

Stark-induced anapole magnetic fields in atoms

Robert R. Lewis*

Department of Physics, University of Michigan, Ann Arbor, Michigan 48109

S. M. Blinder†

Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109

(Received May 12 1995)

We show that a paramagnetic atom with spin polarization \mathbf{S} , in an electric field \mathbf{E} , will have an anapole moment in the direction $\mathbf{E} \times \mathbf{S}$, with magnitude of order $\alpha E a_0^4$. There is a corresponding toroidal magnetic field inside the atom in the direction $\mathbf{r} \times (\mathbf{E} \times \mathbf{S})$, with strength of order αE . As an example, we evaluate exactly the toroidal field and its anapole moment for hydrogenic atoms to first order in \mathbf{E} , using both the Schrödinger and Dirac equations. We also use the calculated electric polarizabilities to estimate the toroidal magnetic fields and anapole moments for the ground states of the alkali-metal atoms and for Rydberg states. We show that the Stark-induced toroidal magnetic fields of atoms will have no influence on their hyperfine structure. However, they can change the direction of the nuclear spins of electron-spin polarized molecules.

PACS number(s): 31.10.+z, 31.90.+s, 31.15.+q

I. INTRODUCTION

Atoms that have symmetry under both space inversion (P) and time inversion (T) can have only a limited variety of multipole moments: electric multipole moments $E(l)$ with l even and magnetic multipole moments $M(l)$ with l odd. Vaks and Zel'dovich [1] asserted that if the atom does *not* have symmetry under P (but does have symmetry under T), then other multipole moments can also be present: toroidal magnetic multipole moments $T(l)$ with l odd. They invented the term "anapole moment" to describe the toroidal dipole moment $T(1)$. It is conventionally defined [2] as either a second moment of the current density or a first moment of the magnetic field of this current

$$\mathbf{t} \equiv (-\pi/c) \int d^3r r^2 \mathbf{j} = \frac{1}{2} \int d^3r \mathbf{r} \times \mathbf{B}. \quad (1)$$

We see that the anapole moment \mathbf{t} is a polar vector that changes sign under P and T . We also see that the current density must have a component that is *even* under space inversion; this component generates a toroidal magnetic field that is *odd* under space inversion. The anapole moment \mathbf{t} is a convenient measure of the strength and orientation of this magnetic field. For an isolated atom with conserved total angular momentum \mathbf{J} , the vector \mathbf{t} must be oriented along \mathbf{J} ; since these two vectors have opposite transformation properties under space inversion, there must be some mechanism for breaking P invariance. By the same reasoning, T invariance can be preserved; we will not consider the further possibilities that arise if we also break the symmetry in time.

In the customary multipole expansion of the magnetic vector potential, Khriplovich [3] has shown that the toroidal dipole moment (TDM) occurs together with the magnetic-quadrupole moment and therefore has the same dimensions

(e cm^2) and the same signature under inversions. He gave a general estimate of the magnitude of t as the product of three parameters of the atom: the magnetic dipole moment μ , the radius R , and the dimensionless parity mixing amplitude η ,

$$t \approx \mu R \eta. \quad (2)$$

The magnitude of t is therefore a sensitive measure of the mechanism for parity nonconservation in the atom.

There is extensive literature on the calculation of TDMs induced by parity-nonconserving weak interactions. Particles such as the nucleons [4] and leptons [5] have been analyzed, as well as complex nuclei [6] and atoms [7]. In each of these cases, the weakly induced TDM is oriented along the spin of the particle

$$\mathbf{t} \propto \mathbf{S} \quad (3)$$

and has magnitude of order

$$t \approx e G_F / \hbar c = 5 \times 10^{-33} \text{ e cm}^2. \quad (4)$$

Chiral molecules also have broken inversion symmetry and are candidates for having anapole moments [8] if they also have an unpaired spin. The moment can be characterized in terms of a tetrahedral structure of four atoms in the molecule,

$$\mathbf{t} \propto (\mathbf{n}_1 \cdot \mathbf{n}_2 \times \mathbf{n}_3) (\mathbf{S} \cdot \mathbf{n}_3) \{f(r_1, r_2) \mathbf{n}_2 - f(r_2, r_1) \mathbf{n}_1\}. \quad (5)$$

Here the unit vectors $\mathbf{n}_{1,2,3}$ give the displacements of three atoms from the fourth atom and \mathbf{S} is the unpaired spin; the quantity $f(r_1, r_2)$ is a certain function of the internuclear distances. If the molecular sample has random orientation, the average anapole moment is in the direction of the spin polarization

$$\langle \mathbf{t} \rangle \propto (\mathbf{n}_1 \cdot \mathbf{n}_2 \times \mathbf{n}_3) \{f(r_1, r_2) (\mathbf{n}_2 \cdot \mathbf{n}_3) - f(r_2, r_1) (\mathbf{n}_1 \cdot \mathbf{n}_3)\} \langle \mathbf{S} \rangle,$$

assuming that $(\mathbf{n}_1 \cdot \mathbf{n}_3)$ and $(\mathbf{n}_2 \cdot \mathbf{n}_3)$ are nonzero. The magnitude of the TDM is estimated to be

*Electronic address: boblewis@umich.edu

†Electronic address: sbinder@umich.edu

$$t \approx \alpha e a_0^2 = 2 \times 10^{-19} \text{ e cm}^2 \quad (6)$$

and the toroidal magnetic field is of order

$$B_{\text{tor}} \approx \alpha e / a_0^2 = 1 \times 10^7 \text{ G}. \quad (7)$$

This is comparable to the strength of the magnetic dipole field in the vicinity of the molecule.

