Physics Letters A 158 (1991) 295–299
North-Holland

PHYSICS LETTERS A

Violation of the Schiff theorem for unstable atomic states

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Received 23 May 1991; revised manuscript received 28 June 1991; accepted for publication 3 July 1991
Communicated by V.M. Agranovich

We discuss the screening of the external static electric field on the nucleus of the neutral atom. It is shown that for the excited atomic states the screening is not complete.

Due to the well-known Schiff theorem [1] for the neutral atom the external static homogeneous electric field is exactly screened on the nucleus by the polarization of the electronic shells. The theorem is valid for relativistic electrons [2,3]. Radiation corrections do not violate the theorem [2]. One can easily understand this theorem: the homogeneous electric field does not accelerate the neutral atom. Therefore the field acting on the nucleus is equal to zero.

The physical arguments as well as formal proof of the theorem are valid only for an atom in a stationary state. For the excited states which decay due to photon emission the situation is not obvious. This problem is connected with the radiation correction to the energy levels.

First of all let us demonstrate simple physical arguments in favor of the Schiff theorem violation for unstable states [#1]. In the present work we will consider the hydrogen atom with an infinitely heavy nucleus to avoid the recoil. Let us consider the $2s_{1/2}$ state which decays via M1-transition to the $1s_{1/2}$ state (in the present work we are interested in one-quantum transitions only). In the external electric field there is a mixing with the $2p_{1/2}$ state which decays via E1 transition (fig. 1). We neglect the mixing with the $2p_{3/2}$ state. The decay amplitude corresponding to fig. 1 equals

[#1] We are grateful to V.V. Flambaum in discussions with whom these arguments were formulated.

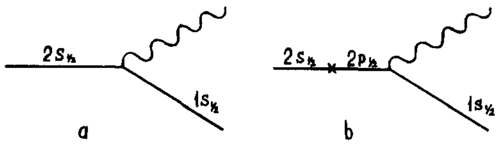

Fig. 1. Amplitude of the $2s_{1/2}$-state decay in the external electric field. The cross corresponds to the states mixing in the field.

$$f_1 = \langle 1s_{1/2} | h_\gamma | 2s_{1/2} \rangle + \frac{\langle 1s_{1/2} | h_\gamma | 2p_{1/2} \rangle \langle 2p_{1/2} | -e\mathscr{E}\cdot\boldsymbol{r} | 2s_{1/2} \rangle}{E_{2s_{1/2}} - E_{2p_{1/2}} + \frac{1}{2}\mathrm{i}\Gamma_p} . \tag{1}$$

Here $\mathscr{E}$ is the external electric field, Γ_p is the radiation width of the $2p_{1/2}$ state,

$$h_\gamma = \sqrt{2\pi/\omega}\, e\boldsymbol{\alpha}\cdot\boldsymbol{\varepsilon}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \tag{2}$$

is the operator of the radiation of the photon with momentum $\boldsymbol{k}$ and polarization $\boldsymbol{\varepsilon}$, $\boldsymbol{\alpha}$ is the Dirac matrix. The use of relativistic notation is technically convenient. A simple linear calculation in the $\mathscr{E}$ approximation gives the angular distribution of the photons averaged over the polarizations of the atomic states (see ref. [4]),

$$\mathrm{d}\dot{W}(\boldsymbol{k}) = \Gamma_{2s}(1+\lambda\boldsymbol{k}\cdot\mathscr{E})\frac{\mathrm{d}\Omega}{4\pi} , \tag{3}$$

where

$$\lambda = \frac{1}{\omega}\frac{\mathrm{E1}}{\mathrm{M1}}\frac{D\Gamma_p}{(E_s-E_p)^2+\frac{1}{4}\Gamma_p^2} .$$

