Effects of parity nonconservation in many-electron atoms

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The contribution from the inner shells to the matrix elements of a parity violating weak interaction is examined. It is shown that the correction thus obtained does not compensate the effect but rather increases it by 20 to 40%.

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The effects of parity violation in atoms, which were predicted by the Weinberg-Salam model, increase rapidly with increasing nuclear charge Z. Therefore, the optical experiments on verification of the Weinberg-Salam model currently focus more attention on the heavy atoms, in particular, on the search of optical activity (rotation of the polarization plane of light) in bismuth pairs.[1-3] The calculation of the sought for effect in terms of the single-configuration approximation for many-electron Bi type atoms is not particularly difficult. Therefore, the applicability of this approximation is the main question in determining the accuracy and reliability of the calculations. The perturbing effect of several nearest excited configurations yields relatively small corrections, of the order of several percent.[4,5] A much larger correction turns out to be for polarization of the electronic core of an atom used in the calculation of the matrix elements of the electric dipole moment. According to Refs. 4 and 6, it comprises 30–50% for the Bi atom and reduces the effect.

In this paper, we examine different types of corrections, associated with the contribution to the matrix elements of the parity-violating weak interaction of electrons of the filled inner shells.

Representing the atomic functions Ψ as an expansion in single-configuration Hartee-Fock functions Φ, we obtain for the matrix element, which mixes the states of opposite parity,

$$V_{ik}' = \langle \Psi_i | V | \Psi_k \rangle = V_{ik} + \sum_m \frac{V_{im}U_{mk} + U_{im}V_{mk}}{E_i - E_m}, \quad (1)$$

where $V_{ik} = \langle \Phi_i | V | \Phi_k \rangle, U_{ik}$ are the matrix elements of interaction of the configurations, and the summation over m extends over all the single-configuration states of the atom, including those corresponding to excitation of the inner-shell electrons. We write Eq. (1) in the form

$$V_{ik}' = V_{ik}\left(1 + \sum_{\nu \geqslant 1} a_{\nu s} + \sum_{\nu \geqslant 2} b_{\nu p}\right), \quad (2)$$

where $a_{\nu s}$ and $b_{\nu p}$ are corrections which describe the contribution of the filled νs^2 and νp^6 shells, and ν are the principal quantum numbers. As an example illustrating further calculations, let us examine the matrix element of the weak interaction, which

adjoins the terms of the ground state $6p^3$ with the excited state $6p^27s$ of the Bi atom $\langle i| = \langle 6p^3SLJ|, |k\rangle = |6p^2[S_1L_1]7sS'L'J\rangle$. Using the standard procedure of isolating the radial parts of the matrix elements of the symmetric tensor operators, summing over the terms of the intermediate states m, and taking into account that the reduced single-electron matrix elements $(vp\|V\|ns) \sim R_{ns}(0)R'_{vp}(0)$, where $R_{ns}(0)$ and $R'_{vp}(0)$ are the values of the radial function of the ns electron and of the derivative of the radial function of the vp electrons as $r \to 0$ (see, for example, Ref. 7), we can obtain (in atomic units)

$$a_{vs} = \frac{1}{I_{vs}} \sum_{n \geq 7} \left(\frac{R_{vs} R'_{np}}{R_{7s} R'_{6p}} \right)_0 \left[\left(F_0 (6pvs, np7s) - \frac{1}{3} F_1 (6pnp, vs\, 7s) \right) \right], \quad (3)$$

$$b_{vp} = \frac{1}{I_{vp}} \sum_{n \geq 7} \left(\frac{R_{ns} R'_{vp}}{R_{7s} R'_{6p}} \right)_0 \left[F_0 (ns\, 6p, 7svp) - \frac{1}{3} F_1 (6p\, vp, ns\, 7s) \right]. \quad (4)$$

Here F_k denotes the two-electron integrals over $r_<^k / r_>^{k+1}$; all the energy denominators in Eq. (1) are close to the binding energy $vp(vs)$ of the electron $-I_{vp}(I_{vs})$ and hence are taken outside the summation sign over $n(I_{vp}, I_{vs} > 0)$. The $6s^2$ shell, for which the above remark does not apply, was examined separately. Moreover, the $vs^26p^3 \to vs6p^4$ excitations were analyzed separately, since in this case a factor, which depends on the orbital quantum numbers of the $vs6p^4$ state, appears at the F_1 integral.