However, chirality is not a necessary condition for molecular anapole moments: inversion symmetry can also be broken in diatomic molecules that have no chirality. Polar diatomic molecules with an unpaired spin also have anapole moments [9] in the direction

$$\mathbf{t} \propto \mathbf{S} \times \mathbf{n}, \quad (8)$$

where \mathbf{n} is the internuclear axis. If spin-dependent forces are neglected, the vector \mathbf{t} is proportional to a product of the magnetic-dipole moment $\boldsymbol{\mu}$ and the intrinsic electric-dipole moment \mathbf{d} of the molecule

$$\mathbf{t} \equiv (2\pi/e) \boldsymbol{\mu} \times \mathbf{d}. \quad (9)$$

The anapole moments and anapole magnetic fields have about the same magnitude as in chiral molecules, but they do not survive the average over molecular orientation.

In this paper, we will add to the above list by considering the breaking of inversion symmetry in atoms by an electric field. The Stark mixing of opposite-parity states will be shown to induce anapole fields in polarized paramagnetic atoms, satisfying the same product rule (9) with the *Stark induced* dipole moment in place of the *intrinsic* dipole moment.

From the transformation properties under P and T , an atom with spin \mathbf{S} in a static electric field \mathbf{E} can have a TDM in the direction

$$\mathbf{t} \propto \mathbf{E} \times \mathbf{S}. \quad (10)$$

The electric field will mix atomic states of opposite parity with amplitude

$$\eta \approx E / (e a_0^2). \quad (11)$$

According to the estimate in Eq. (2), the anapole moment is expected to have magnitude

$$t \approx \alpha E a_0^4 \quad (12)$$

and a toroidal magnetic field of order

$$B_{\text{tor}} \approx \alpha E. \quad (13)$$

Even for strong laboratory fields of 3×10^4 V/cm, this would give toroidal magnetic fields weaker by five orders of magnitude than the intrinsic effects in the molecules discussed above. The direction and strength of \mathbf{t} in atoms can be reconciled with the results for diatomic molecules by noting that the internal electric field in a diatomic molecule is along the molecular axis and approximately five orders of magnitude greater than this laboratory field. The underlying mechanism for inducing the anapole moment in atoms is essentially the same Stark effect, caused by *external* rather than *internal* electric fields.

The plan of this paper is as follows. In Sec. II we will state the basic relations needed for calculation of the toroidal magnetic field of an atom. In Sec. III we will evaluate this field in nonrelativistic hydrogenic atoms to first order in the electric field, using the Sternheimer method. In Sec. IV we will calculate the relativistic corrections to these results, as a test of the product rule. Sections V and VI contain estimates of the anapole moments of alkali atoms and of Rydberg states, using the known electric polarizabilities and the product rule. In Sec. VII we will discuss the experimental consequences of these results, especially in the hyperfine structure of spin-polarized atoms and molecules. Finally, we will summarize our conclusions in Sec. VIII.

II. CLASSICAL THEORY

Previous papers on toroidal multipoles have, in our opinion, overemphasized the role of the toroidal dipole *moment* and said little about the toroidal magnetic *field*. This comes from treating the source as a "point particle," suppressing its internal structure. This is appropriate for the interaction between nuclear anapole moments and atomic electrons because the nuclear dimensions are very small on the atomic scale. But for analyzing anapole effects of the electrons in atoms, we must consider the variation of the toroidal magnetic field over atomic dimensions. Our plan is to calculate first the toroidal magnetic field; it is then relatively easy to get the anapole moment \mathbf{t} by integration,

$$\mathbf{t} \equiv \frac{1}{2} \int d^3r \mathbf{r} \times \mathbf{B}. \quad (14)$$

The basic equation needed for evaluation of this field has been derived by Boston and Sandars [10] and in Ref. [11]. It directly relates the toroidal magnetic field, whose form is

$$\mathbf{B}_{\text{tor}} = g(r) \mathbf{r} \times \mathbf{m} \quad (15)$$

to a poloidal current density varying like

$$\mathbf{j}_{\text{pol}} = (1/r)(df/dr)[\mathbf{r}(\mathbf{r} \cdot \mathbf{m}) - r^2 \mathbf{m}] - 2f \mathbf{m}. \quad (16)$$

Notice that the radial function $f(r)$ can be obtained by evaluating the radial component of this current

$$\hat{\mathbf{r}} \cdot \mathbf{j}_{\text{pol}} = -2f \mathbf{m} \cdot \hat{\mathbf{r}}.$$

Here \mathbf{m} is a fixed vector giving the orientation of the anapole moment. As a prototype, we can picture the toroidal field inside a torus, with a poloidal current flowing on its surface; \mathbf{m} is along the symmetry axis. Insertion of these formulas into Maxwell's relation shows that, within a factor, these two vector fields have the same radial form

$$g(r) = (4\pi/c)f(r). \quad (17)$$

The anapole moment is in the direction of the dummy vector $\hat{\mathbf{m}}$; its magnitude is proportional to the fourth moment of $f(r)$,

$$\mathbf{t} = -(16\pi^2/3c) \mathbf{m} \int_0^\infty dr r^4 f(r). \quad (18)$$

This implies that the toroidal magnetic field is confined to the region of current and has no “long-range” part, like the ordinary magnetic dipole field. This is the main distinguishing feature of toroidal dipole fields and explains why they are hard to detect. We also notice that if the current density remains finite at the origin $f(0) \neq 0$, then the toroidal magnetic field must vanish linearly with r . For the torus, the current density and field will vanish identically in the “hole;” we can also see that the radial component of the surface current, and therefore the magnetic field, vanishes along the equatorial circles.

To summarize these results, one can evaluate the toroidal dipole field of any current density by first finding the poloidal dipole component of the current [Eq. (15)]. The toroidal magnetic field is everywhere proportional to the radial component of this current density. The anapole moment is given by the first moment of the magnetic field.

