Schiff screening of relativistic nucleon electric-dipole moments by electrons

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We show, at leading-order in the multipole expansion of the electron-nucleus interaction, that nucleon electric-dipole moments are completely shielded by electrons so that they contribute nothing to atomic electric-dipole moments, even when relativity in the nucleus is taken into account. It is well known that relativistic electron motion, by contrast, leads to dipole moments that are not screened; we discuss the reasons for the difference.

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Some years ago, Schiff [1] showed that in the limit of a point-like nucleus and nonrelativistic electrons any electric-dipole moments (EDMs) carried by the electrons and nucleus are completely screened by atomic polarization, so that the EDM of the atom vanishes. Shortly thereafter, Sandars [2] pointed out that in heavy polarizable atoms, relativistic corrections to the electron-EDM operator not only survive screening but can enhance atomic EDMs. For nucleons in a nucleus, v/c is about 0.1, and one may wonder whether relativity allows nucleon EDMs to evade screening at some level. Reference [3] claims that it does, at a level much larger than that resulting from the finite size of the nucleus. The authors use the result to argue that the limit on the neutron EDM from experiments in ^{199}Hg should be $|d_n| \lesssim 2.5 \times 10^{-26} e$ cm, a value nearly an order of magnitude tighter than the generally accepted limit, $|d_n| \lesssim 4 \times 10^{-25} e$ cm [4], and comparable to the current best limit from direct measurement, $|d_n| < 2.9 \times 10^{-26} e$ cm [5]. But nucleons are different from electrons in that they are confined to a much smaller volume. This confinement, as we show below, implies that relativistic contributions to nucleon EDMs are just as screened as their nonrelativistic counterparts. To see this, let us divide the parity-and-time-reversal-conserving part of the system's internal Hamiltonian H_0 into a piece that involves electrons only—the electron kinetic energy and electron-electron interactions—a corresponding part that involves nucleons only, and a part that contains the electron-nucleon interaction:

$$H_0 = H_e^{\mathrm{int}} + H_{\mathrm{nuc}}^{\mathrm{int}} + H_{e\text{—nuc}}, \tag{1}$$

where "int" stands for internal. We expand the electron–nucleus part of H_0 (which is the same Hamiltonian as the H_0 in Eq. (2.3) of Ref. [3]) in multipoles:

$$H_{e\text{—nuc}} = \sum_{i=1}^{Z} \frac{Ze^2}{r_i} + \cdots, \tag{2}$$

where $r_i \equiv |\boldsymbol{r}_i|$ is the coordinate of the i^{th} electron. We shall neglect in this discussion the sub-leading terms "...," which involve nuclear moments (static and local) beyond the lowest-order monopole. These higher moments, corresponding to what are often called "finite-size effects," do in fact allow Schiff screening to be evaded, but at a low level that is systematically discussed in Ref. [6]. The effects on the screening of nuclear EDMs due to relativistic electrons, which we also neglect, are not large either: according to Ref. [7], they correct the finite-size effects in heavy atoms by a few tens of percent.

We can now calculate corrections to the ground-state energy induced by the parity- and time-reversal-violating interaction of the nucleon dipole moments with an external electric field $\boldsymbol{E}_{\mathrm{ext}}$. The first-order shift is

$$\Delta E^{(1)} = -\langle \mathrm{g.s.}| \sum_{j=1}^{A} d_N^j \, \gamma_j^0 \, \boldsymbol{\Sigma}_j |\mathrm{g.s.}\rangle \cdot \boldsymbol{E}_{\mathrm{ext}}, \tag{3}$$

where $\gamma_j^0 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ is the Dirac matrix for the j^{th} nucleon, $\boldsymbol{\Sigma}_j = \left(\begin{smallmatrix} \boldsymbol{\Sigma}_j & 0 \\ 0 & \boldsymbol{\Sigma}_j \end{smallmatrix}\right)$ is the spin operator for that nucleon, d_N^j is the magnitude of the EDM for the same nucleon, and $|\mathrm{g.s.}\rangle$ is the ground state of the unperturbed Hamiltonian H_0. Often the relativistic operator in Eq. (3) is divided into two pieces by writing γ^0 as $1 + (\gamma^0 - 1)$; the second piece is then purely relativistic (see, e.g., Ref. [2]). Reference [3] makes this split because it assumes that the relativistic corrections are unshielded, i.e., not canceled by atomic polarization. We do not make the split because in the limit where the nucleus is very small, as we show below, that assumption is not justified.

To see that no portion of the dipole operator is left unscreened in the point-like (lowest-order monopole) limit, we calculate the second-order addition to Eq. (3) from polarization of the electrons. With the nucleus kept in its ground state (see below for justification), this contribution is

$$\begin{aligned}\Delta E^{(2)} &= -\sum_n \frac{1}{E_{\mathrm{g.s.}} - E_n} \langle \mathrm{g.s.}| \left(\sum_{j=1}^{A} d_N^j \, \gamma_j^0 \, \boldsymbol{\Sigma}_j \right) \cdot \left(\sum_{i=1}^{Z} \nabla_i A_0 \right) |n\rangle \\ &\quad \times \langle n| e \sum_{k=1}^{Z} \boldsymbol{r}_k \cdot \boldsymbol{E}_{\mathrm{ext}} |\mathrm{g.s.}\rangle + \mathrm{H.c.},\end{aligned} \tag{4}$$

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where the label n on the states refers to electronic configurations and A_0 denotes the electric potential at the origin (where the nucleus is located) generated by the electrons:

$$A_0 = \sum_{i=1}^{Z} \frac{e}{r_i} = -\frac{1}{Ze} H_{e\text{—nuc}}. \tag{5}$$

The gradient $\nabla_i A_0$ in Eq. (4) is then just the electric field at the origin produced by the i^{th} electron. In writing these expressions we have assumed only that the full wave function factors into products of atomic and nuclear wave functions to good approximation.

