Parity non-conservation in caesium

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Résumé. — L'élément de matrice de transition dipolaire électrique violant la parité pour la transition 6s → 7s de Cs a été évalué en utilisant la théorie des perturbations pour le problème à plusieurs corps. Les diagrammes ne contenant que des excitations à une particule, ont été évalués à tous les ordres par une procédure auto-cohérente, qui donne une équivalence automatique entre les formes de longueur et de vélocité pour l'opérateur dipolaire électrique. Les effets de corrélation, qui exigent l'excitation simultanée de deux particules n'ont pas été inclus. Le résultat final, $0,89 \times 10^{-11}$ iea_0 $Q_W/(- N)$, est compatible avec le résultat expérimental du groupe de Paris pour les valeurs attendues de la charge faible, Q_W.

Abstract. — The parity non-conserving electric dipole transition element for the 6s → 7s transition in Cs has been evaluated using Many-Body Perturbation Theory. Diagrams containing only single excitations were evaluated « to all orders » using a self-consistent procedure, which was found to give an automatic equivalence between the length and velocity forms of the dipole operator. Correlation effects, which require simultaneous excitation of two orbitals, have not been included. The final result, 0.89×10^{-11} (iea_0) $Q_W/(- N)$, is consistent with the experimental results from the Paris group for the expected values of the weak charge, Q_W.

1. Introduction.

More than a decade has now passed since the Bouchiats pointed out [1] that parity non-conservation (PNC) caused by a weak electron-nucleon interaction, as predicted by the Weinberg-Salam theory [2] is strongly enhanced for heavy atoms and might, in fact, be observable. Following the first, sometimes discouraging, experiments, parity non-conservation of the expected magnitude has now been observed in Cs [3, 4], Tl [5], Pb [6] and Bi [7], and the experiments have reached an accuracy where, in some cases, quantitative conclusions can be drawn concerning the weak interaction, provided the atomic calculations are sufficiently accurate and reliable [8]. Several review articles have appeared recently, discussing the experiments [9, 10], calculations [11] and the relation to weak interaction theory [8].

Of the atoms studied so far, Cs is particularly attractive for calculations, not only because it is the lightest ($Z = 55$) but also because it is an alkali atom, which has a single valence electron outside a relatively inert core. A number of semi-empirical estimates of the PNC transition element in Cs have been given [1, 12-14]; the most accurate of them is presented by Bouchiat and coworkers [14]. Recently, Dzuba *et al.* [15] performed an extensive *ab initio* calculation using Many-Body Perturbation Theory (MBPT). Following Sandars' suggestion [16] they included the PNC effect on the orbitals in a self-consistent way, whereas the shielding of the electric field was included only to first order. In addition, certain correlation effects were included directly in the orbitals by modifying them to approximate Brueckner orbitals [17]. Although this had a small effect on the PNC transition element in the length form, it was found to reduce significantly the discrepancy between the length and velocity forms of the dipole operator.

The present work is similar to that of Dzuba *et al.* [15] and the results agree where comparable, but disagree with an earlier MBPT calculation [18]. Correlation effects were not included in the present work but on the other hand the shielding of the electric field has been treated self-consistently together with the PNC interaction, leading to an automatic equivalence between the length and velocity forms. To first order in the core-valence interaction, the treatment is equivalent to the PNC-TDHF procedure [19]. The method used has been applied and described in more detail in an earlier work on Bi [20], except for the simultaneous self-consistent treatment of the PNC interaction and the shielding of the electric field. The method is briefly summarized in section 2, where also some results are presented as an illustration to

the importance of the different effects. Section 3 gives a comparison with experiment and a discussion of the results.

2. Calculation of the parity non-conserving electric dipole transition element.

The weak interaction, described below, between the nucleons and electrons in an atom gives rise to a parity admixture in the orbitals which makes possible an electric dipole transition between states of the same nominal parity. The experiments on heavy atoms aim at determining the size of the transition element, which is then compared to theoretical estimates. This comparison can give information about the interaction parameters within the Weinberg-Salam theory and also impose constraints on alternative models for the electro-weak interaction [10, 21].

2.1 THE PARITY-VIOLATING INTERACTION. — In heavy atoms the parity-violating effect is dominated by [1] the nuclear spin-independent (« nuclear-vector electron-axial current ») part of the parity non-conserving Hamiltonian, which can be written as

$$h^{\text{PNC}} = \frac{G_F}{2\sqrt{2}} Q_W \, \rho_N(r) \, \gamma_5 \qquad (1)$$

where $G_F = G_\mu(\hbar c)^3 = 89.6$ eV/fm^3 = 2.22×10^{-14} a.u., $\rho_N(r)$ is a normalized nuclear density, which has been chosen as a Fermi distribution in the present work (the numerical results are rather insensitive to the choice), γ_5 is the Dirac matrix, which interchanges the upper and lower components of the electron orbitals, thereby changing the parity without affecting the total angular momentum. The « weak charge », Q_W, of the nucleus is related to the coupling constants, C_{1p} of the proton and C_{1n} of the neutron by $Q_W = 2(ZC_{1p} + NC_{1n})$, where Z is the number of protons and N is the number of neutrons in the nucleus. In the Weinberg-Salam theory [2] these coupling constants are given by $C_{1p} = \frac{1}{2}(1 - 4\sin^2\theta_W)$ and $C_{1n} = -\frac{1}{2}$ leading to a nuclear weak charge of

$$Q_W = Z(1 - 4\sin^2\theta_W) - N. \qquad (2)$$

At present, the best value for the weak interaction mixing angle obtained from neutrino-hadron scattering experiments is 0.227 ± 0.015 [22] and the value from electron deuteron scattering [23] as interpreted by Kim et al. [24] gives $\sin^2\theta_W = 0.223 \pm 0.015$. However, radiative corrections make these constants dependent on the momentum transfer [8, 22, 25, 26] leading to a corrected value of $\sin^2\theta_W(M_W) = 0.215 \pm 0.015$ [22]. Using this value, Marciano and Sirlin [25] obtain in the limit of zero-momentum transfer, relevant for atomic physics, $C_{1n} = -0.487$ and $C_{1p} = 0.487 - 1.954\sin^2\theta_W(M_W)$. This leads to $Q_W(^{133}\text{Cs})/(-N) = 0.91 \pm 0.04$.