Here E1 and M1 are the amplitudes of the γ-transitions $2p_{1/2}\to 1s_{1/2}$ and $2s_{1/2}\to 1s_{1/2}$. $D=\langle 2p_{1/2}, \frac{1}{2}| -ez | 2s_{1/2}, \frac{1}{2}\rangle$ is the amplitude of the 2s–2p mixing, $\Gamma_{2s}=\frac{4}{3}\omega^3|\mathrm{M1}|^2$ is the one-photon width of the $2s_{1/2}$-state. Let us stress that correlation of flight direction with the electric field $\boldsymbol{k}\cdot\boldsymbol{\mathscr{E}}$ in (3) is T-odd. Just therefore λ is proportional to Γ_p. With the angular distribution (3) the photon takes away the average momentum directed along the electric field. The recoil force is equivalent to the unscreened electric field at the nucleus,

$$\mathscr{E}_N = \frac{1}{3}\frac{1}{e}\lambda\omega^2\Gamma_{2s}\mathscr{E} . \tag{4}$$

If the nucleus has an electric dipole moment $\boldsymbol{d}$ then one may suppose that a correction to the energy level should arise,

$$\delta E_{2s} = -\mathscr{E}_N\cdot\boldsymbol{d} . \tag{5}$$

Now we would like to understand what the energy shift (5) means and how it can be observed. Let us emphasize once more that $\delta E\sim\Gamma_p\Gamma_{2s}$, i.e. δE arises just due to the instability of the levels. At infinite mass of the nucleus the only probe of an electric field at the origin can be the electric dipole moment of the nucleus. The interaction of this dipole moment with the external field and with the electron is equal to

$$H_d = e\boldsymbol{d}\cdot\boldsymbol{r}/r^3 - \boldsymbol{d}\cdot\boldsymbol{\mathscr{E}} = \frac{\mathrm{i}}{e}\boldsymbol{d}\cdot[\boldsymbol{p}, H] , \tag{6}$$

where

$$H=\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m - e^2/r - e\boldsymbol{\mathscr{E}}\cdot\boldsymbol{r} \tag{7}$$

is the Dirac electron Hamiltonian. The external electric field is included into the Hamiltonian (7). To emphasize this point we will denote its eigenstates by a bar: $H|\bar{n}\rangle = \bar{E}_n|\bar{n}\rangle$. The eigenstates of the total Hamiltonian $H+H_d$ will be denoted by the tilde: $(H+H_d)|\tilde{n}\rangle = \tilde{E}_n|\tilde{n}\rangle$. Due to the Schiff theorem $\tilde{E}_n=\bar{E}_n$. Treating H_d as a perturbation one can easily calculate the matrix element of the radiation operator (2) between the tilde states,

$$\langle\tilde{m}|h_\gamma|\tilde{n}\rangle = \langle\bar{m}|h_\gamma|\bar{n}\rangle + \frac{\mathrm{i}}{e}\boldsymbol{d}\cdot\langle\bar{m}|[h_\gamma, \boldsymbol{p}]|\bar{n}\rangle$$

$$= (1-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{d}/e)\langle\bar{m}|h_\gamma|\bar{n}\rangle . \tag{8}$$

We have used the representation of H_d in the commutator form (6).

Now we can ask the question: Does the correction (5) mean the shift of the 2s energy level which can be observed in the resonant scattering of light on the 1s state of hydrogen? In the leading order in h_γ the amplitude of the resonant scattering is shown in fig. 2, and due to eq. (8) it equals

$$f=(1+\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{d}/e)(1-\mathrm{i}\boldsymbol{k}_2\cdot\boldsymbol{d}/e) \times\frac{\langle 1\bar{s}|h_\gamma(k_2)|2\bar{s}\rangle\langle 2\bar{s}|h_\gamma^+(k_1)|1\bar{s}\rangle}{\omega+E_{1s}-E_{2s}+\mathrm{i}0} , \tag{9}$$

where $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are the momenta of the initial and final photons. The amplitude (9) depends on $\boldsymbol{d}$, but this dependence is not connected with any shift of energy. Moreover $|f|^2$ is independent of $\boldsymbol{d}$. However, it is obvious beforehand that in the leading order in h_γ the shift δE (5) cannot arise, since $\delta E\sim\Gamma_{2s}\Gamma_{2p}$. One should consider at least the Lamb shift (fig. 3a), and even the second order in the Lamb shift (figs. 3b–3d). Nevertheless one can easily verify that in any order in the radiation correction there is no dependence on $\boldsymbol{d}$ in the scattering amplitude except the trivial one (9). Indeed, let us consider for example the amplitude in fig. 3a. The insertion is the self-energy operator

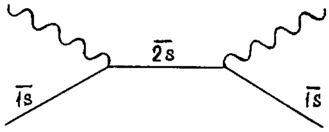

Fig. 2. Amplitude of the photon resonant scattering in leading order in H_γ.

