# Shielding of an external oscillating electric field inside atoms

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According to the Schiff theorem, an external electric field vanishes at the atomic nucleus in a neutral atom, i.e., it is completely shielded by electrons. This makes a nuclear electric dipole moment (EDM) unobservable. In this paper an extension of the Schiff theorem to an oscillating electric field is considered. Such a field can reach the nucleus and interact with the nuclear EDM. An enhancement effect appears if the field is in resonance with an atomic or molecular transition. The shielding by electrons strongly affects low-energy nuclear electric dipole transition amplitudes in different nuclear reactions, including radiative transitions, radiative nucleon capture, photo- or electro-excitation of nuclei, and laser-induced or laser-enhanced nuclear reactions.

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#### I. INTRODUCTION

## A. EDM

The existence of electric dipole moments (EDMs) of elementary particles, nuclei, atoms, and molecules in a state with a definite angular momentum violates time reversal invariance (T) and parity (P). EDM also violates CP invariance if the CPT invariance holds. Very extensive experimental and theoretical activity related to EDM is motivated by the need to test unification theories predicting T, P, and CP violation.

A measurement of the nuclear EDM could provide information about T,P-odd nuclear forces and neutron and proton EDM. However, there is a problem here. A homogeneous static electric field does not accelerate a neutral atom. This means that the total electric field **E** acting on the atomic nucleus is zero since otherwise the charged nucleus would be accelerating, i.e., the external field is completely shielded by atomic electrons. The absence of the electric field means that the nuclear EDM d is unobservable,  $\mathbf{d} \cdot \mathbf{E} = 0$ . One may also say that the nuclear EDM is shielded by the atomic electrons and the atomic EDM is zero even if the nucleus has an EDM.

A quantum-mechanical derivation of this result for an arbitrary nonrelativistic system of pointlike charged particles with EDMs has been done by Schiff [1]. Schiff also mentioned that his theorem is violated by the finite nuclear size. The effect of the finite nuclear size was implemented as the nuclear Schiff moment, which was introduced in Refs. [2–5]. An electrostatic interaction between the nuclear Schiff moment and electrons produces atomic and molecular EDM. References [2,3] calculated the finite nuclear size effect of the proton EDM. References [4,5] calculated (and named) the nuclear Schiff moment produced by the P,T-odd nuclear forces. It was shown in [4] that the contribution of the P,T-odd forces to the nuclear EDM and Schiff moment is  $\sim$ 40 times larger than the contribution of the nucleon EDM.

The suppression factor for the atomic EDM relative to the nuclear EDM, proportional to a very small ratio of the squared nuclear radius to the squared atomic radius, is partly compensated by the factor  $Z^2R_S$ , where Z is the nuclear charge and  $R_S$  is the relativistic factor [4]. However, even in heavy atoms the atomic EDM is ~10<sup>3</sup> times smaller than the nuclear EDM. An additional 2–3 orders of magnitude enhancement appears in nuclei with octupole deformation [6]; however; such nuclei (e.g., <sup>225</sup>Ra) are unstable.

The Schiff theorem is also violated by the magnetic interaction [1,7]. Corresponding atomic EDMs produced by the nuclear EDM and electron-nucleus magnetic interaction have been calculated in Ref. [8]. In light atoms this mechanism of atomic EDM dominates, but in heavy atoms it is smaller than the effect of the finite nuclear size since the latter very rapidly increases with the nuclear charge, as  $Z^2R_s$ , while the magnetic effect increases more slowly, as  $ZR_M$ , where  $R_M$  is the relativistic factor for the magnetic effect [8].

There is no complete shielding in ions. For example, in a molecular ion the shielding factor for the nuclear EDM is  $(Z_i/Z)(M_n/M_m)$ , where  $Z_i$  is the ion charge, Z is the nuclear charge,  $M_n$  is the nuclear mass, and  $M_m$  is the molecular mass [9]. Recently the measurement in the ionic molecule HfF<sup>+</sup> was performed in Ref. [10]. However, they measured electron EDM, which does not have such a shielding factor and actually is strongly enhanced in polar molecules [11–13].

There is another interesting feature of the HfF<sup>+</sup> experiment [10]. To keep the charged molecule in the trap the authors had to use an oscillating electric field. This is not important for the electron EDM measurement since the electron EDM is not shielded. However, for the nuclear EDM the oscillating field makes the shielding incomplete, and the difference with the static case may be important. Indeed, the interval between the opposite parity rotational levels  $\delta E$  in molecules is very small (especially in the case of  $\Omega$  doublets formed by the nonzero electron angular momentum projection  $\Omega$  on the molecular axis; for HfF<sup>+</sup>  $\Omega = \pm 1$ ), and a nonzero frequency effect for  $\omega \sim \delta E/\hbar$  should be considered.

