Calculation of a P- and T-Nonconserving Weak Interaction in Xe and Hg with Many-Body Perturbation Theory

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(Received 10 July 1984)

The electronic part of a possible P- and T-nonconserving neutral-weak-current–induced electric dipole moment in atomic Xe and Hg was calculated with many-body perturbation theory. After the effects of this P- and T-nonconserving interaction on all core orbitals were treated self-consistently, thereby including all single-particle effects to all orders but no correlation effects, the results $\mu_e = (5.2\times10^{-23} e\ \mathrm{m})\, C_T \sigma_N$ and $\mu_e = -(6.0\times10^{-22} e\ \mathrm{m})\, C_T \sigma_N$, respectively, were obtained for Xe and Hg. The value for Xe can be combined with the recent experimental result, $|\mu_e(^{129}\mathrm{Xe})| < 10^{-28} e\ \mathrm{m}$, to give the upper limit $|C_T| < 2\times10^{-6}$.

PACS numbers: 31.20.–d, 11.30.–j

The existence of an electric dipole moment (EDM) of an elementary particle would imply simultaneous nonconservation of both parity (P) and time (T) reversal symmetry.[1] Nevertheless, the search for a neutron EDM[2] was initiated several years before the discovery of the nonconservation of parity in weak interactions.[3] The only evidence for T nonconservation so far is the CP nonconservation in the decay of the neutral kaons[4] and it would, of course, be of interest to establish T nonconservation in other systems. The search for a proton EDM has led to the study of thallium fluoride,[5,6] where a nonzero result could be evidence for a proton EDM but also for a short-range P- and T-nonconserving electron-nucleon interaction which for nonrelativistic nucleons has the form[5,7]

$$h^T = \sqrt{2} i G_F (\gamma_0\gamma_5\boldsymbol{\sigma})_e \cdot \Big[\sum_p C_{Tp}\delta(\mathbf{r}-\mathbf{r}_p)\boldsymbol{\sigma}_p + \sum_n C_{Tn}\delta(\mathbf{r}-\mathbf{r}_n)\boldsymbol{\sigma}_n\Big],$$

where G_F is the weak-interaction constant and the two sums run over all the protons and neutrons in the nucleus. Such an interaction, h^T, would lead to an EDM in atomic systems, and experiments to detect a linear Stark effect in ^{129}Xe have been performed by Vold, Raab, Heckel, and Fortson.[8] The results of atomic many-body calculations of this effect for Xe and Hg is presented here.

A full calculation will require a detailed treatment also of the nuclear part of h^T. However, at present it is adequate to note that h^T can be written as

$$h^T = \sqrt{2} i G_F C_{TN} \boldsymbol{\sigma}_N \cdot (\gamma_0\gamma_5\boldsymbol{\sigma})_e \rho_N(\mathbf{r}_e),$$

where C_{TN} is a constant which depends on the particular nucleus but may be related to the more fundamental coupling constants, C_{Tn} and C_{Tp}, by a nuclear-structure calculation. $\rho_N(r_e)$ is a normalized nuclear density. A Fermi distribution is used in the present work, but since the electronic density is essentially constant at the nucleus, the numerical results are insensitive to the choice.

The presence of the perturbation h^T induces a correction $|a^T\rangle$ to orbital $|a\rangle$, given by

$$|a^T\rangle = \sum_s^{\mathrm{exc}} \frac{|s\rangle\langle s|h^T|a\rangle}{(\epsilon_a - \epsilon_s)}, \tag{1}$$

which can be represented diagrammatically as in Fig. 1. This correction is obtained as the solution to the inhomogeneous differential equation

$$(\epsilon_a - h_0)|a^T\rangle = h^T|a\rangle - \sum_c^{\mathrm{core}} |c\rangle\langle c|h^T|a\rangle \tag{2}$$