III. NONRELATIVISTIC HYDROGENIC ATOMS

We can convert the classical relations to quantum theory by inserting the appropriate current densities. For the Schrödinger equation, the current density can be split into “orbital” and “spin” parts [12]

$$\mathbf{j} = \mathbf{j}_L + \mathbf{j}_S,$$

defined as

$$\mathbf{j}_L = (1/2i)[(\nabla\Psi)^*\Psi - \Psi^*(\nabla\Psi)], \quad (19a)$$

$$\mathbf{j}_S = -\frac{1}{2}\nabla \times [\Psi^* \boldsymbol{\sigma} \Psi]. \quad (19b)$$

These are given in atomic units, which will be used throughout this section. We will denote the perturbed wave function as Ψ and the unperturbed as ψ , in order to distinguish them. For the *unperturbed* ground state of a hydrogenlike atom

$$\psi_{1S} = (Z^3/\pi)^{1/2} e^{-Zr} \chi \quad (20)$$

the spin current density is

$$\mathbf{j}_S = (2Z^4/\pi) \hat{\mathbf{r}} \times \mathbf{S} e^{-2Zr}, \quad (21)$$

where $\mathbf{S} = \langle \boldsymbol{\sigma} \rangle / 2$ is the atomic spin in units of \hbar and $\hat{\mathbf{r}}$ is a unit vector. This current results from the nonuniform distribution of the magnetic moment of the electron. It is a toroidal current, odd under inversions, that generates the ordinary magnetic dipole field of the electron. The orbital current in this state is zero because of reality (T invariance).

We can evaluate the effect of an applied E field on the ground state using the Sternheimer method [13], writing the perturbed wave function as

$$\Psi_{1S} \equiv \psi_{1S} + \psi'_{1S}.$$

The “response function” ψ' satisfies the inhomogeneous equation

$$[H_{\text{Sch}} - E_{1S}] \psi'_{1S} = -(\mathbf{E} \cdot \mathbf{r}) \psi_{1S},$$

where H_{Sch} is the Schrödinger Hamiltonian. The notation used here denotes perturbed wave functions by Ψ , unperturbed by ψ , and response functions by ψ' .

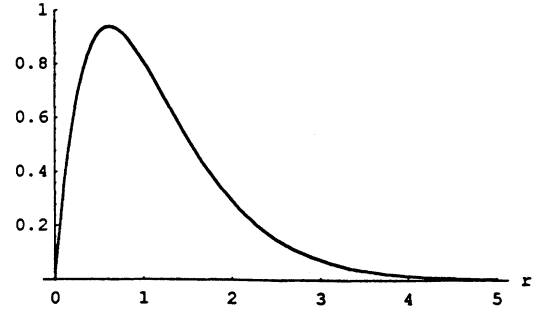


FIG. 1. Radial dependence of the toroidal magnetic field of the Schrödinger hydrogen atom, in units of $\alpha(\mathbf{E} \times \mathbf{S}) \sin \theta$, versus the radial distance in a.u.

turbed by ψ , and response functions by ψ' . The solution for the hydrogen atom is well known [14],

$$\psi'_{1S} = -(\mathbf{E} \cdot \mathbf{r}/Z^2)(1 + Zr/2) \psi_{1S} \quad (22)$$

so that the first-order wave function is

$$\Psi_{1S} = [1 - (\mathbf{E} \cdot \mathbf{r})(1 + Zr/2)/Z^2] \psi_{1S}, \quad (23)$$

which no longer has even parity. The electron is pushed in a direction opposite to \mathbf{E} and the atom acquires an induced electric dipole moment $\mathbf{d} = \alpha_E \mathbf{E}$, corresponding to a polarizability

$$\alpha_E = 9/2Z^4. \quad (24)$$

The same distortion of the wave function also changes the current density and the magnetic field. The current density acquires an additional *poloidal* component

$$\mathbf{j}'_S = (2Z/\pi)[(1 + Zr/2)\mathbf{E} \times \mathbf{S} - Z(3/2 + Zr)(\mathbf{E} \cdot \mathbf{r})\hat{\mathbf{r}} \times \mathbf{S}] e^{-2Zr}. \quad (25)$$

It is even under inversions and proportional to the electric field. This spin current density generates the toroidal magnetic field. The orbital current remains zero.

The radial function of the poloidal current $f(r)$ can be found by evaluating its radial component

$$-2f(r)\hat{\mathbf{r}} \cdot \mathbf{m} \equiv \hat{\mathbf{r}} \cdot \mathbf{j}'_S = (2Z/\pi)(1 + Zr/2)e^{-2Zr}[\hat{\mathbf{r}} \cdot (\mathbf{E} \times \mathbf{S})]. \quad (26)$$

If we identify \mathbf{m} with $\mathbf{E} \times \mathbf{S}$, then the radial function is

$$f(r) = -(Z/\pi)(1 + Zr/2)e^{-2Zr}. \quad (27)$$

We find for the toroidal magnetic field,

$$\mathbf{B}_{\text{tor}} = (4\alpha Z)(1 + Zr/2)e^{-2Zr}[(\mathbf{E} \times \mathbf{S}) \times \mathbf{r}]. \quad (28)$$

It has strength of order αE , with field lines that are circles around the direction $(\mathbf{E} \times \mathbf{S})$; the dependence on r is shown in Fig. 1. It decreases exponentially at large distance and is zero at the origin. Equations (15)–(17) show that this latter property is a general feature of toroidal dipole fields for any

current density that remains finite at the origin; there is no field in the “hole” of the donut.