### **B.** Nuclear reactions

Shielding of an external electric field by electrons strongly affects low-energy nuclear electric dipole transition amplitudes. This may happen in low-energy radiative transitions, radiative nucleon capture, photo- or electro-excitation of nuclei, and in laser-induced or laser-enhanced nuclear reactions. Activity in the latter field has been motivated by the theoretical papers [14,15], wherein the laser-induced *s*-wave neutron capture to a *p*-wave resonance was suggested. Capture of a low energy (e.g., thermal) neutron to a *p*-wave resonance is kinematically suppressed  $10^6$  times, but the laser field allows an unsuppressed *s*-wave neutron capture to the *p*-wave resonance (note that such kinematic enhancement, combined with the enhanced mixing of close *s*- and *p*-wave compound states (resonances) by the weak interaction, leads to a  $10^6$  enhancement of parity violating effects in neutron reactions predicted in Ref. [16], confirmed in experiment [17], and then studied in numerous experiments involving hundreds of *p*-wave resonances in many nuclei; see reviews [18–20]).

These works initiated intensive theoretical and experimental activity; see, e.g., numerous references in [21,22]. However, in striking contrast to the success in the study of the enhanced parity violating effects in *p*-wave resonances, experiments with the laser field [23–25] failed to find the predicted effect. Note that these theoretical predictions have not taken into account the electron shielding of the laser field and therefore overestimated the effect.

The availability of new high power lasers and a significant increase of their frequency range due to an efficient method of high harmonic generation (the atomic antenna mechanism [26,27]) provide an incentive for a proper account of the electron shielding effect, which will be done in the present work.

### II. SHIELDING THEORY: NONRESONANT OSCILLATING ELECTRIC FIELD

In our paper [28] the shielding of an external electric field in an ion described by the relativistic Dirac Hamiltonian for atomic electrons was considered. It was demonstrated that the Schiff theorem for the nuclear EDM is still valid both in the "exact" Dirac equation treatment and in the Dirac-Hartree-Fock approximation if the external electric field is included in the self-consistent equations. This allowed us to perform the Dirac-Hartree-Fock numerical calculations for a static electric field and for an oscillating electric field in Tl<sup>+</sup>.

The screened field  $E = E_0 + \langle E_e \rangle$  oscillates in space, has a maximal magnitude  $E \approx -3E_0$  near the radius of the 1s shell,  $r = a_B/Z$  ( $a_B$  is the Bohr radius), and becomes very small near the nucleus. It was concluded that the deviation of the electric field at the nucleus from zero in a neutral system is proportional to  $\omega^2$ , where  $\omega$  is the electric field oscillation frequency. However, there was no formula derived for the shielding factor in the case of the oscillating field. The aim of the present paper is to derive such formula and extend the Schiff theorem to the case of the oscillating electric field.

The Hamiltonian of an atom in an external electric field along the z axis  $E_z = E_0 \cos(\omega t)$  may be presented as

$$H_E = H_0 - E_z D_z, \tag{1}$$

$$D_z = e \sum_{k=1}^N z_k,\tag{2}$$

where  $H_0$  is the Schrödinger or the Dirac Hamiltonian for the atomic electrons in the absence of the external field  $E_z$ , N is the number of the electrons,  $Z_i = Z - N$ , e = -|e| is the

electron charge, and  $z_k$  is the z-axis projection of the electron position relative to the nucleus. We assume that the nuclear mass is infinite and neglect very small effects of the Breit and magnetic interactions. The electric field on the nucleus may be presented as  $E_n = (E_0 + \langle E_e \rangle) \cos(\omega t)$ , where the electron electric field on the nucleus is

$$E_e = -e \sum_{k=1}^{N} \frac{z_k}{r_k^3} = -\frac{i}{Ze\hbar} [P_z, H_0], \qquad (3)$$

where  $P_z = \sum_{k=1}^{N} p_{z,k}$  is the total momentum of the atomic electrons. The second equality follows from the differentiation of the nuclear Coulomb potential in the Dirac or Shrodinger Hamiltonian  $H_0$  since the total electron momentum  $P_z$  commutes with the electron kinetic energy and the electron-electron interaction. Using the time-dependent perturbation theory [29] for the oscillating perturbation  $D_z E_z$ , we obtain

$$\langle E_e \rangle = -E_0 \sum_n \frac{(\epsilon_0 - \epsilon_n)}{(\epsilon_0 - \epsilon_n)^2 - \epsilon^2} \\ \times \left( \langle 0 | E_e | n \rangle \langle n | D_z | 0 \rangle + \langle 0 | D_z | n \rangle \langle n | E_e | 0 \rangle \right) \\ = -\frac{iE_0}{Ze\hbar} \sum_n \frac{(\epsilon_0 - \epsilon_n)^2}{(\epsilon_0 - \epsilon_n)^2 - \epsilon^2} \\ \times \left( \langle 0 | P_z | n \rangle \langle n | D_z | 0 \rangle - \langle 0 | D_z | n \rangle \langle n | P_z | 0 \rangle \right).$$
(4)

