BRIEF REPORTS

Brief Reports are accounts of completed research which do not warrant regular articles or the priority handling given to Rapid Communications; however, the same standards of scientific quality apply. (Addenda are included in Brief Reports.) A Brief Report may be no longer than four printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.

Computation of correlation effects on the parity-nonconserving electric-dipole transition in atomic ytterbium

B. P. Das
Non-Accelerator Particle Physics Group, Indian Institute of Astrophysics, Bangalore 560034, India
(Received 2 April 1996)

A high-precision experiment to measure parity-nonconservation in atomic Yb has been proposed recently [D. De Mille, Phys. Rev. Lett. **74**, 4165 (1995)]. We use a relativistic configuration-interaction approach to highlight the importance of correlation effects in the $6s^2(^1S_0)\rightarrow 6s5d(^3D_1)$ parity-nonconserving electric transition amplitude for Yb. Our result shows that this transition amplitude is dramatically altered by the strong mixing between some of the configurations that make up the odd-parity $6s6p(^1P_1)$ atomic state. [S1050-2947(97)03305-2]

PACS number(s): 32.80.Ys, 11.30.Er, 12.15.Ji, 32.70.Cs

In a recent paper, De Mille has proposed that the $6s^2(^1S_0)\rightarrow 6s5d(^3D_1)$ transition in atomic Yb can be used for studying parity nonconversation (PNC) [1]. He points out that (i) the aforementioned transition has a very large electric-dipole ($E1$) amplitude arising from PNC, a strongly suppressed magnetic dipole ($M1$) amplitude, and a moderate Stark-induced $E1$ amplitude; (ii) extremely high-precision measurements of PNC in Yb using the well-developed technique of Stark PNC interference appear possible; and (iii) a comparison of PNC between the large number of stable isotopes of Yb may provide a unique test of the standard model. In this paper we are concerned with only the theoretical aspects of the PNC-induced $E1$ amplitude of the $6s^2(^1S_0)\rightarrow 6s5d(^3D_1)$ transition in atomic Yb.

The $E1$ transition amplitude arising from a parity-nonconserving weak interaction can, in general, be written using first-order perturbation theory as

$$E1_{\rm PNC}=\sum_I\left(\frac{\langle\Psi_f|D|\Psi_I\rangle\langle\Psi_I|H_{\rm PNC}|\Psi_i\rangle}{E_i-E_I}+\frac{\langle\Psi_f|H_{\rm PNC}|\Psi_I\rangle\langle\Psi_I|D|\Psi_i\rangle}{E_f-E_I}\right),$$

where $|\Psi_i\rangle$ and $|\Psi_f\rangle$ are, respectively, the initial and final atomic states and $|\Psi_I\rangle$ is an intermediate atomic state whose parity is opposite that of the initial and the final atomic states. The energies of these states are given by E_i, E_f, and

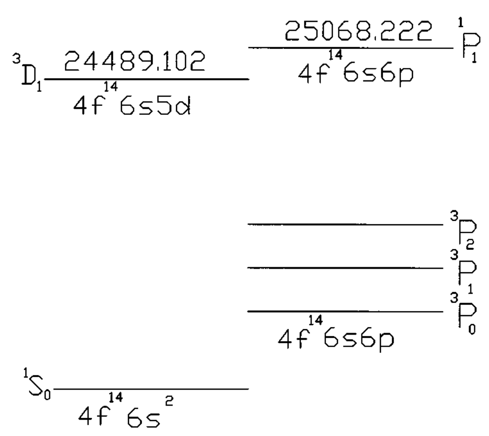

FIG. 1. Some low-lying energy levels of Yb in cm^{-1} (not to scale).

TABLE I. CI results for the reduced matrix element of the parity-nonconserving $6s^2(^1S_0)\rightarrow 6s5d(^3D_1)$ transition amplitude in Yb. Units are in $iea_0Q_W\times 10^{-11}$.

Case	Configurations	$E1_{\rm PNC}$
1	even: $4f^{14}6s^2$,$4f^{14}6s5d(J=1)$ odd: $4f^{14}6s6p(J=0)$	0.355
2	even: $4f^{14}6s$,$4f^{14}6s5d(J=1)$ odd: $4f^{14}6s6p(J=0)$,$4f^{14}6s6p(J=1)$, $4f^{14}6p5d(J=1)$	3.284
3	even: $4f^{14}6s^2$,$4f^{14}6s5d(J=1)$; $4f^{14}5d^2(J=0)$; $4f^{14}5d^2(J=1)$; $4f^{14}6p^2(J=0)$; $4f^{14}6p^2(J=1)$; $4f^{13}6p5d(J=1)$; $4f^{13}6s^26p(J=1)$ odd: $4f^{14}6s6p(J=0)$; $4f^{14}6s6p(J=1)$ $4f^{14}6p5d(J=1)$, $4f^{13}6s5d^2(J=1)$, $4f^{13}6s6p^2(J=1)$, $4f^{13}6s^25d(J=0)$	2.765

TABLE II. Comparison between theoretical and experimental energies of atomic states. Units are in cm^{-1}.