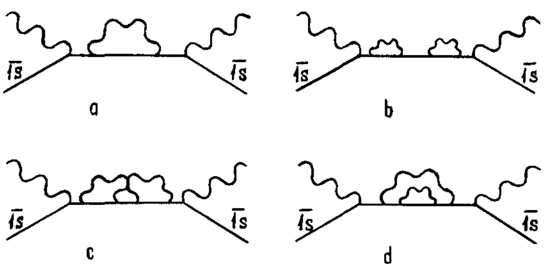

Fig. 3. Amplitude of the photon resonant scattering with the Lamb-shift insertion.

$$\Sigma(E)=\sum_n\int\frac{d^3q}{(2\pi)^3}\frac{\langle 2\bar{s}|h_\gamma(q)|\tilde{n}\rangle\langle\tilde{n}|h_\gamma^+(q)|2\bar{s}\rangle}{E-\tilde{E}_n+i0}, \tag{10}$$

but due to eq. (8), the dependence on $\boldsymbol{d}$ in the matrix element of h_γ exactly compensates that in the matrix element h_γ^+. In the same way we can prove the independence of $\boldsymbol{d}$ of the insertions in the diagrams presented at figs. 3b–3d. Thus, there is no energy shift proportional to $\boldsymbol{d}$ which can be observed in the resonant scattering of light in the atomic ground state. Then the question arises: what does formula (5) mean?

To answer this question let us first of all answer a more simple one: What is the usual pressure of light? Thus without any external static electric field the laser shines on an atom in resonance with the transition $1s_{1/2}\to 2s_{1/2}$. The interaction of an electron with the classical electromagnetic wave is of the form (cf. with eq. (2))

$$\hat{V}=V^{(+)}+V^{(-)},$$

$$V^{(+)}=\tfrac{1}{2}e\boldsymbol{A}\cdot\boldsymbol{\alpha}e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\omega t},\quad V^{(-)}=(V^{(+)})^+. \tag{11}$$

$\boldsymbol{A}$ is the wave vector potential. The rescattering is isotropic and therefore light pressure arises. This is equivalent to a static electric field acting on the nucleus. Due to balance of momentum at a small saturation parameter $\langle 2p|V|1s\rangle/\Gamma_p \ll 1$,

$$\mathscr{E}_N=-\frac{1}{e}\boldsymbol{k}\frac{\Gamma_p}{(\omega-\omega_0)^2+\frac{1}{4}\Gamma_p^2}\times\frac{1}{2}\sum_{\alpha,\beta}|\langle 2p_{1/2},\alpha|V^{(+)}|1s_{1/2},\beta\rangle|^2, \tag{12}$$

$\omega_0=E_{2p_{1/2}}-E_{1s_{1/2}}$, $\alpha,\beta=\pm\frac{1}{2}$ are the projections of the angular momentum. Similar to (5), an energy shift proportional to $\boldsymbol{d}$ must arise. However, we argue above (eq. (10)) that there are no corrections to the photon scattering amplitude proportional to $\boldsymbol{d}$. Thus we can conclude that the photon which prepares the unstable quantum state cannot measure by itself the recoil electric field (4), (12) on the nucleus. However, a different experiment is possible. Let the laser field (11) prepare the unstable quantum state and the other field probe the atom. Say, using the microwave field one can search for the dependence of the nuclear-magnetic-resonance (NMR) frequency on the nucleus electric dipole moment $\boldsymbol{d}$. Just in such an experiment the recoil electric field (4), (12) can be measured and exactly in this sense the Schiff theorem is violated for the unstable quantum states.