The Weinberg angle, θ_W, is related to the masses of the Intermediate Vector Bosons, $W^\pm$ and Z^0

recently observed at CERN [27-29] as $\cos\theta_W = M_W/M_Z$. By using expressions for the muon decay lifetime [30] it is possible to obtain relations containing only one of the masses [8, 25]

$$\sin\theta_W(M_W) = 38.5 \text{ GeV}/M_W$$

or, equivalently

$$\sin 2\theta_W = 77.1 \text{ GeV}/M_Z.$$

The direct measurement of the W boson mass, $M_W = (80.9 \pm 1.5)$ GeV [27] gives $\sin^2\theta_W(M_W) = (0.226 \pm 0.008 \pm 0.143\,(\text{syst}))$ leading to a weak charge of $Q_W(^{133}\text{Cs})/(-N) = 0.91 \pm 0.022 \pm 0.038$, whereas the range 90 GeV $\leq M_Z \leq 98$ GeV [29] from the direct observation of the Z boson leads to $Q_W(^{133}\text{Cs})/(-N) = -0.88 \pm 0.08$ [8].

The atomic physics experiments can give a competitive indirect determination of the boson masses provided the combined error of theory and experiment is sufficiently small. With the increasing accuracy of the experimental results [9], it seems worthwhile to pursue the atomic physics calculations of the PNC, which is also in itself an interesting and challenging problem.

All values in the present work are given in terms of the ratio $Q_W/(-N)$. As Lynn has pointed out, this ratio is very close to a constant, $\eta = -2(C_{1n} + 2\,C_{1p}/3)$ for all the heavy atoms studied, since $Z/N \approx 2/3$ and C_{1p} is very small. Atomic units $(e = m_e = \hbar = 4\pi\varepsilon_0 = 1)$ are used throughout the paper unless otherwise specified.

2.2 THE ZEROTH-ORDER PARITY NON-CONSERVING ELECTRIC DIPOLE ELEMENT. — The presence of the PNC interaction (1) leads to admixtures to opposite parity into all orbitals. In this way electric dipole transitions may occur between states of the same nominal parity, such as the 6s → 7s transition in Cs, studied by Bouchiat and coworkers [3, 4], who observe the presence of the PNC electric dipole element, E_1^{PNC}, through its interference with the parity allowed Stark induced electric dipole transitions in an electric field.

In zeroth order, the PNC transition element between two states, i and f, is given by

$$E_1^{\text{PNC}} = \sum_j^{\text{all}} \left(\frac{\langle f | \mathbf{d} | j \rangle \langle j | h^{\text{PNC}} | i \rangle}{\varepsilon_i - \varepsilon_j} + \frac{\langle f | h^{\text{PNC}} | j \rangle \langle j | \mathbf{d} | i \rangle}{\varepsilon_f - \varepsilon_j} \right) \qquad (3)$$

where the sum runs over all orbitals j, excited as well as occupied. In this way the two diagrams in figure 1a and c (b and d) are automatically included in the first (second) term. We observe that in (3) the energy denominator is evaluated towards the dipole operator. The terms $j = i$ or $j = f$, which would lead to zero energy denominators, are automatically excluded
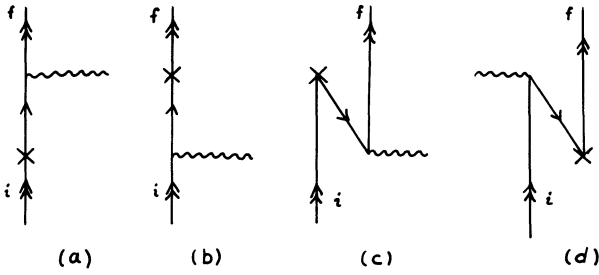
Fig. 1. — Graphical illustration of the zeroth-order E_1^{PNC} given by equation (3). Lines with double arrows represent a valence orbital and lines with a single arrow pointing up (down) represent excited (core) orbitals. A cross represents h^{PNC} and a wavy line the electric dipole operator.

since both the dipole operator, $\mathbf{d}$, and the parity violating operator, h^{PNC}, have odd parity.

To avoid the explicit summation in (3) over an infinite number of states, we use the inhomogeneous differential equation technique, first introduced by Sternheimer for hyperfine structure calculations [31]. It can be applied to the evaluation of the transition element (3) in two different ways. Let us first consider the parity admixture $|\,a^{PNC}\,\rangle$ into the orbital $|\,a\,\rangle$. This is given to lowest order by

$$(\varepsilon_a - h_0)\,|\,a^{PNC}\,\rangle = \sum_j |\,j\,\rangle\,\langle\,j\,|\,h^{PNC}\,|\,a\,\rangle = h^{PNC}\,|\,a\,\rangle.$$

$$(4)$$

The closure relation is used to remove the infinite summation over j. (This means that also states in the negative energy continuum are included, although the large energy denominators reduce the importance of these contributions.) The transition element is evaluated using these functions as

$$E_1^{PNC} = \langle\,f\,|\,\mathbf{d}\,|\,i^{PNC}\,\rangle + \langle\,f^{PNC}\,|\,\mathbf{d}\,|\,i\,\rangle.$$

$$(5)$$

The second possibility is to consider first the effect of the applied electric field on the orbitals

$$(\varepsilon_a \pm \omega - h_0)\,|\,\rho_a^{\pm}\,\rangle = \sum_j |\,j\,\rangle\,\langle\,j\,|\,\mathbf{d}\,|\,a\,\rangle = \mathbf{d}\,|\,a\,\rangle$$

$$(6)$$

and the transition element is then evaluated as

$$E_1^{PNC} = \langle\,\rho_f^-\,|\,h^{PNC}\,|\,i\,\rangle + \langle\,f\,|\,h^{PNC}\,|\,\rho_i^+\,\rangle.$$

$$(7)$$

To obtain the same element as in (3), the approximation $\omega = \varepsilon_f - \varepsilon_i$ is used for the transition frequency. We have then neglected correlation effects on the binding energies, which enter in second order of the electrostatic interaction.