State	Theory	Experiment
$6s6p(3P_0)$	13 839.179	17 288
$6s6p(3P_1)$	14 373.477	17 992
$6s5d(3D_1)$	24 582.682	24 489.102
$6s6p(^1P_1)$	24 217.839	25 068.222

E_I. D is the electric-dipole operator and H_{PNC} is the nuclear-pin-independent neutral weak current interaction Hamiltonian given by [2]

$$H_{\mathrm{PNC}}=\frac{G_F}{2\sqrt{2}}\,Q_W\sum_e \gamma_5\rho(r_e),$$

where G_F is the Fermi constant and Q_W is the weak nuclear change given by $Q_w=2[ZC_{1p}+NC_{1n}]$. Z and N^x are the number of protons and neutrons, respectively. C_{1p} and C_{1n} are the vector (nucleon)–axial vector (electron) coupling coefficients, $\rho(r_e)$ is the normalized nucleon number density, and γ_5 is the usual pseudoscalar Dirac matrix. We use a relativistic configuration interaction (CI) approach [3] to determine the strong correlation (many-body) effects that characterize $E1_{\mathrm{PNC}}$ for atomic Yb. An atomic state in this approach is written as a linear combination of configuration states

$$|\Psi_\alpha(JM\pi)\rangle=\sum_r c_{r\alpha}|\Phi_r(JM\pi)\rangle,$$

where $|\Psi_\alpha\rangle$ is a general atomic state with angular momentum (J,M) and parity (π). Note that $|\Phi_r\rangle$ is a configuration state with the some angular momentum and parity as $|\Psi_\alpha\rangle$. The configuration mixing coefficients are given by $c_{r\alpha}$. The diagonalization of the atomic Hamiltonian in the space spanned by all the configurations required to describe the initial, final, and intermediate atomic states yields its eigenvalues and eigenvectors, which are, respectively, the energies and the mixing coefficients of the atomic states. The occupied orbitals used in the determination of $E1_{\mathrm{PNC}}$ for the transition of experimental interest in the case of Yb were obtained by performing a single-configuration $(1s^2 2s^2 \ldots 6s^2)$ Dirac-Fock calculation. The $6p_{1/2}$, $6p_{3/2}$, $5d_{3/2}$, and $5d_{5/2}$ virtual orbitals were generated from a V_{N-1} potential [4] that was constructed by exciting a $6s$ orbital. All these calculations were carried out using the GRASP code [5].

The dominant contribution to $E1_{\mathrm{PNC}}$ comes from the odd-parity $6s6p(^1P_1)$ intermediate state, which differs in energy from the $6s5d(^3D_1)$ state by only 579.12 cm^{-1} (see Fig. 1). In the present work we consider the effect of this and several other low-lying configurations built out of the occupied $5d$ and $6p$ orbitals. Some of the residual shielding configurations will be taken into account through an effective Hamiltonian. Table I gives the contributions to the reduced matrix element $E1_{\mathrm{PNC}}$ for three different cases. The Dirac-Fock approximation (no configuration mixing) yields $0.355\times10^{-11}iea_0Q_W$ (note that all the subsequent values will be given in this unit). The odd-parity configurations $6s6p_{1/2}(J=1)$, $6s6p_{3/2}(J=1)$, $6p_{1/2}5d_{3/2}(J=1)$, $6p_{3/2}5d_{5/2}(J=1)$, and $6p_{3/2}5d_{3/2}(J=1)$ have dramatic effects on $E1_{\mathrm{PNC}}$. The addition of the first three configurations changes its value to -0.228×10^{-11} with the largest contribution (-0.635×10^{-11}) coming from the $6s6p(^1P_1)$ intermediate state. The reason for the change in sign of $E1_{\mathrm{PNC}}$ is because of the change in ordering of the $6s5d(^3D_1)$ and $6s6p(^1P_1)$ energy levels relative to the Dirac-Fock case. The addition of the $6p_{3/2}5d_{5/2}$ configuration produces another change in the ordering of those two levels and the very small energy separation (70.2 cm^{-1}) between them leads to a very large contribution (7.13×10^{-11}) once again from the $6s6p(^1P_1)$ state. The total contribution from all the intermediate states in this case is 7.522×10^{-11}. The effect of the $6p_{3/2}5d_{3/2}$ configuration is to reduce this value to 3.284×10^{-11}. The result of the 14 (odd plus even) nonrelativistic or 54 relativistic configurations calculation clearly shows that the effect of electron correlation on $E1_{\mathrm{PNC}}$ is much weaker from the initial and final states than it is for some of the intermediate states. Table II gives the energies obtained for the atomic states in this case and the corresponding experimental energies [6]. The agreement between these energies can be improved by introducing an effective Hamiltonian that contains adjustable shielding factors. The electron-electron interaction part of this Hamiltonian can be written as [7]