The truncation of the multipole expansion at leading order—the point-like approximation—allows us to restrict attention to the electric field at the origin and write $H_{e\text{—nuc}}$ in terms of electron operators only in Eq. (5). As a consequence, the nuclear state is not perturbed; excited nuclear states do not contribute to Eq. (4), even if the coupling of nucleons to $\boldsymbol{E}_{\text{ext}}$ is included (nuclear polarization). For there to be a contribution, the excitations would have to be created by a nuclear operator with positive parity (i.e., $\boldsymbol{\Sigma}$) and destroyed by one with negative parity (i.e., $\boldsymbol{r}$). That can not happen, however, because $H_{\text{nuc}}^{\text{int}}$ is symmetric under reflection so that all unperturbed nuclear states have good parity.

These facts allow us to evaluate the sum in $\Delta E^{(2)}$. From Eq. (5) it follows that

$$\begin{aligned}
&\left(\sum_{j=1}^{A} d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j\right) \cdot \left(\sum_{i=1}^{Z} \nabla_i A_0\right) \\
&= -\frac{1}{Ze}\left[\sum_{j=1}^{A}\sum_{i=1}^{Z} d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j \cdot \nabla_i,\, H_{e\text{—nuc}}\right] \\
&= -\frac{1}{Ze}\left[\sum_{j=1}^{A}\sum_{i=1}^{Z} d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j \cdot \nabla_i,\, H_0 - H_e^{\text{int}} - H_{\text{nuc}}^{\text{int}}\right].
\end{aligned} \tag{6}$$

Now, noting that

(i) the electron-electron interaction is pair-wise, so that

$$\sum_{i=1}^{Z} \left[d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j \cdot \nabla_i,\, H_e^{\text{int}}\right] = \sum_{i=1}^{Z} d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j \cdot \left[\nabla_i,\, H_e^{\text{int}}\right] = 0, \tag{7}$$

and

(ii) the nucleus is not excited so that the commutator of any nuclear operator with H_{nuc} yields a vanishing expectation value,

$$\begin{aligned}
&{}_{\text{nuc}}\langle \text{g.s.}|\left[d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j \cdot \nabla_i,\, H_{\text{nuc}}^{\text{int}}\right]|\text{g.s.}\rangle_{\text{nuc}} \\
&\quad = {}_{\text{nuc}}\langle \text{g.s.}|\left[d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j,\, H_{\text{nuc}}^{\text{int}}\right]|\text{g.s.}\rangle_{\text{nuc}} \cdot \nabla_i = 0,
\end{aligned} \tag{8}$$

we can eliminate the energy denominators in $\Delta E^{(2)}$ and perform the sum over intermediate state in closure. The result is

$$\begin{aligned}
\Delta E^{(2)} &= \frac{1}{Z}\langle \text{g.s}|\left[\left(\sum_{j=1}^{A}\sum_{i=1}^{Z} d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j \cdot \nabla_i\right),\, \sum_{k=1}^{Z} \boldsymbol{r}_k \cdot \boldsymbol{E}_{\text{ext}}\right]|\text{g.s.}\rangle \\
&= \langle \text{g.s.}|\sum_{j=1}^{A} d_N^j\, \gamma_j^0\, \boldsymbol{\Sigma}_j|\text{g.s.}\rangle \cdot \boldsymbol{E}_{\text{ext}} = -\Delta E^{(1)},
\end{aligned} \tag{9}$$

so that the first- and second-order contributions cancel each other exactly. Thus, atomic polarization screens the nucleon EDMs even in relativistic quantum theory. The finite size of the nucleus, leading to a difference between the monopole and dipole charge densities, is still the dominant nuclear contribution to the atomic EDM. Relativistic corrections to nuclear wave functions affect the result only a little because their contributions to densities are of $\mathcal{O}(v^2/c^2) \approx 1\%$.

Why then do relativistic corrections to *electron* EDM operators evade screening? The reason is that the γ^0 in the relativistic operator does not commute with the relativistic free-electron Hamiltonian $\gamma_0(m_e + \boldsymbol{p} \cdot \boldsymbol{\gamma})$, so that the first commutator in Eq. (7) does not vanish if the Dirac matrices act on electrons (see Refs. [2,6,8] for details). By contrast, Eq. (8) vanishes even if one uses a relativistic form for the nuclear Hamiltonian because of the expectation value. And as mentioned above, off-diagonal nuclear matrix elements contribute nothing because of the parity symmetry of $H_{\text{nuc}}^{\text{int}}$.

In summary, at leading-order in the multipole expansion for $H_{e\text{—nuc}}$, where the electrons see the nucleus as a point particle, even fully relativistic nucleon EDMs are screened by electron polarization. The effects of relativity in the nucleus will only add small corrections to the usual finite-size effects encoded in the nuclear "Schiff moment."

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