The result for E_1^{PNC} depends on the choice of single-electron Hamiltonian, h_0. The present work uses the Dirac-Hartree-Fock potential from the Cs^+ core, given by

$$v^{HF}\,|\,j\,\rangle = \sum_a^{core} (\langle\,a\,|\,r_{12}^{-1}\,|\,a\,\rangle\,|\,j\,\rangle - \langle\,a\,|\,r_{12}^{-1}\,|\,j\,\rangle\,|\,a\,\rangle).$$

$$(8)$$

This potential was used also in the earlier MBPT calculations on the PNC in Cs [15, 18]. As a non-local potential, it has the disadvantage that it depends on the orbital it operates on through the « exchange » term on the right-hand side of (8) and iterative solutions are necessary. However, it also has the advantage of reducing the number of diagrams in higher orders of perturbation theory. Omitting the valence electrons from the potential in (8) makes the summation run over closed shells only. An additional advantage is that the same potential describes both the initial and final states. Since the valence electron is excluded from the summation in (8) over occupied orbitals, the core orbitals are not aware of the presence of the valence electron. The correction of the core orbitals (as well as the subsequent correction of the valence orbitals) is taken into account together with correlation effects in higher orders of perturbation theory, but the effects due to the correction of the central one-electron potential for the core orbitals are usually quite small for the alkalis.

Sucher has pointed out [32] that in a proper treatment the electrostatic interaction, $1/r_{12}$, should be surrounded by projection operators for positive energy states to avoid the so-called Brown-Ravenhall disease [33]. (A state consisting of two bound electrons is degenerate with an infinite number of states consisting of one electron in the positive and one in the negative energy continuum. If the electrostatic interaction is allowed to couple positive and negative energy states, all bound states will « dissolve into the continuum » [32] and no lower bound can be obtained for the energy.) However, Mittlemann has demonstrated [34] that the proper projection operators are implicitly included through the boundary conditions used in the numerical solution of the relativistic HF equations. All equations used in the present work can be considered as generalizations of the HF equation (8) and we will not consider this problem any further.

Table I shows the zeroth-order results using the local Optimized Hartree-Fock-Slater (OHFS) potential [35] as well as for the Dirac-Hartree-Fock potential (8) together with corresponding results obtained in other work. The results given are the transition elements between $m = 1/2$ states. Both the length form, $\mathbf{d}_L = -\mathbf{r} = -r\mathbf{C}^1$, and the velocity form, $\mathbf{d}_V = ic\alpha/\omega = [H, \mathbf{d}_L]/\omega$ of the dipole operator have been used. The two forms always give the same results in a local potential (if $\omega = \varepsilon_f - \varepsilon_i$ is used) whereas the equivalence does not hold in the non-local Hartree-Fock potential, as seen from the second and third lines of table I. The discrepancy is removed when the effect of the electric dipole field on the core orbitals is treated in a self-consistent way, as discussed below.

Table I. — *Comparison between the results for E_1^{PNC} in the length and velocity form obtained with different PNC functions (in units of 10^{-11} (iea_0) $Q_W/(-N)$).*

| | | $\langle$ 7s $\vert$ **d** $\vert$ $6s^{PNC}$ $\rangle$ | $\langle$ $7s^{PNC}$ $\vert$ **d** $\vert$ 6s $\rangle$ | Total | |
				This work	Other works
Local potential	$L = V$	− 0.384	1.214	0.930 [a]	1.10 [b]
					1.15 [c]
					1.05 [d]
Dirac-Hartree-Fock potential	L	− 0.274	1.010	0.736	0.975 [e]
					0.740 [f]
	V	− 0.338	0.928	0.590	0.504 [f]
					(0.590 [f])
Coupled PNC-functions					
First-order v^{PNC}	L	− 0.326	1.201	0.875	0.960 [e]
					0.872 [f]
	V	− 0.381	1.130	0.750	0.635 [f]
					(0.743 [f])
Self-consistent v^{PNC}	L	− 0.344	1.267	0.924	0.920 [f]
					0.92 [g]
					0.912 [h]
	V	− 0.385	1.210	0.825	0.700 [f]
					(0.820 [f])

[a] Result obtained using the local OHFS potential defined in [32].

[b] Bouchiat and Bouchiat [1].

[c] Loving and Sandars [13].

[d] Bouchiat et al. [14]. Their final result, 0.972, was obtained using and effective dipole operator, thereby including some of the shielding effects discussed in section 2.3.

[e] Das et al. [18].

[f] Dzuba et al. [15]. Their values for the velocity form were obtained using the experimental transition energies whereas our values were obtained with the Hartree-Fock values. The values in brackets have been renormalized by the corresponding ratio.

[g] Schäfer et al. [35].

[h] Johnson et al. [36].