We can easily evaluate the first moment of this field to obtain the anapole moment (in cgs units)

$$\mathbf{t} = \mathbf{t}_S = (9\pi\alpha/Z^4)\mathbf{E} \times \mathbf{S}a_0^4. \quad (29)$$

As we found in diatomic molecules [9], this result for the anapole moment can be expressed as a product of the magnetic dipole moment ($\boldsymbol{\mu} = -\alpha e a_0 \mathbf{S}$) and the induced electric dipole moment ($\mathbf{d} = \alpha_E \mathbf{E}$)

$$\mathbf{t} = (2\pi/e)\boldsymbol{\mu} \times \mathbf{d}. \quad (9')$$

This relationship comes from the separability of space and spin factors in the wave function and the neglect of spin-dependent forces. It is useful approximation valid for light atoms, to order $(\alpha Z)^2$. To leading order in αZ , the anapole moment can be predicted from the better known electric and magnetic dipole moments. We would like to use relation (9) to survey anapole moments of other atomic states, but will first examine its accuracy by considering corrections coming from the spin-orbit interaction and other relativistic effects.

IV. RELATIVISTIC HYDROGENIC ATOMS

The presence of the spin-orbit interaction and other relativistic effects makes significant corrections to the toroidal magnetic field. These can be obtained in one-electron atoms by repeating the above derivation with the Dirac Hamiltonian. The principal reason for doing this is to assess the accuracy of the “product rule,” which we want to use as the basis for estimating anapole moments in other atoms.

As in the nonrelativistic theory, we can find the first-order change in the ground-state wave function by solving the Sternheimer equation

$$[H_D - E_{1S}]\psi' = -(\mathbf{E} \cdot \mathbf{r})\psi_{1S}, \quad (30)$$

where H_D is the Dirac Hamiltonian. The calculation of anapole moments in Dirac theory has been discussed by Boston and Sandars in Ref. [10]; we will use the same notation as these authors. The toroidal magnetic field and the anapole moment are derived by the general procedure in Sec. III, using the poloidal current density induced by the electric field

$$\mathbf{j}' = c\psi_{1S}^\dagger \boldsymbol{\alpha} \psi' + \text{H.c.} \quad (31)$$

In order to simplify the discussion, we neglect hyperfine structure terms of order α/M . This suppresses the role of the nuclear spin, leaving a hydrogenic atom with only electronic variables. We choose the electric field with strength \mathcal{E} along the quantization axis, $\mathbf{E} = \mathcal{E}\hat{\mathbf{z}}$. The electronic wave functions are written in the form of four-component spinors

$$\psi_\kappa^m = (1/r)\{P_\kappa(r)u_\kappa^m, iQ_\kappa(r)u_{-\kappa}^m\}, \quad (32)$$

where u_κ^m is the normalized two-component spinor with quantum numbers ljm , and $u_{-\kappa}^m$ is the corresponding spinor for the state with the same j [15]. The eigenvalues and wave functions of the unperturbed states are well known.

In the presence of the electric field, the spin and orbital angular momentum are no longer conserved separately but are coupled together. The Sternheimer equation (27) must be decomposed into a sum of terms with the angular dependence of $p_{1/2}$ and $p_{3/2}$ states and then solved separately. The inhomogeneous term of the Sternheimer equation is a linear combination of $p_{1/2}, p_{3/2}$ states,

$$\begin{aligned} \mathcal{E}r \cos\theta \psi_{-1}^m &= A_m \mathcal{E}\{P_{-1}u_{+1}^m, iQ_{-1}u_{-1}^m\} \\ &+ B_m \mathcal{E}\{P_{-1}u_{-2}^m, iQ_{-1}u_{+2}^m\}, \end{aligned} \quad (33)$$

where

$$A_m = \mp \frac{1}{3}, \quad B_m = \sqrt{2}/3.$$

We parametrize the response function in a similar way,

$$\psi_{-1}^m \equiv A_m \psi_{+1}^m + B_m \psi_{-2}^m, \quad (34)$$

where

$$\begin{aligned} \psi_{+1}^m &\equiv (1/r)\{P'_{+1}(r)u_{+1}^m, iQ'_{+1}(r)u_{-1}^m\}, \\ \psi_{-2}^m &\equiv (1/r)\{P'_{-2}(r)u_{-2}^m, iQ'_{-2}(r)u_{+2}^m\}. \end{aligned}$$

The Sternheimer equation is now separated into two portions with common angular factors

$$\begin{aligned} (\gamma c^2 - H_D)\psi_{+1}^m &= \mathcal{E}\{P_{-1}u_{+1}^m, iQ_{-1}u_{-1}^m\}, \\ (\gamma c^2 - H_D)\psi_{-2}^m &= \mathcal{E}\{P_{-1}u_{-2}^m, iQ_{-1}u_{+2}^m\}. \end{aligned} \quad (35)$$

This reduces the problem to finding four new radial functions, satisfying inhomogeneous radial equations. For the $p_{1/2}$ response we have

$$\begin{aligned} [(\gamma - 1)/\alpha + \alpha Z/r]P'_{+1} + [d/dr - 1/r]Q'_{+1} \\ = \alpha \mathcal{E} N_{-1} r^{\gamma+1} e^{-Zr}, \\ -[(\gamma + 1)/\alpha + \alpha Z/r]Q'_{+1} + [d/dr + 1/r]P'_{+1} \\ = [\alpha^2 Z/(1 + \gamma)] \mathcal{E} N_{-1} r^{\gamma+1} e^{-Zr} \end{aligned} \quad (36)$$

and for $p_{3/2}$ we find

$$\begin{aligned} [(\gamma - 1)/\alpha + \alpha Z/r]P'_{-2} + [d/dr + 2/r]Q'_{-2} \\ = \alpha \mathcal{E} N_{-1} r^{\gamma+1} e^{-Zr}, \\ -[(\gamma + 1)/\alpha + \alpha Z/r]Q'_{-2} + [d/dr - 2/r]P'_{-2} \\ = [\alpha^2 Z/(\gamma + 1)] \mathcal{E} N_{-1} r^{\gamma+1} e^{-Zr}. \end{aligned} \quad (37)$$

The $p_{1/2}$ response function has already been constructed by Sandars in Ref. [16]; we will just restate the results. The solution can be written in closed form as a polynomial multiple of $r^\gamma e^{-Zr}$,

$$\begin{aligned} P'_{+1} &= (a + br + cr^2)r^\gamma e^{-Zr}, \\ Q'_{+1} &= (a' + b'r + c'r^2)r^\gamma e^{-Zr}. \end{aligned} \quad (38)$$

The coefficients are given in Ref. [16].

