_0^2=J_3(r)/J_1(r)$$



The proton component of the Schiff moment. Solid curve is the renormalized operator after subtraction of the ghost mode, dashed curve is the bare operator.



The neutron component of the renormalized Schiff moment.

Results for Mercury nucleus.

$$S = -0.0004 g_\pi g_0 - 0.055 g_\pi g_1 + 0.009 g_\pi g_2 \left[e \cdot fm^3\right]$$

J. H. de Jesus and J. Engel (2005)

$$S = -0.007 g_\pi g_0 - 0.071 g_\pi g_1 + 0.018 g_\pi g_2 \qquad 0.057 \div 0.090$$

For atomic EDM we have the upper bound $d(Hg) < 2.1 \times 10^{-28} e \cdot cm$

Combining our result with calculations of the atomic EDM (Flambaum et al.) we obtain $g_1 < 0.5 \times 10^{-11}$.

The standard model estimates is $g_1 \approx 10^{-17}$

Nucleon dipole moments contribution

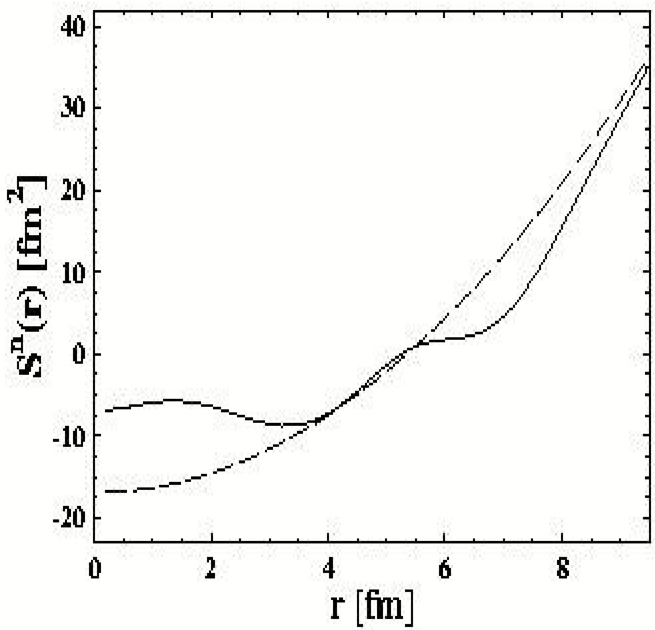
$$\tilde{\phi}(\boldsymbol{r}) = \int d^3r' \frac{\rho_c(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + \frac{d\cdot\nabla}{Ze}\int d^3r' \frac{\rho_c(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} \qquad \vec{d}=\sum_a \vec{d}_a$$

$$\rho_c(\vec{r})=\sum_p e\,\delta(\vec{r}-\vec{r}_p)-\sum_a \vec{d}_a\cdot\vec{\nabla}\,\delta(\vec{r}-\vec{r}_a)$$

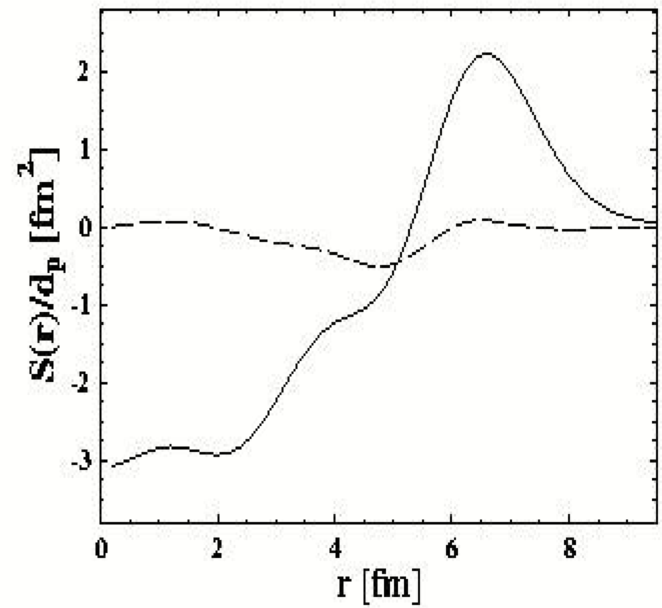
Repeating the expansion over nucleon coordinates and separating the dipole component we obtain for the Schiff moment

$$S^i=\frac{1}{6}\sum_a d_a^i(r_a^2-\langle r^2\rangle_c)+\frac{1}{15}\sum_a d_a^j[(3\mathrm{r}_a^i r_a^j-\delta^{ij} r_a^2)-\frac{\langle Q_{ij}\rangle}{Ze}]$$

$$\langle \nu'|\tilde{S}|\nu\rangle = \langle \nu'|S^0|\nu\rangle + \sum_{\mu'\mu} \langle \mu|\tilde{S}|\mu'\rangle \frac{n_\mu - n_{\mu'}}{\epsilon_\mu - \epsilon_{\mu'}} \langle \nu'\mu'|F|\mu\nu\rangle$$



Polarization effects for the neutron component of the Schiff moment.