The second equality follows from Eq. (3) and the relation  $\langle 0|[P_z, H_0]|n\rangle = -(\epsilon_0 - \epsilon_n)\langle 0|P_z|n\rangle$ ,  $\epsilon = \hbar\omega$ . The energy-dependent factor may be presented as

$$\frac{(\epsilon_0 - \epsilon_n)^2}{(\epsilon_0 - \epsilon_n)^2 - \epsilon^2} = 1 + \frac{\epsilon^2}{(\epsilon_0 - \epsilon_n)^2 - \epsilon^2}.$$
 (5)

The energy-independent term 1 in the right-hand side allows us to sum over states  $|n\rangle$  in Eq. (4) using the closure and then use the commutator relation  $[P_z, D_z] = -ie\hbar N$ . The result is

$$\langle E_e \rangle = -E_0 \frac{N}{Z} - \frac{iE_0}{Ze\hbar} \sum_n \frac{\epsilon^2}{(\epsilon_0 - \epsilon_n)^2 - \epsilon^2} \\ \times (\langle 0|P_z|n \rangle \langle n|D_z|0 \rangle - \langle 0|D_z|n \rangle \langle n|P_z|0 \rangle).$$
 (6)

Using the nonrelativistic commutator relation  $P_z = \frac{im}{e\hbar}[H_0, D_z]$  (here *m* is the electron mass) we can express the induced electron field on the nucleus in terms of the atomic dynamical polarizability  $\alpha_{zz}(\omega)$ :

$$\langle E_e \rangle = -E_0 \frac{N}{Z} - E_0 \alpha_{zz} \frac{\epsilon^2 m}{Z e^2 \hbar^2},$$
  
$$\alpha_{zz} = 2 \sum_n \frac{(\epsilon_n - \epsilon_0) \langle 0 | D_z | n \rangle^2}{(\epsilon_n - \epsilon_0)^2 - \epsilon^2}.$$
 (7)

The values of the dynamical polarizabilities are measured and calculated for many atoms; they appear in the expression for the refractive index. There are high precision computer codes for the calculations of the dynamical polarizabilities; see, e.g., [30,31].

It may be instructive to present the formula for the total electric field amplitude  $E_t$  at the nucleus using the energy and the polarizability in atomic units,  $\tilde{\epsilon} = \frac{\epsilon}{e^2/a_b}$  and  $\tilde{\alpha}_{zz} = \frac{\alpha_{zz}}{a_z^2}$ :

$$E_t = E_0 \left( \frac{Z_i}{Z} - \frac{\tilde{\epsilon}^2 \tilde{\alpha}_{zz}}{Z} \right).$$
(8)

If  $\epsilon^2 = (\hbar \omega)^2 \ll (\epsilon_0 - \epsilon_n)^2$  we have the static-type screening of the external field,  $E_0 + E_e = E_0(1 - N/Z) = E_0 Z_i/Z$ , i.e., the complete shielding of the external field in neutral systems where the ion charge  $Z_i = Z - N = 0$ .

The shielded field is proportional to 1/Z, so it may seem that the shielding is stronger in heavy atoms. However, this is not necessarily the case, since in hydrogen and helium  $\tilde{\alpha}_{zz} \sim 1$ while in cesium (Z = 55)  $\tilde{\alpha}_{zz} \sim 400$ . Indeed, the numerical value of the polarizability  $\tilde{\alpha}_{zz}$  in atomic units often exceeds the value of the nuclear charge Z, therefore the suppression of the field mainly comes from the frequency of the field oscillations in atomic units,  $\tilde{\epsilon}$ .

As an illustration, let us consider a numerical example. One of the largest parity violating effects (7%) has been observed in the 0.734 eV *p*-wave resonance in <sup>139</sup>La, Z = 70. This means that the kinematic factor and the mixing of *s* and *p* compound states by the weak interaction are large. Therefore, it looks natural to use this resonance to search for the capture of neutron in a laser field, which also may provide mixing of the *s* and *p* compound states and enhance capture of neutron to the p-wave resonance.

The static scalar polarizability of La is  $\tilde{\alpha}_s = 213.7$  [30]. Thus, in a low frequency laser field, s  $\tilde{\epsilon} = 1/27.2$  (1 eV), the shielding factor is 0.005. However, it rapidly increases with  $\tilde{\epsilon}$  and reaches the pole of  $\tilde{\alpha}_{zz}$  at the position of the La atom energy level  $\tilde{\epsilon} = 0.0604$  (1.64 eV).