The shift of the NMR frequency due to the nucleus electric dipole moment is equal to $\delta E=\mathrm{Tr}(H_d\rho)$. Here ρ is the density matrix of an atom in the laser field (11) and H_d is defined by eq. (6). We will solve the equation for the density matrix by iterations in the perturbation $\hat{V}$ (see e.g. ref. [5]),

$$(i\,\partial/\partial t-\omega_{ik})\rho_{ik}+i\Gamma_{ik}(\rho_{ik}-\rho_{ik}^{(e)})=[\hat{V},\rho]_{ik}, \tag{13}$$

$\rho_{ik}^{(e)}$ is the equilibrium density matrix. In our case $\rho^{(e)}$ corresponds to the equal population of the states $|1s_{1/2},\pm\frac{1}{2}\rangle$. In first approximation the positive and negative frequency components of ρ arise:

$$\rho_{ik}^{(1\pm)}=\frac{[\hat{V}^{(\pm)},\rho^{(e)}]_{ik}}{\pm\omega-\omega_{ik}+i\Gamma_{ik}}. \tag{14}$$

The effect we are interested in arises in the second approximation. The time-independent components of $\rho^{(2)}$ are equal to

$$\rho_{ik}^{(2)}=-\frac{1}{\omega_{ik}}([V^{(+)},\rho^{(1-)}]_{ik}+[V^{(-)},\rho^{(1+)}]_{ik}). \tag{15}$$

The further calculation is straightforward:

$$\begin{aligned}\delta E&=\mathrm{Tr}(H_d\rho^{(2)})=\frac{i}{e}\boldsymbol{d}\cdot\sum_{ik}[\boldsymbol{p},H]_{ik}\rho_{ik}^{(2)}\\&=-\frac{i}{e}\boldsymbol{d}\cdot\mathrm{Tr}([\boldsymbol{p},V^{(+)}]\rho^{(1-)}+[\boldsymbol{p},V^{(-)}]\rho^{(1+)})\\&=-\frac{i}{e}\boldsymbol{d}\cdot\boldsymbol{k}\,\mathrm{Tr}(V^{(+)}\rho^{(1-)}-\rho^{(1+)}V^{(-)}).\end{aligned} \tag{16}$$

After the substitution of $\rho^{(1)}$ from eq. (14) we really get $\delta E=-\boldsymbol{d}\cdot\mathscr{E}_N$ with $\mathscr{E}_N$ from eq. (12).

We now return to the Schiff theorem (formulae (4) and (5)). Here the situation is very similar to the consideration of the light pressure. However, in this case the indices i, k in the density matrix ρ_{ik} numerate not only the states of an atom, but the states of a photon as well. This is a rather unusual situation and therefore we emphasize it once more. Usually in the density-matrix description one averages over all photon states and keeps explicit the electron degrees of freedom only. To spot the Schiff-theorem violation (eqs. (4) and (5)) we should keep explicit the states of an atom with one photon and average over the states with more than one photon.

Let the laser (11) be tuned to the transition $1s_{1/2} \to 2s_{1/2}$. It produces some population of the $2s_{1/2}$ level which corresponds to a stationary density matrix $\rho^{(0)}$. Say that at saturation the populations of all four states $|1s_{1/2}, \pm\frac{1}{2}\rangle$, $|2s_{1/2}, \pm\frac{1}{2}\rangle$ are equal. We will solve eq. (13) starting from $\rho^{(0)}$. First of all let us take into account the interaction with the external static electric field $U=-e\boldsymbol{\mathscr{E}}\cdot\boldsymbol{r}$ which mixes $2s_{1/2}$ and $2p_{1/2}$ levels,

$$\rho_{ik}^{(1)} = -\frac{[U,\rho^{(0)}]_{ik}}{\omega_{ik}-\mathrm{i}\Gamma_{ik}}\,. \tag{17}$$

More explicitly,

$$\rho_{sp}^{(1)} = \frac{\langle s|U|p\rangle}{\omega_{sp}-\frac{1}{2}\mathrm{i}\Gamma_p}\rho_{ss}^{(0)}\,, \quad \rho_{ps}^{(1)} = (\rho_{sp}^{(1)})^+\,. \tag{18}$$

Here s, p denotes $2s_{1/2}$ and $2p_{1/2}$, and $\rho_{sp}^{(1)}$ still is a matrix in the projections of angular momenta.