Using the property of completeness of single-electron functions, we can write Eqs. (3) and (4) in a different form after eliminating the summation over the highly excited states n and the continuous spectrum.

Thus, for b_{vp}, in addition to Eq. (4), we have

$$b_{vp} = \frac{1}{I_{vp}} \left\{ \left(\frac{R'_{vp}}{R'_{6p}} \right)_0 \langle R_{6p} | \frac{1}{r} | R_{vp} \rangle - \sum_{n=1}^{6} \left(\frac{R_{ns} R'_{vp}}{R_{7s} R'_{6p}} \right) \left[F_0 (ns\, 6p, 7svp) - \frac{1}{3} F(6p\, vp, ns\, 7s) \right] \right\}. \quad (5)$$

By recording a_{vs} and b_{vp} in two different ways in the numerical calculations, we obtain additional monitoring of the calculations.

The probability of finding the electron near the nucleus, and hence the R_{vs} and R'_{vp} functions, increases with decreasing v. Therefore, the small values of F_k/I_{vp} and F_k/I_{vs} are compensated for to a certain extent by the factors R_{vs}/R_{7s} and R'_{vp}/R'_{6p} in Eqs. (3) and (4) and also by the large number of correction terms in Eqs. (2)–(4). The corrections for a_{vs} and b_{vp} were numerically calculated for the matrix elements $\langle 6s^26p^3|V|6s^26p^27s\rangle$, $\langle 6s^26p^3|V|6s^26p^28s\rangle$, and $\langle 6s^26p^3|V|6s6p^4\rangle$ using two kinds of radi-

al functions–Hartree-Fock[8] and semiempirical.[9] Since the relative correction turned out to be almost identical for the first two of these matrix elements, the same relative correction was introduced into the matrix elements $\langle 6s^2 6p^3 | V | 6s^2 6p^2 \epsilon s \rangle$, where ϵs is the state of the continuous spectrum. We used primarily expressions such as (5) for $a_{\nu s}$ and $b_{\nu s}$. To check the procedure, we calculated the first terms of the sum over n in Eqs. (3) and (4).

The calculations yielded the following results.[1)] The total correction for each matrix element and also for the value $R = \mathrm{Im} E1/M1$ determined experimentally, where $E1$ and $M1$ are the matrix elements of the electric and magnetic moments of the transition, is positive, i.e., it increases the effect. The largest contribution to the correction comes from the $5p^6$, $5s^2$, and $6s^2$ shells. The contribution from the $5p^6$ and $6s^2$ shells can be reduced by using the semiempirical functions. The total correction for R is 20–40% (the upper value, which was obtained with the Hartree-Fock functions,[8] apparently is slightly overestimated), i.e., it partially compensates for the decrease of R due to the correction for polarization of the electron core in the matrix element of the electric dipole.[4,6] We see no possibility of appreciably suppressing the parity-violating effect in the heavy Bi type atoms in comparison with the results of calculations in the single-configuration approximation.

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[1)]A detailed description of the results of calculations will be published separately.

[1]P.E.G. Baird *et al.*, Phys. Rev Lett. **39**, 798 (1977).
[2]L.L. Lewis, *et al.*, Phys. Rev. Lett. **39**, 795 (1977).
[3]L.M. Barkov and M.S. Zolotarev, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 379 (1978); **28**, 544 (1978) [JETP Lett. **27**, 357 (1978); **28**, 503 (1978)].
[4]V.N. Novikov, O.P. Sushkov, and I.B. Khriplovich, Zh. Eksp. Teor. Fiz. **71**, 1665 (1976) [Sov. Phys. JETP **71**, 872 (1976)].
[5]E.M. Henley, M. Klapisch, and L. Wilets, Phys. Rev. Lett. **39**, 994 (1977).
[6]M.J. Harris, C.E. Loving and P.G.H. Sanders, J. Phys. B, L749 (1978).
[7]V.A. Alekseev, B. Ya. Zel'dovich, and I.I. Sobel'man, Usp. Fiz. Nauk **118**, 385 (1976) [Sov. Phys. Usp. **19**, 207 (1976)].
[8]F. Herman and S. Skillman, Atomic Structure Calculations, Prentice Hall, Englewood Cliffs, N.J., 1963.
[9]L.A. Vaĭnshteĭn, Trudy FIAN **15**, 3 (1961).