The $p_{3/2}$ response function is more difficult to construct than the $p_{1/2}$. The underlying difficulty is that the homogeneous differential equation has indicial behavior $\delta = \sqrt{4 - \alpha^2}$, while the inhomogeneous term has power law $\gamma = \sqrt{1 - \alpha^2}$. This difference arises because the unperturbed $1s_{1/2}$ state doesn't have the same angular momentum barrier as the $p_{3/2}$ response function. The solutions are *not* given exactly by polynomial multiples of $r^\delta e^{-Zr}$; the power series do not terminate. The inhomogeneous term has a radial factor $r^{\gamma - \delta + 1}$, whose exponent $\gamma - \delta + 1 \cong -3\alpha^2 Z^2/8$ is small and negative, leading to a logarithmic singularity at $r=0$. This is a familiar situation in Coulomb problems [17] and it is usually handled by evaluating this factor at a small radius R ,

$$\rho \equiv R^{\gamma - \delta + 1} \cong e^{-(3\alpha^2 Z^2/8)\ln R},$$

replacing the slowly varying factor ρ by a constant.

Writing the response functions in the form

$$P_{-2}(r) = p(r)r^\delta e^{-Zr}, \quad Q_{-2}(r) = q(r)r^\delta e^{-Zr}, \quad (39)$$

the radial equations are

$$\begin{aligned} [(\gamma - 1)/\alpha + \alpha Z/r]p + [d/dr + (\delta + 2)/r - Z]q &= \alpha \mathcal{E} N_{-1} \rho, \\ -[(\gamma + 1)/\alpha + \alpha Z/r]q + [d/dr + (\delta - 2)/r - Z]p & \\ = [\alpha^2 Z/(1 + \gamma)] \mathcal{E} N_{-1} \rho. & \end{aligned} \quad (40)$$

These equations have polynomial solutions of the form

$$p(r) = (d + er), \quad q(r) = (d' + e'r), \quad (41)$$

where

$$\begin{aligned} d &= -\mathcal{E} N_{-1} \rho [(\delta - 2\gamma + 1)(\delta + 2)/Z^2(\delta - \gamma + 1)^2], \\ e &= -\mathcal{E} N_{-1} \rho [\gamma/(Z)(\delta - \gamma + 1)], \\ d' &= \alpha \mathcal{E} N_{-1} \rho [(\delta - 2\gamma + 1)/Z(\delta - \gamma + 1)^2], \\ e' &= \alpha \mathcal{E} N_{-1} \rho [\gamma/[(\delta - \gamma + 1)(\gamma + 1)]. \end{aligned} \quad (42)$$

The difference between these two response functions already shows that the polarization of the atom is affected by the fine-structure splitting of the excited p states.

The next step is to evaluate the toroidal magnetic field

$$\mathbf{B}_{\text{tor}} = (4\pi/c)f(r)\mathbf{r} \times \mathbf{m}, \quad (43)$$

where $f(r)$ is obtained from the radial component of the poloidal current density. Once again, we must do this as a sum of $p_{1/2}$ and $p_{3/2}$ terms. For $p_{1/2}$ we get

$$-2f_{1/2}\mathbf{m} \cdot \hat{\mathbf{r}} = (c/6\pi)\langle \boldsymbol{\sigma} \cdot \hat{\mathbf{E}} \times \hat{\mathbf{r}} \rangle [Q_{-1}P'_{+1} - P_{-1}Q'_{+1}]/r^2.$$

Inserting the radial functions and identifying $\mathbf{m} = \mathbf{E} \times \boldsymbol{\sigma}/2$, we find

$$\begin{aligned} f_{1/2}(r) &= -[Z(1 + \gamma)/3\pi\Gamma(2\gamma + 1)](2Zr)^{2\gamma - 2} \\ &\times [(2\gamma + 1) + 2Zr]e^{-2Zr}. \end{aligned} \quad (44)$$

Repeating this for $p_{3/2}$, we get

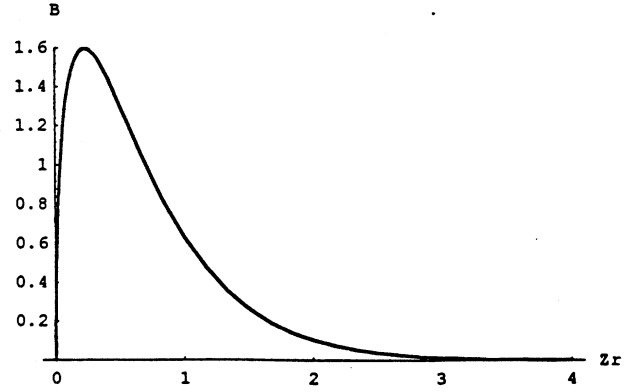


FIG. 2. Radial dependence of the toroidal magnetic field of the Dirac hydrogenic uranium ion, in units of $\alpha(\mathbf{E} \times \mathbf{S})\sin\theta$, versus the radial distance Zr in a.u.