2.3 PARITY ADMIXTURES IN THE CORE ORBITALS. —

The parity non-conserving interaction (1) between the nucleus and the core electrons causes also the core orbitals to have a PNC part given to lowest order by (4). However, a PNC admixture in one core orbital affects all other core orbitals through the Hartree-Fock potential (8) [16]. The correction to the potential due to PNC is obtained by inserting the parity-mixed orbital $\vert b^{PM} \rangle = \vert b \rangle + \vert b^{PNC} \rangle$ in the expression for the HF potential and keeping terms to first order in h^{PNC}. This leads to

$$v^{PNC} \vert i \rangle = - \sum_b^{core} (\langle b \vert r_{12}^{-1} \vert i \rangle \vert b^{PNC} \rangle +$$

$$+ \langle b^{PNC} \vert r_{12}^{-1} \vert i \rangle \vert b \rangle). \quad (9)$$

The corresponding corrections to the direct potential cancel each other due to sign inversion associated with the conjugation of the imaginary correction, $\vert b^{PNC} \rangle$. In addition, the direct terms are individually zero when summed over closed shells due to angular-momentum restrictions.

Inclusion of v^{PNC} in the equation (4) for the parity admixture in the orbitals leads to a system of coupled equations

$$(\varepsilon_a - h_0) \vert a^{PNC} \rangle = h^{PNC} \vert a \rangle + v^{PNC} \vert a \rangle = h^{PNC} \vert a \rangle - \sum_b^{core} (\langle b \vert r_{12}^{-1} \vert a \rangle \vert b^{PNC} \rangle + \langle b^{PNC} \vert r_{12}^{-1} \vert a \rangle \vert b \rangle) \quad (10)$$

which can be illustrated by the diagrams in figure 2. This approach has now been used by several groups [15, 19, 20, 36-38]. Inserting the core orbital admixtures from (4) on the right-hand side of (10) for $|6s^{PNC}\rangle$ and $|7s^{PNC}\rangle$ leads to the results shown in the fourth and fifth line of table I. Of course, also the core orbitals will be affected by the presence of v^{PNC} in (10) and those new core orbital admixtures are then in turn inserted on the right-hand side of (10) and the procedure is repeated until a self-consistent solution is obtained, leading to the results shown in the last two lines of table I.

2.4 SHIELDING OF THE ELECTRIC FIELD. — The application of an oscillating electric field affects the .core electrons as well as the valence electrons. Taking
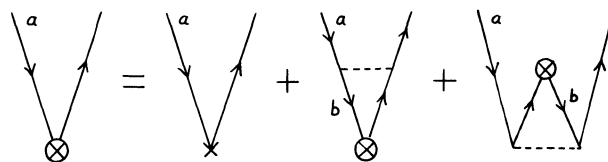

Fig. 2. — Graphical illustration of the coupled equation (10) for the parity admixtures into the orbitals. The dotted line is the electrostatic interaction. The first-order admixture is represented by the first diagram on the right-hand side.

these orbital modifications into account in the Hartree-Fock potential (8) leads to a set of coupled equations for the electric dipole perturbed functions

$$(\varepsilon_a \pm \omega - h_0)|\rho_a^{\pm}\rangle = \mathbf{d}|a\rangle + v^{\pm}|a\rangle = \mathbf{d}|a\rangle + \sum_b^{core} (\langle b|r_{12}^{-1}|\rho_b^{\pm}\rangle|a\rangle + \langle \rho_b^{\mp}|r_{12}^{-1}|b\rangle|a\rangle -$$
$$- \langle b|r_{12}^{-1}|a\rangle|\rho_b^{\pm}\rangle - \langle \rho_b^{\mp}|r_{12}^{-1}|a\rangle|b\rangle) \quad (11)$$

illustrated diagrammatically in figure 3. Explicit expressions for the additional diagrams have been given in the case of hyperfine interactions [40] and hold here, as well. The first two terms in the sum, the « direct » terms, can be transformed to a screening function which changes the dipole operator in the length form from $-r\mathbf{C}^1$ to $-(r + f(r))\mathbf{C}^1$, as demonstrated by Sandars and coworkers [39, 41]. In the calculations for bismuth [20], it was found that the direct shielding was responsible for the dominant contributions. In the present work, the relative importance of the direct and exchange terms was not investigated and only the complete set of equations (11) was solved, although this is a rather (computer-) time consuming procedure, since already for Cs there are 84 different core excitations of the type $a \rightarrow lj \pm$, which all have to be coupled.

The PNC transition element can then be evaluated as

$$E_1^{PNC} = \langle f|h^{PNC}|\rho_i^+\rangle + \langle \rho_f^-|h^{PNC}|i\rangle \quad (12a)$$

or as

$$E_1^{PNC} = \langle f^{PNC}|\mathbf{d} + v^+|i\rangle + \langle f|\mathbf{d} + v^+|i^{PNC}\rangle. \quad (12b)$$

If the « uncoupled » PNC functions from (4) are used in (12b) the same result as in (12a) is obtained, $(1.023 - 0.316) \times 10^{-11}$ $iea_0 Q_W/(-N)$ for the $6s \rightarrow 7s$ transition in Cs, both in the length and velocity forms. We note that although the effect of the shielding is rather small, the discrepancy between the length and velocity forms for the zeroth order Hartree-Fock result is removed when the coupled equations (11) are used to obtain ρ_i^+ and ρ_f^-. By using the relation, $\mathbf{d}_V = [h^{HF}, \mathbf{d}_L] - [v^{HF}, \mathbf{d}_L]$ and the fact that $\mathbf{d}_L$ com-
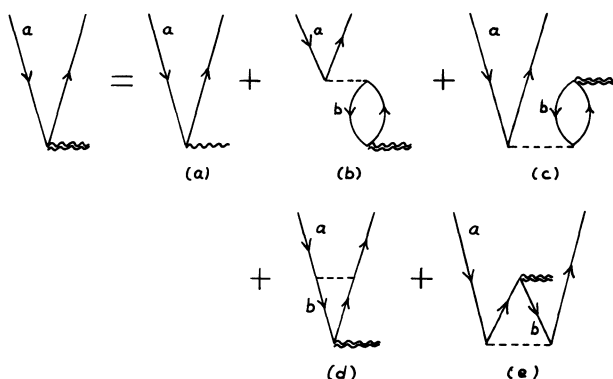

Fig. 3. — The coupled equation (11) for the electric-dipole excitation of the core orbitals.

mutes with r_{12}^{-1} one finds

$$\rho_V^{\pm} = \rho_L^{\pm} \mp \mathbf{d}_L|a\rangle/\omega.$$

This relation holds irrespective of ω. Since $\mathbf{d}_L$ commutes also with h^{PNC}, (12a) leads to the same value for E_1^{PNC} if the approximation $\omega = \varepsilon_f - \varepsilon_i$ is used.