where the closure relation, $\sum_i^{\mathrm{all}} |i\rangle\langle i| = 1$, has been used to remove the infinite summation over excited states. The second term on the right-hand side of (2) makes the whole right-hand side orthogonal to the core orbitals. The correction $|a^T\rangle$ leads to an EDM, μ_e, given by

$$\mu_e = \sum_a (\langle a|\mathbf{d}|a^T\rangle + \langle a^T|\mathbf{d}|a\rangle), \tag{3}$$

represented by the diagrams in Figs. 1(b) and 1(c). The length form of the dipole operator, $\mathbf{d} = -e\mathbf{r} = -er\mathbf{C}^1$, has been used here.

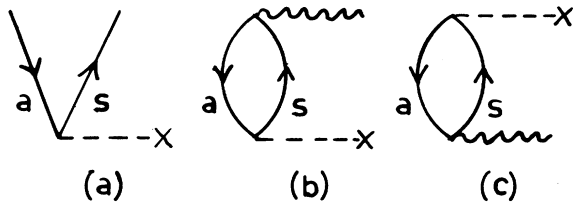

FIG. 1. (a) is the correction $|a^T\rangle$ to orbital $|a\rangle$, given by (1). (b) and (c) correspond to the two terms in the EDM (3). A down- (up-) going line represents a core (excited) orbital, a dashed line with a cross is used to denote h^T and a wavy line represents the dipole operator, $\mathbf{d}$.

The modification of one orbital affects all other orbitals through the electrostatic interaction. This leads to a coupled set of equations,

$$(\epsilon_a - h_0)|a^T\rangle = h^T|a\rangle + \sum_b^{\text{core}}[(\langle b|r_{12}^{-1}|b^T\rangle + \langle b^T|r_{12}^{-1}|b\rangle)|a\rangle - (\langle b|r_{12}^{-1}|a\rangle|b^T\rangle - \langle b^T|r_{12}^{-1}|a\rangle|b\rangle)] - (\text{orthogonality terms})$$

$$= h^T|a\rangle + v^T|a\rangle - (\text{orthogonality terms}), \tag{4}$$

which is solved iteratively. (Only terms to first order in h^T have been kept.) The diagrammatic form of (4) is shown in Fig. 2.

In calculations of new properties, where comparison with experiment will not immediately show if a calculation is correct or not, it is extremely valuable to have consistency checks. One check is obtained by dropping the orthogonality terms in (2) and (4). This will lead to admixtures of the occupied orbitals $|c\rangle$ in $|a^T\rangle$. However, since both h^T and v^T [defined in (4) above] are Hermitian operators with real matrix elements the contributions from this admixture to the EDM and to v^T are exactly canceled by the contributions from the admixture of $|a\rangle$ into $|c^T\rangle$, given by $\langle a|c^T\rangle = -\langle c|a^T\rangle$. Thus, neglect of the orthogonality terms leaves the results unchanged, although we have found that it has negative effects on the convergence properties of the system of coupled equations (4). A second check is obtained by interchanging $\mathbf{d}$ and h^T in all equations.

Before solving Eq. (2) for the P- and T-nonconserving parts of the orbitals, the equation is separated into radial and angular parts. The P- and T-conserving parts of the orbitals are written in the usual two-component form,

$$|a\rangle = \frac{1}{r}\begin{pmatrix} P_a(r)|l_a s j_a m_a\rangle \\ iQ_a(r)|\bar{l}_a s j_a m_a\rangle \end{pmatrix},$$

where $j_a = l_a \pm \frac{1}{2}$ and $\bar{l}_a = 2j_a - l_a$. The P- and T-nonconserving part is somewhat more complicated:

$$|a^T\rangle = \sum_{l_s j_s m_s}\sum_q (-1)^q (\sigma_N)_q (-1)^{j_s - m_s}\begin{pmatrix} j_s & 1 & j_a \\ -m_s & -q & m_a \end{pmatrix}\frac{1}{r}\begin{pmatrix} S_{a\to l_s j_s}(r)|l_s s j_s m_s\rangle \\ T_{a\to l_s j_s}(r)|\bar{l}_s s j_s m_s\rangle \end{pmatrix}.$$