$$-2f_{3/2}\mathbf{m} \cdot \hat{\mathbf{r}} = (c/6\pi)\langle \boldsymbol{\sigma} \cdot \hat{\mathbf{E}} \times \hat{\mathbf{r}} \rangle [P_{-1}Q'_{-2} - Q_{-1}P'_{-2}]/r^2.$$

Once again, we evaluate the logarithmic factor $r^{\gamma - \delta + 1} \cong \rho$ at the radius R . It is interesting to notice that the quantity ρ *cancels out* of the current density; the value of the small radius R does not appear in our final answer for $f_{3/2}(r)$

$$\begin{aligned} f_{3/2}(r) &= [Z/3\pi\Gamma(2\gamma + 1)](2Zr)^{2\gamma - 1} \\ &\times [(\delta - 2\gamma + 1)/(\delta - \gamma + 1)]e^{-2Zr}. \end{aligned} \quad (45)$$

Combining the $p_{1/2}$ and $p_{3/2}$ parts, we get

$$\begin{aligned} f(r) &= -K(2Zr)^{2\gamma - 2}[(2\gamma + 1) + 2Zr \\ &\quad - 2Zr(\delta - 2\gamma + 1)/(\delta - \gamma + 1)(1 + \gamma)]e^{-2Zr}, \end{aligned} \quad (46)$$

where the constant K is

$$K \equiv Z(1 + \gamma)/3\pi\Gamma(2\gamma + 1).$$

The radial dependence of B_{tor} is shown in Fig. 2 for the extreme relativistic case of hydrogenic uranium, with $\alpha Z = 0.672$. It resembles the nonrelativistic (NR) result, but with a stronger peak field occurring at a smaller radius.

The final step is to evaluate the anapole moment using the toroidal magnetic fields above,

$$\mathbf{t} = -(16\pi^2/3c)\mathbf{E} \times \mathbf{S} \int_0^\infty dr r^4 f(r).$$

The radial integrals all involve integrals of the form

$$\int dr r^{2\gamma + s} e^{-2Zr} = \Gamma(2\gamma + s + 1)/(2Z)^{2\gamma + s + 1},$$

with $s = 2, 3$. The final results are

$$\mathbf{t}_{1/2} = [4\pi\alpha/9Z^4](\mathbf{E} \times \mathbf{S})(\gamma + 1)^3(2\gamma + 1), \quad (47)$$

$$\begin{aligned} \mathbf{t}_{3/2} &= -[\pi\alpha/9Z^4][(2\gamma + 3)(\gamma + 1)(2\gamma + 1) \\ &\quad \times (\delta - 2\gamma + 1)/(\delta - \gamma + 1)](\mathbf{E} \times \mathbf{S}). \end{aligned} \quad (48)$$

TABLE I. Estimates for the alkali-metal ground states, based on the product rule Eq. (8). The entries marked with an asterisk and those with a dagger are estimated; the others are taken from the literature.

Element	r_0 (units of a_0)	α_E (units of a_0^3)	t (units of a_0^4)	$B_{\max}(\alpha E)$
H	1.7	4.5	0.103	0.47
Li	4.22 ^a	163.7 ^b	3.75	0.48
K	5.61 ^a	295.6 ^c	6.78	0.28
Rb	6.01 ^a	330.0 ^c	7.57	0.24
Cs	6.71 ^a	413.7 ^c	9.49	0.19
Fr	7.83 [†]	326	7.48	0.08

^aReference [23]

^bReference [24]

^cReference [25]

Combining these, the total moment approaches the correct NR limit Eq. (29). An expansion of (47) and (48) in powers of αZ shows that the relativistic effects reduce the NR value of \mathbf{t} by a factor

$$[1 - 271\alpha^2 Z^2/216 + 2785\alpha^4 Z^4/10368 + O(\alpha Z)^6].$$

Before comparing this with the product rule (9), we must also recalculate the electric dipole moment (EDM) and magnetic dipole moment (MDM) using the same relativistic wave functions; they will change slightly from the NR values. The EDM is defined by the matrix element

$$d = \langle \Psi_{-1} | r \cos \theta | \Psi_{-1} \rangle \equiv \langle \psi_{-1} | r \cos \theta | \psi'_{-1} \rangle + \text{H.c.}, \quad (49)$$

which separates into two portions

$$\begin{aligned} d_{1/2} &= \gamma(\gamma+1)(2\gamma+1)(4\gamma+5)/36Z^4, \\ d_{3/2} &= (\gamma+1)(2\gamma+1)[\gamma(2\gamma+3)(\delta-\gamma+1) \\ &\quad + (\gamma+1)(\delta-2\gamma+1)(\delta-\gamma+3)]/[9Z^4(\delta-\gamma+1)^2]. \end{aligned} \quad (50)$$

An expansion in powers of αZ gives a correction factor that slightly *reduces* the electric dipole moment [18]

$$[1 - 28\alpha^2 Z^2/27 + 631\alpha^4 Z^4/5184 + \mathcal{O}(\alpha Z)^6].$$

The MDMD involves the expectation value of an operator *even* under space inversion; it only acquires a Stark correction *quadratic* in \mathcal{E} , which we will ignore. In the ground state, the magnetic moment is [14]

$$\mathbf{M} = -\frac{1}{2} \langle \Psi | \mathbf{r} \times \boldsymbol{\alpha} \cdot \hat{\mathbf{z}} | \Psi \rangle = -[(2\gamma+1)/3]\alpha/2, \quad (51)$$

which is also slightly *reduced* by binding, by a correction factor $1 - \alpha^2 Z^2/3$.