The approach (11) above differs from the time-dependent Hartree-Fock (TDHF) method [42] through the presence of the inhomogeneous term $\mathbf{d}|a\rangle$ in equation (11). However, it leads to the same result if terms beyond first order in the core-valence interaction (such as normalization and energy corrections) are neglected in the TDHF approach. It is then not so surprising that it gives the same result both in the length and velocity forms. However, $\mathbf{d}_L$ does not commute with the non-local potential v^{PNC} and the expression (12b) leads to different results in the length and velocity forms, $(1.279 - 0.391)$ and $(1.363 -$

0.311) $\times 10^{-11}$ $iea_0 Q_W/(- N)$, respectively, if the coupled PNC-functions from (10) are used in the evaluation. To restore the length-velocity equivalence, it is necessary to treat both the dipole and the PNC perturbation at the same time, as described below.

2.5 THE PNC SHIELDING. — A natural extension of the treatment described in the two previous subsections is to allow parity admixtures also in the electric dipole excitations. This leads to a new set of coupled equations

$$(\varepsilon_a \pm \omega - h_0) | \rho_a^{\pm PNC} \rangle = \mathbf{d} | a^{PNC} \rangle + v^{\pm} | a^{PNC} \rangle + h^{PNC} | \rho_a^{\pm} \rangle + v^{PNC} | \rho_a^{\pm} \rangle + v^{\pm PNC} | a \rangle \qquad (13a)$$

where $v^{\pm}$ and $\rho_a^{\pm}$ are defined in equation (11), v^{PNC} and $| a^{PNC} \rangle$ are defined in equations (9) and (10) and $v^{\pm PNC}$ is given by

$$v^{\pm PNC} | a \rangle = - \sum_b^{core} (\langle b^{PNC} | r_{12}^{-1} | a \rangle | \rho_b^{\pm} \rangle + \langle \rho_b^{\mp} | r_{12}^{-1} | a \rangle | b^{PNC} \rangle +$$

$$+ \langle b | r_{12}^{-1} | a \rangle | \rho_b^{\pm PNC} \rangle + \langle \rho_b^{\mp PNC} | r_{12}^{-1} | a \rangle | b \rangle). \qquad (13b)$$

Equations (13) are illustrated in figure 4. Only the exchange terms enter due to angular-momentum restrictions when summing over closed shells. This set of coupled equations must be solved iteratively. The first time the equations are solved, the last two terms in $v^{\pm PNC}$ are omitted since they depend on $\rho_b^{\pm PNC}$, whereas all other terms can be evaluated using the PNC and electric-dipole functions already obtained as solutions to equations (10) and (11), respectively. When approximate functions $\rho_b^{\pm PNC}$ have been obtained in this way, they are used to evaluate the last two, previously omitted, terms in $v^{\pm PNC}$. The equations are then solved again to obtain better functions $\rho_b^{\pm PNC}$ and the procedure is continued until a self-consistent solution is obtained.

2.5.1 *Orthogonalization to occupied orbitals.* — The equations for $| a^{PNC} \rangle$, $| \rho_a^{\pm} \rangle$ and $| \rho_a^{\pm PNC} \rangle$ all contain an implicit summation on the right-hand side over excited as well as occupied orbitals. In applying perturbation theory it is customary to exclude excitations to the core orbitals. This exclusion can be achieved by orthogonalizing either the right-hand side or the functions obtained to all core orbitals. E.g., the orthogonalized electric-dipole function $| \rho_a^{\pm} \rangle_{ort}$

Fig. 4. — The coupled equation (13) for $\rho_a^{\pm PNC}$, which includes both the PNC interaction and the interaction with the electric field. The last two diagrams enter through the orthogonalization procedure as discussed in section 2.5.

(without excitations into the core orbitals) can be obtained from the non-orthogonalized function $| \rho_a^{\pm} \rangle$ as

$$| \rho_a^{\pm} \rangle_{ort} = | \rho_a^{\pm} \rangle - \sum_c^{core} | c \rangle \langle c | \rho_a^{\pm} \rangle. \qquad (14a)$$

However, by using the hermiticity of the dipole operator and the relation $\langle a | v^{\pm} | c \rangle = \langle c | v^{\mp} | a \rangle$, it is easy to see from equation (11) that $\langle c | \rho_a^{\pm} \rangle = - \langle a | \rho_c^{\mp} \rangle$. One then finds that the contribution to $v^{\pm}$ from the admixture of orbital c into $\rho_a^{\pm}$ is exactly cancelled by the contribution from the admixture of orbital a into $\rho_c^{\mp}$. Thus, $v^{\pm}$ is independent of the orthogonalization. The choice of orthogonalization in (13) is not quite so arbitrary since (13) must be considered as an extension of (11). In order to treat the orthogonalities in a consistent way the parity-mixed dipole excitations $| \rho_a^{\pm PM} \rangle = | \rho_a^{\pm} \rangle + | \rho_a^{\pm PNC} \rangle$ are orthogonalized to the parity-mixed core orbitals, $| c^{PM} \rangle = | c \rangle + | c^{PNC} \rangle$. Keeping terms to lowest order in the weak interaction gives

$$| \rho_a^{\pm PNC} \rangle_{ort} = | \rho_a^{\pm PNC} \rangle - \sum_b^{core} | b \rangle \langle b | \rho_a^{\pm PNC} \rangle -$$

$$- \sum_b^{core} | b \rangle \langle b^{PNC} | \rho_a^{\pm} \rangle - \sum_c^{core} | c^{PNC} \rangle \langle c | \rho_a^{\pm} \rangle \qquad (14b)$$

to be used together with (14a)