Radial dependence of the proton component of the Schiff moment induced by core polarization. Dashed curve is the tensor component.

Results for Hg

$$S = s_p d_p + s_n d_n \qquad s_p = 0.20 \pm 0.02\, fm^2 \qquad s_n = 1.895 \pm 0.035\, fm^2$$

From the atomic calculations, cited above, we have

$$d = -2.8 \times 10^{-17} S \; \left[e\, fm^3 \right]$$

From the experiment this implies for the Schiff moment

$$|S(Hg)| < 0.75 \times 10^{-11}\, e\, fm^3$$

$$|d_p| < 3.8 \times 10^{-24}\, e\, cm, \quad |d_n| < 4.0 \times 10^{-25}\, e\, cm.$$

Existing upper limit for the neutron dipole moment is: $d_n < 0.63 \times 10^{-25}\, e\, cm$

For the proton dipole moment the existing upper limit was:

$$d_p < (-4 \pm 6) \times 10^{-23}\ e\,cm$$

Theoretical uncertainty

The value +- 0.02 cited above does not reflects the real accuracy of the theory. It came from the differences in adopted values of the residual interaction constants. The uncertainty in calculations of the core polarization using RPA with effective forces can be estimated from the following considerations. Using RPA with effective forces we can fit different nuclear moments in one nucleus. Then, in neighbor nuclei the calculated moments will differ from the data. This difference can be regarded as an uncertainty in our theory. In our experience this difference is of the order of 20% on average, reaching sometimes the value of 30%. To be safe we can adopt a conservative 30% uncertainty in calculations of s_p. It gives

$$s_p = 0.2 \pm 0.06\ fm^2$$

For the proton dipole moment we obtain $|d_p| < 5.4 \times 10^{-24}\ e\,cm$

Relativistic corrections

Relativistic corrections appear in higher order terms of charge density expansion. The first correction comes from

$$-\frac{1}{120}\sum_p r_p^i r_p^j r_p^k r_p^l r_p^m \nabla^i \nabla^j \nabla^k \nabla^l \nabla^m \delta\left(\boldsymbol{r}\right)$$

The atomic matrix element for the correction contains higher order derivatives of the electron wave functions at r= 0.
It is convenient to expand the product of radial wave functions near r= 0.
For Dirac wave functions

$$f_s\left(r\right) f_p\left(r\right) + g_s(r) g_p\left(r\right) = \sum_{k=1} b_k r^k$$

With this expansion all the corrections can be summed in a new P- and T- odd so called LOCAL DIPOLE MOMENT

$$\boldsymbol{L} = e \sum_{k=1,3,5...} b_k \frac{1}{(k+1)(k+4)}\left[\langle \boldsymbol{r} r^{k+1}\rangle - \frac{k+4}{3}\langle \boldsymbol{r}\rangle\langle r^{k+1}\rangle\right]$$

The first term is just the Schiff moment and the other terms are the relativistic corrections. The coefficients b_k can be calculated analytically for a uniformly charged sphere. For the first correction we have

$$b_3 = -\frac{3}{5}\frac{(Z\alpha)^2}{R_N^2} b_1 \text{ for } s - p_{1/2} \text{ atomic transition}$$

$$b_3 = -\frac{9}{20}\frac{(Z\alpha)^2}{R_N^2} b_1 \text{ for } s - p_{3/2} \text{ atomic transition}$$

Results for the first correction

$$\boldsymbol{L}' = \frac{1}{28}\left(\langle \boldsymbol{r} r^4 \rangle - \frac{7}{3} \langle \boldsymbol{r} \rangle \langle r^4 \rangle \right)$$

	^{205}Tl				^{199}Hg			
	S_0	L'_0/S_0	S_{tot}	L'_{tot}/S_{tot}	S_0	L'_0/S_0	S_{tot}	L'_{tot}/S_{tot}
g_0	-0.075	-0.09	0.014	-0.18	-0.085	-0.1	-0.006	-0.05
g_1	-0.028	-0.39	-0.082	-0.18	-0.085	-0.1	-0.036	-0.15
g_2	0.237	-0.08	-0.007	-0.51	0.17	-0.1	0.019	-0.08

Table 1: Schiff moment S and the ratio of relativistic correction L' to S ($L = S + L'$) for proton odd ^{205}Tl and neutron odd ^{199}Hg nuclei. S_0 and L'_0 are the bare values, without strong residual nuclear forces. S_{tot} and L'_{tot} are the total results with full account of core polarization effects. The values of L'/S are given for $s - p_{1/2}$ transition. For $s - p_{3/2}$ transition they differ by the factor $3/4$. To obtain values of L and S one should sum up contributions of three interaction constants g_0, g_1 and g_2.

Conclusions

Calculations of nuclear Schiff moments combined with atomic structure calculations and data from atomic experiments can bring new information about such fundamental quantities like nucleon dipole moments.
Effects of nuclear polarization are important and should be taken into consideration in calculations of the Schiff moment.
Relativistic corrections are sizable for heavy atoms and should not be ignored either.