#### **III. ATOMIC RESONANCE**

When the frequency increases and approaches the resonance,  $\epsilon^2 = (\hbar \omega)^2 \approx (\epsilon_0 - \epsilon_n)^2$ , the induced electron field may become much larger than the external field amplitude  $E_0$ . The field remains finite for  $\epsilon^2 = (\epsilon_0 - \epsilon_n)^2$  due to the widths of the excited states, which should be added to the energy denominators (where we should have  $\epsilon_n - i\Gamma_n/2$  instead of  $\epsilon_n$ ).

If the width is small  $(\Gamma_n \ll eE_0\langle 0|D_z|n\rangle)$  and may be neglected, Rabi oscillations between the two resonating states happen (the electron oscillates between the ground state and excited state and at any instant the wave function is a superposition of two states).

The solution for a two-level system with energies  $E_0$ and  $E_n$  subjected to a periodic perturbation is presented in the textbook [29]. We just calculate the electron field  $E_e$ using this two-state wave function. Use of the commutator relations in Eq. (3),  $\langle 0|[P_z, H_0]|n \rangle = -(\epsilon_0 - \epsilon_n) \langle 0|P_z|n \rangle$ , and  $P_z = \frac{im}{e\hbar} [H_0, D_z]$  leads to the following expression for the resonance contribution to the electric filed at the nucleus for  $\epsilon^2 = (\hbar\omega)^2 = (\epsilon_0 - \epsilon_n)^2$ :

$$\langle E_e \rangle = E_r \sin(\Omega t) \sin(\omega t),$$
 (9)

$$\Omega = 2eE_0\langle 0|D_z|n\rangle/\hbar, \qquad (10)$$

$$E_r = \frac{\tilde{\epsilon}^2 D_z}{Z} \frac{e}{a_B^2} = \frac{\tilde{\epsilon}^2 D_z}{Z} \times 5.14 \times 10^9 \,\mathrm{V/cm},\qquad(11)$$

 L. I. Schiff, Measurability of nuclear electric dipole moments, Phys. Rev. 132, 2194 (1963). where  $\tilde{D}_z = \frac{\langle 0|D_z|n \rangle}{ea_B}$ . The frequency of these Rabi oscillations  $\Omega$  is determined by the strength of the external field  $E_0$ , but the field on the nucleus does not depend on  $E_0$  and is defined by the electron field, which has a scale  $e/a_B^2 = 5.14 \times 10^9 \text{ V/cm}$ .

Again, the suppression of the field at the nucleus  $\sim \tilde{\epsilon}^2$ appears if the field oscillation frequency is small. This may be the case if we want to use a resonance between close opposite parity levels (e.g., in a molecule) to measure the nuclear EDM. The frequency of the oscillations should not be too high since one has to separate the oscillating signal at this frequency. For example, one may rotate the nuclear spin in a unison with the rotating electric field. Using a very optimistic estimate  $\tilde{\epsilon} = 10^{-4}$  (658 GHz) and  $Z \sim 1$  we obtain  $E_r \sim 50$  V/cm. This field does not look large, and the experiment itself looks too complicated to do.

However, there are two arguments in favor of such attempt. Nuclear EDM in light nuclei such as  ${}^{1}$ H,  ${}^{2}$ H, and  ${}^{3}$ He may be calculated more reliably than the Schiff moment in heavy nuclei. Indeed, the formula for the Schiff moment contains two terms of opposite sign (the second term comes from the electron shielding effect). As a result, the sophisticated many-body calculations for  ${}^{199}$ Hg [32] failed to predict the magnitude and even the sign of the Schiff moment.

The second argument is that the static effective field (the screened external field which is not zero due to the magnetic interaction) for the nuclear EDM in light atoms is very small. According to [1] the suppression factor for <sup>3</sup>He is  $10^{-7}$ , i.e., an external filed 30 KV/cm corresponds to an effective field acting on the <sup>3</sup>He EDM of only 0.003 V/cm. Therefore, if someone were to decide to do a measurement of a theoretically "clean" light nucleus EDM in a neutral molecule or atom, an oscillating electric field is possibly not the worst option.

As an example of the strong field at the nucleus, we take the lanthanum resonance case Z = 57,  $\tilde{\epsilon} = 0.0604$  (1.64 eV) and use a rough estimate  $\tilde{D}_z \sim 0.3$ . This gives the field at the nucleus  $E_r \sim 10^5$  V/cm. In the higher-energy resonances the field may be an order of magnitude larger due to the larger  $\tilde{\epsilon}^2$ and  $\tilde{D}_z$ . Such a very strong field gives an incentive to study laser-induced nuclear reactions using atomic resonances; for example, to repeat the laser-induced neutron capture experiments [23–25].

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