Since the formula (3) for E_1^{PNC} must contain a summation over all orbitals in order to include automatically all diagrams in figure 1, we have found it convenient to leave all functions non-orthogonalized as far as possible. This caused no problem for the PNC functions or the electric-dipole functions, whereas the self-consistent procedure encountered severe convergence problems when applied to equation (13). These problems are caused by a strong divergence of the $5p_{1/2} \rightarrow p_{3/2}$ and $5p_{3/2} \rightarrow p_{1/2}$ excitations, since $\varepsilon_{5p_{1/2}} - \varepsilon_{5p_{1/2}}$ is close to ω, leading to very small energy denominators for excitations
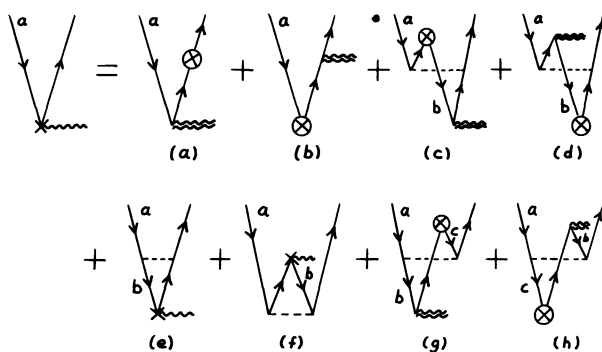
within the 5p shell. Although these contributions should cancel, this cancellation is not very helpful after the convergence is destroyed and we should thus like to enforce orthogonality to the core orbitals. This can be done without affecting the solution for $| \rho_a^{\pm} \rangle$ by observing that in the summations in (14), above, b runs over all core orbitals with the same nominal parity as a, whereas c runs over orbitals with opposite nominal parity. This makes it possible to perform a partial orthogonalization leaving $| \rho_a^{\pm} \rangle$ non-orthogonalized while omitting also the last term in (14b) and we have chosen to orthogonalize in this way. The third term on the right-hand side of (14b) must still be included and leads to two extra terms in $v^{\pm PNC}$ illustrated by the diagrams 4g and 4h.

2.5.2 *Evaluation of E_1^{PNC} from the coupled equations.* — Since only the core orbitals are used in $v^{\pm PNC}$, there is no need to obtain $\rho_{6s}^{\pm PNC}$ of $\rho_{7s}^{\pm PNC}$. However, the transition element is evaluated either as the overlap between $\langle 7s |$ and the right-hand side of the equation for $| \rho_{6s}^{+PNC} \rangle$ i.e.

$$E_1^{PNC} = \langle 7s | d + v^+ | 6s^{PNC} \rangle +$$
$$+ \langle 7s | h^{PNC} + v^{PNC} | \rho_{6s}^+ \rangle + \langle 7s | v^{+PNC} | 6s \rangle$$

or as the overlap between $| 6s \rangle$ and the right-hand side

of the equation for $\langle \rho_{7s}^{-PNC} |$

$$E_1^{PNC} = \langle 7s^{PNC} | d + v^+ | 6s \rangle +$$
$$+ \langle \rho_{7s}^- | h^{PNC} + v^{PNC} | 6s \rangle + \langle 7s | v^{+PNC} | 6s \rangle .$$

By expanding the diagrams for v^+ and v^{+PNC} it is easy to see that the two expressions are equivalent. This provides a consistency check in addition to the equivalence between the length and velocity forms which holds for the procedure described here, since it is a generalization of (11).

All matrix elements needed for the evaluation of E_1^{PNC}, in addition to those presented in table I, are given in tables II and III for the length and velocity forms, respectively. The sum of all these matrix elements can be added directly to the zeroth-order result, except for the fourth column where both the electric dipole functions and the PNC functions are coupled. In this case the terms

$$\sum (\langle 7s | v^+ | r \rangle \langle r | v^{PNC} | 6s \rangle / (\varepsilon_{6s} - \varepsilon_r) +$$
$$+ \langle 7s | v^{PNC} | 6s \rangle \langle r | v^+ | 6s \rangle / (\varepsilon_{7s} - \varepsilon_r))$$

have been counted twice and must be subtracted as indicated in the tables. The results will be discussed in the next section.

Table II. — *Summary of contributions to E_1^{PNC} for the length form of the dipole operator (in units of 10^{-11} (iea_0) $Q_W/(-N)$).*

PNC functions	Zeroth order (4)		Coupled (10)	
E_1 functions	Zeroth order (6)	Coupled (11)	Zeroth order (6)	Coupled (11)
$\langle 7s | v^{PNC} | \rho_{6s}^+ \rangle$	0.191	0.191	0.257	0.256
$\langle 7s^{PNC} | v^+ | 6s \rangle$ overcounting (^{a})	0.023	0.014	0.024	0.012 0.0014 (^{b})
$\langle \rho_{7s}^- | v^{PNC} | 6s \rangle$	− 0.052	− 0.057	− 0.070	− 0.076
$\langle 7s | v^+ | 6s^{PNC} \rangle$ overcounting (^{a})	− 0.054	− 0.042	− 0.064	− 0.047 0.0055 (^{c})
$\langle 7s | v^{+PNC} | 6s \rangle$ first order higher orders	0.0006	− 0.0005	0.0006	− 0.0013 − 0.0002
Total correction	0.108	0.106	0.147	0.150
+ zeroth order value (0.736)	0.844	0.842	0.883 0.880 (^{d})	0.886
+ Brueckner orbital correction			0.856 (^{d})	