Combining these results, we see that the product rule is *not* exactly satisfied spin-orbit coupling is included: the TDM, EDM, and MDM are each reduced, but by different factors. To leading order in αZ , the reduction of the TDM is by $1 - 1.255\alpha^2 Z^2$ and the product of EDM and MDM is reduced by $[1 - 1.037\alpha^2 Z^2][1 - 0.333\alpha^2 Z^2] \equiv 1 - 1.370\alpha^2 Z^2$. Thus the product rule slightly *underestimates* the anapole moment by a factor $1 - 0.115\alpha^2 Z^2$. This small discrepancy is really a measure of how *well* the rule works. We will use the product rule to continue our discussion, surveying other states and other atoms.

V. ALKALI ATOMS

The results of the preceding section give precise predictions for the toroidal magnetic fields of the hydrogenic atoms with arbitrary Z , but this result is not particularly useful. It would be more interesting to learn about the fields of the ground states of other neutral atoms. It would take a major effort to repeat this method precisely for a list of atoms. It is more practical to get an approximate overview by estimating the *anapole moment* rather than the *toroidal magnetic field*, using Eq. (8) with either the calculated or measured electric polarizabilities. There is probably a corresponding rule for relating the radial dependence of the field to the electron density. Instead, we will roughly estimate it from Fig. 1 by assuming that the *form* of the field is universal and scaling the distances according to the rms radius of the valence electron r_0 .

The electric polarizability α_e is the largest for a closed shell plus one electron, so we only consider the alkali-metal atoms. We have included estimates for francium, although the data are poorer and the relativistic corrections larger. The relevant information is summarized in Table I. The atomic radii r_0 in column 2 are *calculated* rather than measured; they increase by a factor of 3.9 over the table. They are taken from the rms radii of the valence electrons in the Hartree-Fock method. In column 3, we have also used *calculated* polarizabilities rather than *measured*; there is little difference between theory and experiment on these data.

The anapole moments in column 4 are calculated from the product rule, using one Bohr magneton as the magnetic moment of each atom. The entries show an increase by a factor of 92 between hydrogen and cesium. In column 5, we have estimated the maximum toroidal magnetic field in units of αE , by assuming that Fig. 1 is a universal graph of its radial dependence with abscissas scaled according to the size of the atom. Knowing the anapole moment, we can estimate the maximum strength of the field from the hydrogen results. Thus we set

$$B_{\max} \equiv B_{\max}(H)[t/t(H)][r_0(H)/r_0^4].$$

This estimate predicts a slow *decrease* of the maximum toroidal field with increasing Z . All considered, we conclude that Li or Na would be the best candidate for the study of anapole effects.

VI. RYDBERG STATES

Polarizabilities and anapole moments also become very large in Rydberg states, due to the close spacing of opposite parity states. We can use the product rule again to estimate how the anapole moments of excited states depend on the principal quantum number n . The polarizability in nS states in hydrogen is known to be [19]

$$\alpha_E = n^4(n^2 + 7/2) \rightarrow n^6 \quad (52)$$

for $n \gg 1$. By scaling from the $1S$ state of hydrogen, we estimate the anapole moments of Rydberg state in other neutral atoms to have the same dependence on n

$$t \cong 0.130n^6. \quad (53)$$

The mean-square radii of these states also grow with n ,

$$\langle r^2 \rangle_{nS} = n^2(5n^2 + 1)/2 \rightarrow 5n^4/2. \quad (54)$$

Using the same scaling law as before, the maximum toroidal magnetic field decreases like

$$B_{\max} \approx (0.15/n^2)\alpha E. \quad (55)$$

These estimates are very preliminary, but indicate that Rydberg states are good candidates for studying toroidal magnetic fields.

There would also be Stark-induced anapole effects for molecular free radicals and other polarizable systems with unpaired spins. The presence of an electric field breaks inversion symmetry and the unpaired spin provides a sense of time. These are the two general requirements for the existence of anapole fields.

We could leave the discussion at this point, but some comment is required on the problem of observing these effects. To our knowledge, the only experimental evidence for the existence of toroidal magnetic fields in *in quantum systems* concerns the existence of *nuclear* anapole moments. Parity-nonconserving transitions in heavy atoms have been analyzed for the presence of weak-induced nuclear anapole moments, where they contribute to the nuclear spin-dependent transitions. The current evidence is marginal: a 2σ result is reported in cesium [20] and upper limits have been set in thallium [21]. However, anapole fields are a classical concept that is easily transcribed into quantum mechanics; it should not be necessary to invoke weak interactions to make them appear. In the next section we will look to ordinary atomic physics for evidence of their existence.

VII. EXPERIMENTAL CONSEQUENCES

The general requirement for detecting anapole magnetic fields is that some “test charge” should interact with the toroidal magnetic field inside the atom. For example, the nuclear spin could interact through its magnetic-dipole coupling with the field at the nucleus. This would result in an energy shift

$$\Delta E = -\langle \boldsymbol{\mu}_N \cdot \mathbf{B}_{\text{tor}} \rangle_N = -\langle g(r) \boldsymbol{\mu}_N \cdot \mathbf{r} \times (\mathbf{E} \times \mathbf{S}) \rangle_N. \quad (56)$$

This vanishes as $\mathbf{r} \rightarrow 0$; we have already shown the field at the nucleus to be zero. There should be no linear Stark shift in hyperfine intervals of atoms. This is confirmed by measurements on the hydrogen maser [22], which show a quadratic Stark shift in hydrogen; they would surely have seen a linear shift had it been present at the same level.