The interaction with the photon with momentum $\boldsymbol{q}$ and polarization $\boldsymbol{\varepsilon}$ due to eq. (2) is of the form

$$H_\gamma(\boldsymbol{q},\boldsymbol{\varepsilon}) = H_\gamma^{(+)} + H_\gamma^{(-)}\,,$$

$$H_\gamma^{(+)} = h_\gamma a_{q,\varepsilon}\,, \quad H_\gamma^{(-)} + h_\gamma^+ a_{q,\varepsilon}^+\,. \tag{19}$$

Here a^+ and a are the creation and annihilation operators of the photon. In the second approximation

$$\rho_{ik}^{(2\pm)} = \frac{[H_\gamma^{(\pm)},\rho^{(1)}]_{ik}}{\pm\omega-\omega_{ik}+\mathrm{i}\Gamma_{ik}}\,. \tag{20}$$

Similarly to eq. (15) the time independent part of $\rho^{(3)}$ is equal to

$$\rho_{ik}^{(3)} = -\frac{1}{\omega_{ik}}([H_\gamma^{(+)},\rho^{(2-)}]_{ik} + [H_\gamma^{(-)},\rho^{(2+)}]_{ik})\,. \tag{21}$$

Analogously to eq. (16) the correction to the energy is of the form

$$\delta E = \mathrm{Tr}(H_d\rho^{(3)})$$
$$= -\frac{\mathrm{i}}{e}\mathrm{Tr}[\boldsymbol{d}\cdot\boldsymbol{q}(H_\gamma^{(+)}\rho^{(2-)} - \rho^{(2+)}H_\gamma^{(-)})]$$
$$= -\frac{\mathrm{i}}{e}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\boldsymbol{d}\cdot\boldsymbol{q}$$
$$\times\sum_{ik}\left(\frac{h_{ki}[h^+,\rho^{(1)}]_{ik}}{-\omega-\omega_{ik}+\mathrm{i}0} - \frac{[h,\rho^{(1)}]_{ki}h_{ik}^+}{\omega-\omega_{ki}+\mathrm{i}0}\right). \tag{22}$$

One can verify that due to the relation $\omega_{ik}=-\omega_{ki}$ the real parts of the Green functions in (22) are cancelled out, and only δ-functions survive: $(\omega-\omega_0-\mathrm{i}0)^{-1}\to\mathrm{i}\pi\delta(\omega-\omega_0)$. Using eq. (18) δE can be transformed to the form

$$\delta E = \frac{4\pi}{e}\mathrm{Re}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\boldsymbol{d}\cdot\boldsymbol{q}\,\delta(\omega-\omega_0)$$
$$\times\mathrm{Tr}(\rho_{sp}^{(1)}\langle p|h|1s\rangle\langle 1s|h^+|s\rangle)\,. \tag{23}$$

The trace in this formula is over the projections of the angular momentum. Comparing with eqs. (1)–(5) we see that expression (23) identically coincides with the energy shift (5) which is derived from the balance of momenta.

In conclusion we formulate the results of the present work. The Schiff theorem (screening of an external static homogeneous electric field on the nucleus of a neutral atom) is violated for the excited (unstable) atomic states. As a matter of principle this violation cannot be observed in the scattering of a photon on the ground state of an atom. In other words there is no effect if one uses as a probe the photon which itself prepares the unstable quantum state. The violation takes place if the photons (laser field) are used to prepare the unstable quantum state and the other field probes the atom. Say using the microwave field one can observe the dependence of nuclear magnetic response frequency on the nucleus electric dipole moment $\boldsymbol{d}$. Just in this sense the Schiff theorem is violated for the unstable quantum states.

The main subject of the present paper is to point out the Schiff theorem violation for unstable atomic states. Besides that we would like to draw the attention of the reader to an interesting principal possibility. We mean the use of the effective electric field [12] due to the light pressure for the experimental search for the electric dipole moment of the nucleus in nuclear magnetic resonance experiments. This method is more suitable for light atoms.

We are grateful to V.F. Dmitriev, M.G. Kozlov, J. Sucher, V.B. Telitsin, V.F. Yezhov, and especially to V.V. Flambaum and I.B. Khriplovich for the numerous helpful discussions and stimulating questions.

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