(^{a}) When both the PNC and E_1-functions are coupled, certain diagrams are counted twice, as discussed in section 2.5. The correction for this is obtained as :
(^{b}) $\langle 7s_0^{PNC} | v^+ | 6s \rangle - \langle 7s_c^{PNC} | v^+ | 6s \rangle = \langle 7s | v^{PNC} | \rho_{6s,0}^+ \rangle - \langle 7s | v^{PNC} | \rho_{6s,c}^+ \rangle$. The subscripts denote zeroth order and coupled functions, respectively.
(^{c}) $\langle 7s | v^+ | 6s_0^{PNC} \rangle - \langle 7s | v^+ | 6s_c^{PNC} \rangle = \langle \rho_{7s,0}^- | v^{PNC} | 6s \rangle - \langle \rho_{7s,c}^+ | v^{PNC} | 6s \rangle$.
(^{d}) Dzuba *et al.* [15].

Table III. — *Summary of contributions to* E_1^{PNC} *for the velocity form of the dipole operator* (*in units of* 10^{-11} (iea_0) $Q_W/(-N)$).

PNC functions	Zeroth order (4)		Coupled (10)	
E_1 functions	Zeroth order (6)	Coupled (11)	Zeroth order (6)	Coupled (11)
$\langle 7s \mid v^{PNC} \mid \rho_{6s}^+ \rangle$	0.202	0.240	0.282	0.340
$\langle 7s^{PNC} \mid v^+ \mid 6s \rangle$	0.069	0.095	0.108	0.153
overcounting [a]				-0.058 [a]
$\langle \rho_{7s}^- \mid v^{PNC} \mid 6s \rangle$	-0.043	-0.011	-0.047	0.005
$\langle 7s \mid v^+ \mid 6s^{PNC} \rangle$	0.011	0.022	0.043	0.074
overcounting [a]				-0.052 [a]
$\langle 7s \mid v^{+PNC} \mid 6s \rangle$ first order	-0.056	-0.095	-0.107	-0.178
higher orders				0.012
Total correction	0.183	0.251	0.279	0.296
$+$ zeroth order value (0.590)	0.773	0.841	0.869 0.739 [b] (0.866 [b])	0.886
$+$ Brueckner orbital correction			0.854 [b]	

[a] See footnote to table II.

[b] Dzuba *et al.* [15]. The value in brackets has been renormalized to the use of the Hartree-Fock value for ω in the dipole operator.

3. Discussion.

3.1 COMPARISON WITH OTHER CALCULATIONS. — The $j = 1/2$ states of the alkalis can often be quite well described by a central-field model using a well-chosen local potential, as demonstrated e.g. by Bouchiat and coworkers [14] in their extensive semi-empirical study of Cs. It is also possible to obtain quite accurate results by starting from the non-local Hartree-Fock potential and applying perturbation theory [15]. We will here discuss the relations between the different types of approach.

The discrepancy between zeroth-order results obtained in different potentials should, of course, be taken into account in higher orders of perturbation theory. An important term is the potential correction, described by single-particle excitations from the wave functions obtained in the local potential, as seen e.g. from the calculations for Bi [20, 39, 41]. However, semi-empirical orbitals may also include some correlation effects, which would require double excitations in the HF wave function. Lindgren *et al.* [17] have demonstrated that important correlation effects can be included in the orbitals by modifying them to approximate « Brueckner » or « natural » orbitals. These effects may of course be included also in semi-empirical orbitals, whereas other correlation effects are not so easily included. In the related case of hyperfine structure of the s states of the alkali atoms

[15, 43, 44] and alkali-like systems [45, 46] it has been found that this is, indeed the dominating part of the correlation effects and increases significantly the density at the nucleus for the valence electron compared to the HF value. For the 6s → 7s transition in Cs, Dzuba *et al.* [15] find a surprisingly small effect of this modification, a reduction of about 3 %. Possibly, the contraction of the orbitals in the « Brueckner potential » leads to a reduction in the dipole matrix element which compensates the increase in the PNC matrix element.

The picture of an inert core whose only function is to provide a potential for the valence electron responsible for all interactions with additional perturbations is, however, not entirely correct — not even for such a « text-book » one-electron system as the alkali s-states. The corrections shown in tables II and III to the zeroth-order results are all effects which cannot be included in a central-field model although their size would depend on the orbital basis used. (Nevertheless, the procedure described in section 2 is still within the Independent-Particle Model, with orbitals of the form

$$\mid a^{TOT} \rangle = \mid a \rangle + \mid a^{PNC} \rangle + \mid \rho_a^+ + \rho_a^{+PNC} \rangle e^{i\omega t} + \mid \rho_a^- + \rho_a^{-PNC} \rangle e^{-i\omega t}.$$

As discussed in section 2.4, the (parity-conserving) shielding of the electric field can be approximated by

including a screening correction in the dipole length operator. Bouchiat *et al.* [14] use the form $d_L = - r(1 - \alpha_d/r^3) C^1$, where α_d is the dipole polarizability, and find that this form reduces the transition element by about 6 %, which is in reasonable agreement with our reduction, 4 %, but an order of magnitude larger than the result given in [18]. Bouchiat *et al.* suggest that the neglect of excitations from orbitals with $n < 5$ may be the cause of the under-estimate, but we have found that excitations from these orbitals account for only 1 % of the total shielding. (In the more sensitive velocity form, they contribute about 3 % of the parity-conserving shielding).

The PNC correction to the potential, v^{PNC}, has not been included in the semi-empirical calculation [14]. As seen from table II, this effect increases the transition element by 24 % compared to the zeroth-order HF result. The situation is quite similar for the hyperfine structure where the polarization of the core due to the exchange interaction with the valence electron is not included. This has been found to increase the hfs for ground state in Cs by a slightly smaller amount, about 17 % [41] compared to the HF value. Bouchiat find that their potential gives a 5 % overestimate of the hfs, which is thus of about the right size to compensate for the neglect of core-polarization terms both for the PNC and hyperfine interactions. Probably, there is also a large cancellation between these terms and the potential correction terms in a local potential, as observed for Bi [20, 39, 41].