The Wigner-Eckart theorem can be used to write the right-hand side of (2) in a similar form and the corresponding radial equation becomes

$$\begin{pmatrix} (\epsilon_a - v^{\text{HF}}) & \alpha^{-1}(d/dr - \mathscr{K}/r) \\ -\alpha^{-1}(d/dr + \mathscr{K}/r) & (\epsilon_a + 2\alpha^{-2}v^{\text{HF}}) \end{pmatrix}\begin{pmatrix} S_{a\to l_s j_s}(r) \\ T_{a\to l_s j_s}(r) \end{pmatrix} = -\sqrt{2}G_F\rho_N(r)\begin{pmatrix} Q_a(r)\langle l_s j_s||\sigma||\bar{l}_a j_a\rangle \\ P_a(r)\langle \bar{l}_s j_s||\sigma||l_a j_a\rangle \end{pmatrix}. \tag{5}$$

From the reduced matrix elements on the right-hand side of (5) it is easy to see that the selection rules are the same as for the electronic dipole operator, i.e., $l_s = l_a \pm 1$, $j_s = j_a$, $j_a \pm 1$. The presence of the nuclear density, $\rho_N(r)$, makes the first-order contributions very much smaller if $j_a \neq \frac{1}{2}$ or $j_r \neq \frac{1}{2}$. For Xe with 17 orbitals there are 42 possible excitations which have all been coupled together in the equation system (4). The angular-momentum graph technique[9] makes the evaluation of the radial parts of the remaining terms in (5) straightforward. The expression given in detail for the hyperfine interaction[10] holds here as well.

After the radial equations are solved the EDM is evaluated as

$$\mu_e = -2\sigma_N C_T \sum_{a l_s j_s} \tfrac{1}{3}(-1)^{j_s - j_a}\langle j_a||\mathbf{C}^1||j_s\rangle \int [P_a(r)S_{a\to l_s j_s}(r) + Q_a(r)T_{a\to l_s j_s}(r)]r\,dr. \tag{6}$$

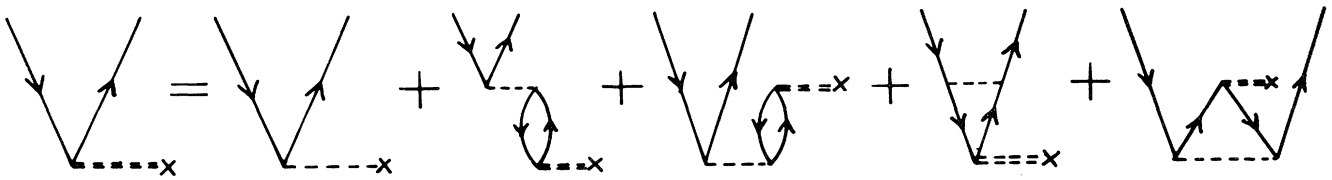

FIG. 2. Diagrammatic representation of Eq. (4). The double dashed line with a cross represents the self-consistent solution $|a^T\rangle$ and the dashed line the electrostatic interaction.