Although this effect vanishes in atoms, it should be present in spin-polarized molecular radicals since their nuclei experience a toroidal magnetic field transverse to the anapole moment. In a diatomic molecule, the hyperfine interaction has the form

$$H = \langle g(r) (\mathbf{I} \times \mathbf{r}) \cdot (\mathbf{E} \times \mathbf{S}) \rangle \propto (\mathbf{I} \times \mathbf{n}) \cdot (\mathbf{E} \times \mathbf{S}). \quad (57)$$

We can crudely estimate the magnitude of this interaction by assuming the toroidal magnetic field at one of the nuclei has “typical” strength αE

$$-\boldsymbol{\mu}_N \cdot \mathbf{B}_{\text{tor}} \approx (e\hbar/Mc)(\alpha E),$$

much smaller than a typical hyperfine splitting. Clearly, the direction of the nuclear spin will be influenced by the applied electric field. There is no linear Stark shift in the hyperfine interval because the toroidal field is transverse to the hyperfine field; furthermore, it averages to zero for free molecular rotations. There should be similar terms in the hyperfine structure of chiral radicals, with much larger magnitude. We intend to explore the consequences of these interactions in subsequent work.

VIII. CONCLUSIONS

We have shown that there is a toroidal magnetic field induced in the interior of paramagnetic atoms when an external electric field is applied, breaking inversion symmetry. The internal fields have *odd* symmetry under inversions and strengths of order αE (atomic units). The external magnetic fields of these atoms are *even* under inversions and have strength of order α (atomic units).

This represents a curious kind of “mixed polarizability” of atoms having unpaired spins, in which a laboratory electric field induces a change in the internal magnetic field

$$\mathbf{B}_{\text{tor}} \propto (\mathbf{E} \times \mathbf{S}) \times \mathbf{r}.$$

This is a straightforward consequence of electromagnetism and quantum mechanics, which results from an asymmetric distortion of the current density in the atom giving a poloidal term. The first moment of this toroidal magnetic field is called the anapole moment; to a good approximation, it is proportional to the cross product of the (intrinsic) magnetic-dipole moment and the (induced) electric-dipole moment.

We have presented a detailed calculation of the field in hydrogenic atoms and have estimated the fields in other alkali atoms and in Rydberg states. The methods could be accurately extended to other atoms; a prediction of these effects in molecules and complex atoms is feasible. There is at present only marginal experimental evidence for such fields; the situation clearly calls for some new experiments.

- [1] Ya. B. Zel'dovich, Zh. Éksp. Teor. Fiz. **33**, 1531 (1957) [Sov. Phys. JETP **6**, 184 (1958)].
- [2] V. M. Dubovik and A. A. Cheshkov, Fiz. Elem. Chastits At. Yadra **5**, 791 (1974) [Sov. J. Part. Nucl. **5**, 31 (1975)].
- [3] I. B. Khriplovich, *Parity Nonconservation in Atomic Phenomena* (Gordon and Breach, New York, 1991), Chap. 8.
- [4] E. M. Henley, A. H. Huffman, and D. U. L. Yu, Phys. Rev. D **7**, 943 (1973).
- [5] M. A. Gongora-T and R. G. Stuart, Z. Phys. C **55**, 101 (1992).
- [6] E. M. Henley *et al.*, Phys. Lett. **88B**, 349 (1979); V. V. Flambaum and I. B. Khriplovich, Zh. Éksp. Teor. Fiz. **79**, 1656 (1980) [Sov. Phys. JETP **52**, 835 (1980)].
- [7] S. M. Apenko and Y. E. Lozovik, J. Phys. B **15**, L57 (1982); E. R. Boston and P. G. H. Sandars, *ibid.* **23**, 2663 (1990); R. R. Lewis, Phys. Rev. A **48**, 4107 (1993).
- [8] I. B. Khriplovich and M. E. Pospelov, Z. Phys. D **17**, 81 (1990).
- [9] R. R. Lewis, Phys. Rev. A **49**, 3376 (1994).
- [10] E. R. Boston and P. G. H. Sandars, J. Phys. B **23**, 2663 (1990).
- [11] R. R. Lewis, Comments At. Mol. Phys. **31**, 67 (1995).
- [12] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, 2nd ed. (Pergamon, Oxford, 1975), p. 241.
- [13] R. M. Sternheimer, Phys. Rev. **84**, 244 (1951); **96**, 951 (1954); **105**, 158 (1957).
- [14] A. Dalgarno and J. T. Lewis, Proc. R. Soc. London Ser. A **233**, 70 (1956); C. Schwartz, Ann. Phys. (N.Y.) **2**, 156 (1959); P. G. H. Sandars, Proc. Phys. Soc. London **92**, 857 (1967).
- [15] M. E. Rose, *Relativistic Electron Theory* (Wiley, New York, 1961), Chap. V.
- [16] P. G. H. Sandars, J. Phys. B **1**, 511 (1968).
- [17] J. J. Sakurai, *Advanced Quantum Mechanics* (Addison-Wesley, Reading, MA, 1967), p. 129.
- [18] B. A. Zon, N. L. Manakov, and L. P. Rapaport, Yad. Fiz. **15**, 508 (1972) [Sov. J. Nucl. Phys. **15**, 282 (1972)].
- [19] B. L. Jhanwar and W. J. Meath, Mol. Phys. **40**, 713 (1980).
- [20] M. C. Noecker, B. P. Masterson, and C. E. Wieman, Phys. Rev. Lett. **61**, 310 (1988).
- [21] N. H. Edwards *et al.*, Phys. Rev. Lett. **74**, 2654 (1995); P. A. Vetter *et al.*, *ibid.* **74**, 2658 (1995).
- [22] P. C. Gibbons and N. F. Ramsey, Phys. Rev. A **5**, 73 (1972).
- [23] C. Froese-Fischer, *Hartree-Fock Method of Atoms* (Wiley, New York, 1977).
- [24] W. Müller *et al.*, J. Chem. Phys. **80**, 3297 (1984).
- [25] V. Kellö *et al.*, Phys. Rev. A **47**, 1715 (1993).