The difference between the columns in table II is due to contributions of second and higher order in the electrostatic interaction — all columns include the complete first-order correction. Thus, the difference may give an indication of the importance of omitted terms. For the length form, the completely coupled results, which correspond to the solution of (9), (11) and (13), is only 5 % larger than the first-order result, whereas for the velocity form the difference is nearly 15 %. However, one might also argue that the effect of higher orders will be somewhat overestimated by this comparison. The use of the Hartree-Fock potential for excited states is known to lead to unphysical results, since these states still interact with the orbital excited [47]. In the HF potential (8) the valence orbital is not included, so there is no problem with the zeroth-order result, whereas the first-order corrections involve excitations from core-orbitals. The corrections for the self-interaction is taken into account by the terms $b = a$ in the coupled equations (10), (11) and (13) as discussed e.g. in [47, 48]. The idea behind Kelly's V^{N-1} potential is to include these terms directly in the potential for the excited states, since these are not defined by the energy-minimization criterion leading to the HF equations. (In the more recent literature, the term « V^{N-1} potential » has sometimes been used also for the HF potential defined by (8)). There is thus a certain degree of arbitrariness in the first-order result, due to the choice of potential. This ambiguity is

removed when the complete set of coupled equations are used.

We turn now to the calculation of Dzuba *et al.* [15]. Their final results, both for the HF and Brueckner orbitals are given in tables II and III for the length and velocity forms, respectively. (Their intermediate results without shielding were given in table I). They include the PNC correction to the potential to all orders and the shielding (both the parity conserving and the parity non-conserving shielding) to first order only. Thus, their results are comparable to our results in the third column of tables II and III, respectively. The results in the length form agree very well, whereas there is a large discrepancy in the velocity case. This is due to their use of the experimental value for ω, whereas we have used the HF value. For comparison their « renormalized » value, which agrees well with our result, is also given in table III.

As expected from the discussion in section 2.4, the length and velocity forms give the same results when the shielding is included to all orders, although, as seen from tables II and III, the equivalence is not at all trivial. This provides a useful check of the computational procedure. As seen from the tables, the length formula is much less sensitive than the velocity formula to higher-order corrections. In addition, there are more fundamental reasons, based on gauge invariance, to prefer the length formula [49]. Nevertheless, the use of both formulae can give an estimate of the theoretical uncertainty [15, 50] (if the equivalence is not built into the procedure).

The small contributions from the Brueckner-orbital modifications [15] as well as from higher-order corrections to v^{PNC}, to the shielding and PNC-shielding reflects the fact that the core of an alkali atom is relatively inert and gives reason to believe that the neglected correlation effects will not contribute more than a few percent.

3.2 COMPARISON WITH EXPERIMENT. — The Paris group has now observed PNC in two hyperfine components of the 6s → 7s transition in Cs; from $F = 4$ to $F' = 4$ [3] and from $F = 4$ to $F' = 3$ [4], with the result

$$\mathrm{Im}\,(E_1^{PNC})/\beta = (1.56 \pm 0.17(\mathrm{stat}) \pm 0.12(\mathrm{syst}))$$

$$(\mathrm{mV/cm})$$

where β is the vector polarizability. In order to compare the experimental and theoretical results, we assume the value $\beta = 27\,a_0^3$, which is consistent both with the result of a calculation using a semi-empirical potential [14] and with a determination based on a parametric analysis of experimental data [51, 52]. This leads to an experimental value

$$E_{1,\mathrm{exp}}^{PNC} = (0.819 \pm 0.089 \pm 0.063) \times 10^{-11}(iea_0)$$

which, together with our calculated value, $E_1^{PNC} =$ 0.886 $\times$ $10^{-11}(iea_0)(Q_W/-N)$, gives a weak charge of

$$Q_W/(-N) = 0.92 \pm 0.10 \pm 0.07$$

if we omit the uncertainty in the theoretical value which is not expected to be larger than a few percent. This result for Q_W is consistent with the values deduced from the direct measurements of the boson masses [26-28] and from neutrino-hadron scattering [21, 23] and from electron-deuteron scattering [22, 23] as discussed in section 2.1.

4. Conclusion.

The calculation presented here of the parity non-conserving electric-dipole element for the 6s → 7s transition in Cs includes to all orders the terms which contain only single excitations. Correlation effects, which require double excitations, have not been included, but the calculation is complete to first order in the electrostatic interaction. The self-consistent method used to sum certain classes of diagrams to all orders is an attractive alternative to the strict order-by-order approach and has been found to lead to an automatic, non-trivial equivalence between the results

for the length and velocity forms of the electric dipole operator.

Whereas a large number of calculations complete to second order in the electrostatic interaction have been performed for the hyperfine structure, no such calculation has yet been attempted for the PNC problem, which is more complicated than the hyperfine structure due to the presence of two perturbations in addition to the electrostatic interaction. The study of PNC is still a relatively young branch of atomic many-body theory and a complete second-order calculation would require a considerable amount of work, although Dzuba et al. [14] have included in an elegant way the second-order correlation diagrams that are expected to dominate.

In view of the smallness of the second- and higher-order effects so far obtained for the 6s → 7s transition in Cs, there is reason to believe that the omitted terms will not give any drastic contribution and that the final result, $E_1^{PNC} = 0.89 \times 10^{-11} (iea_0) Q_W/(-N)$ will not change by more than a few percent. Many-Body Perturbation Theory is a powerful tool in atomic physics and the need for atomic calculations in order to interprete the result of the PNC experiments on heavy atoms does not necessarily exclude quantitative conclusions.

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