First, the lowest-order corrections $|a^T\rangle$ to the orbitals were obtained from Eq. (2) by use of both the local optimized Hartree-Fock Slater (OHFS) potential[11] and the nonlocal Hartree-Fock (HF) potential, leading to an electric dipole moment of $\mu_e = 13.08\times10^{-13} \times C_{TN}\sigma_N$ (atomic units are used unless otherwise specified) and $\mu_e = 7.76\times10^{-13}C_{TN}\sigma_N$, respectively, for Xe. For Hg the local potential gave $\mu_e = -1.17 \times10^{-11}C_{TN}\sigma_N$ and the Hartree-Fock potential $\mu_e = -0.38\times10^{-11}C_{TN}\sigma_N$. The contributions to the electric dipole moment for Xe from different shells are shown in Table I, with the orthogonality terms kept in the equations (when they are neglected certain cancellations occur between the shells). The lowest-order corrections, $|b^T\rangle$, obtained in the HF potential were then inserted on the right-hand side of Eq. (4) as a first approximation. The set of coupled equations was then solved iteratively. After 15 iterations the results had converged to $\mu_e = 9.81\times10^{-13}C_{TN}\sigma_n = (5.2\times10^{-23}\ e\ \mathrm{m})C_{TN}\sigma_N$ for Xe and $\mu_e = -1.13 \times10^{-11}C_{TN}\sigma_N = (-6.0\times10^{-22}\ e\ \mathrm{m})C_{TN}\sigma_N$ for Hg. We note that the result for Hg is about 10 times larger than that for Xe, but also that it is more sensitive to perturbations. Both of these observations can be ascribed to the presence of the two loosely bound $6s$ electrons in Hg, which are much more easily perturbed than the $5s^25p^6$ configuration in Xe. The $6s$ electrons are also responsible for the negative sign in Hg; the $6s \rightarrow p_{1/2}$ excitation gives a large negative contribution $\{(-1.4\times10^{-11},\ -0.56\times10^{-11},$ and $-1.8\times10^{-11}C_{TN}\sigma_N$, respectively, in the local potential and in the uncoupled [Eq. (2)] and coupled [Eq. (4)] HF approaches$\}$, whereas all the inner shells give positive contributions just like in Xe.

The result for Xe is relatively stable and we do not expect drastic changes as a result of correlation effects, which have not been included in the present work. Combining our final value with the recent experimental result, $\mu_e(^{129}\mathrm{Xe}) = -(0.3\pm1.1)\times10^{-28}\ e\ \mathrm{m}$,[8] gives $C_{TN} = (-0.6\pm2.1)\times10^{-6}/\langle\sigma_N\rangle$. To relate C_{TN} to C_{Tn} and C_{Tp} in an accurate way requires a nuclear structure calculation. However, a first approximation of C_T is obtained by the assumption that the nuclear spin arises solely from the spin of the unpaired neutron, which is in an $s_{1/2}$ state according to the shell model, giving[12] $C_{TN} \approx C_{Tn}$. We thus obtain[13] $|C_{Tn}| < 2\times10^{-6}$. This can be compared to the estimate $C_{Tp} = (6\pm9)\times10^{-6}$ obtained in a recent experiment on thallium fluoride.[7]

I have benefitted from discussions and correspondence with Professor E. N. Fortson concerning this work and I would also like to thank him for sending me the experimental results prior to publication. This work has been supported by the U. S. Department of Energy and by the Swedish Natural Science Research Council.

TABLE I. Individual contributions to the electric dipole moment (6) for Xe from various shells in units of $\sigma_N C_T 10^{-13}$ a.u.

	OHFS Eq. (2)	HF Eq. (2)	Coupled Eq. (4)
$n=1$	0.0895	0.0886	0.0894
$n=2$	0.2459	0.2380	0.2440
$n=3$	0.5897	0.5550	0.5921
$n=4$	1.6948	1.4290	1.7325
$n=5$			
$5s_{1/2} \rightarrow p_{1/2}$	0.9463	0.8238	1.0981
$5p_{1/2} \rightarrow s_{1/2}$	9.5094	4.6298	8.0424
Other	(0.038)[a]	(0.018)[a]	−1.9903
Total	13.076	7.764	9.808

[a]These contributions involve matrix elements of h^T between states with $j \neq \frac{1}{2}$ and have been neglected.

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[13]The discrepancy of a factor of 2 between the result for C_T given in the present work and in Ref. 8 appears to be due to confusion in the correspondence.