TABLE III. Comparison between theoretical and experimental energies of atomic states for $\alpha_0=0.997$, $\alpha_1=0.654$, and $\alpha_2=0.98$. Units are in cm^{-1}.

State	Theory	Experiment
$6s6p(^3P_0)$	16 882.601	17 288
$6s6p(^3P_1)$	17 641.244	17 992
$6s5d(^3D_1)$	24 497.245	24 489.102
$6s6p(^1P_1)$	25 075.991	25 068.222

$$H_{\mathrm{eff}}^{ee}=\sum_k \alpha_k\frac{4\pi}{2k+1}\sum_{q=-k}^{k} Y_k^{q*}(\theta_1,\phi_1)Y_k^q(\theta_2,\phi_2)\frac{r_<^k}{r_>^{l+1}},$$

where α_k's are multipole shielding factors and if chosen properly they can account for certain types of shielding effects that are not included in our calculations described earlier (see Table I). For $\alpha_0=0.99$, $\alpha_1=0.654$, and $\alpha_2=0.98$, we get our best fit for energies (see Table III). The agreement between our calculated and experimental $^3D_1$ and $^1P_1$ experimental energies is indeed very good for this case and we obtain $E1_{\mathrm{PNC}}=-0.768\times10^{-11}iea_0Q_W$. The contribution of the $6s6p(^1P_1)$ state is $-0.895\times10^{-11}iea_0Q_W$. Our result is in reasonable agreement with De Mille's estimate of $|\mathrm{Im}\,E1_{\mathrm{PNC}}|=1.1(4)\times10^{-1}ea_0$ [1], which takes into consideration only the dominant contribution to $E1_{\mathrm{PNC}}$, which comes from the $6p5d$ configuration, which strongly mixes with the $6s6p$ configuration in the $^1P_1$ state. His estimate is based on information obtained from previous atomic structure calculations on Yb [8–10]. It is not straightforward to determine the accuracy of the present calculation even though it contains the most important correlation contribution arising from the mixing of $6s6p$ and $6p5d$ configurations. We are presently exploring other nonperturbative methods that will incorporate the unusually strong correlation effects that make the parity-nonconserving $E1$ transition amplitude in Yb larger than in other atoms of experimental interest.

The author is grateful to Dr. David De Mille, Professor Eugene Commins, and Professor Dmitry Budker for very valuable discussions. He would also like to thank Dr. De Mille for drawing his attention to a calculation of PNC in Yb by Porsev *et al.* [11] after this paper was submitted for publication. The result of that calculation is in reasonable agreement with this calculation before adding the shielding factors.

[1] David De Mille, Phys. Rev. Lett. **74**, 4165 (1995).
[2] E. D. Commins and P. H. Bucksbaum, *Weak Interactions of Quarks and Leptons* (Cambridge University Press, Cambridge, 1983), p. 345.
[3] B. P. Das, Phys. Scr. **36**, 487 (1987).
[4] H. P. Kelly, Phys. Rev. **131**, 674 (1963).
[5] F. A. Parpia, C. F. Fischer, and I. P. Grant (unpublished).
[6] W. C. Martin, R. Zalubas, and L. Hagan, *Atomic Energy Levels—The Rare Earth Elements*, Natl. Bur. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) Circ. No. 60 (U.S. GPO, Washington, DC, 1978).
[7] Swati Malhotra, Angom D. Singh, and B. P. Das, Phys. Rev. A **51**, R2665 (1995).
[8] J. Migdalek and W. E. Baylis, J. Phys. B **24**, L99 (1991).
[9] J. F. Wyart and P. Camus, Phys. Scr. **20**, 43 (1979).
[10] B. Budick and J. Snir, Phys. Rev. **178**, 18 (1969).
[11] S. G. Porsev, Yu. G. Rakhlina, and M. G. Kozlov, Pis'ma Zh. Eksp. Teor. Fiz. **61**, 449 (1995) [JETP Lett. **61**, 459 (1995)].