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

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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)→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]

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In a recent paper, De Mille has proposed that the 6s^2(^1S_0)→6s5d(^3D_1) transition in atomic Yb can be used for studying parity nonconservation (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)→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

\[ E_{1PNC} = \sum_i \left( \frac{\langle \Psi_i|D|\Psi_i\rangle\langle \Psi_i|H_{PNC}|\Psi_i\rangle}{E_i - E_f} + \frac{\langle \Psi_i|H_{PNC}|\Psi_f\rangle\langle \Psi_f|D|\Psi_f\rangle}{E_f - E_i} \right), \]

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 \( E_j \).

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

<table>
<thead>
<tr>
<th>Case</th>
<th>Configurations</th>
<th>( E_{1PNC} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>even: ( 4f^{14}6s^2,4f^{14}6s5d(J=1) ); odd: ( 4f^{14}6s6p(J=0) )</td>
<td>0.355</td>
</tr>
<tr>
<td>2</td>
<td>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) )</td>
<td>3.284</td>
</tr>
<tr>
<td>3</td>
<td>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^{14}6p5d(J=1); 4f^{14}6s6p(J=1); 4f^{14}6s6p(J=1) ); odd: ( 4f^{14}6s6p(J=0); 4f^{14}6s6p(J=1) ); ( 4f^{14}6p5d(J=1),4f^{14}6s5d^2(J=1),4f^{14}6s6p^2(J=1),4f^{14}6s5d^2(J=0) )</td>
<td>2.765</td>
</tr>
</tbody>
</table>

FIG. 1. Some low-lying energy levels of Yb in cm\(^{-1}\) (not to scale).
TABLE II. Comparison between theoretical and experimental energies of atomic states. Units are in cm\(^{-1}\).

<table>
<thead>
<tr>
<th>State</th>
<th>Theory</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>6s6p(3P(_o))</td>
<td>13 839.179</td>
<td>17 288</td>
</tr>
<tr>
<td>6s6p(3P(_i))</td>
<td>14 373.477</td>
<td>17 992</td>
</tr>
<tr>
<td>6s5d(3D(_i))</td>
<td>24 582.682</td>
<td>24 489.102</td>
</tr>
<tr>
<td>6s6p(1P(_i))</td>
<td>24 217.839</td>
<td>25 068.222</td>
</tr>
</tbody>
</table>

\(E_1, D\) is the electric-dipole operator and \(H_{PNC}\) is the nuclearpin-independent neutral weak current interaction Hamiltonian given by [2]

\[ H_{PNC} = \frac{G_F}{2\sqrt{2}} Q_W \sum r \gamma_5 \rho(r_e), \]

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 \(N\) 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 \(\gamma_5\) 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 \(E_{1PNC}\) for atomic Yb. An atomic state in this approach is written as a linear combination of configuration states

\[ |\Psi_\alpha(JM \pi)\rangle = \sum_r c_{ra} |\Phi_\alpha(JM \pi)\rangle, \]

where \(|\Psi_\alpha\rangle\) is a general atomic state with angular momentum \((J,M)\) and parity \((\pi)\). Note that \(|\Phi_\alpha\rangle\) is a configuration state with the same angular momentum and parity as \(|\Psi_\alpha\rangle\). The configuration mixing coefficients are given by \(c_{ra}\). 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 \(E_{1PNC}\) for the transition of experimental interest in the case of Yb were obtained by performing a single-configuration \((1s^22s^2...6s^2)\) 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 \(E_{1PNC}\) comes from the odd-parity \(6s6p(1P\(_i\))\) intermediate state, which differs in energy from the \(6s5d(3D\(_i\))\) 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 given in this unit). The odd-parity configurations \(6s6p\_{2/2}(J=1), 6s6p\_{3/2}(J=1), 6p\_{10/2}5d\_{3/2}(J=1),\) and \(6p\_{3/2}5d\_{5/2}(J=1)\) have dramatic effects on \(E_{1PNC}\). The addition of the first three configurations changes its value to \(-0.228 \times 10^{-11}\) with the largest contribution \((-0.635 \times 10^{-11})\) coming from the \(6s6p(1P\(_i\))\) intermediate state. The reason for the change in sign of \(E_{1PNC}\) is because of the change in ordering of the \(6s5d(3D\(_i\))\) and \(6s6p(1P\(_i\))\) energy levels relative to the Dirac-Fock case. The addition of the \(6p\_{10/2}5d\_{5/2}\) 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 \((7.13 \times 10^{-11})\) once again from the \(6s6p(1P\(_i\))\) state. The total contribution from all the intermediate states in this case is \(7.52 \times 10^{-11}\). The effect of the \(6p\_{10/2}5d_{5/2}\) configuration is to reduce this value to \(3.284 \times 10^{-11}\). The result of the 14 (odd plus even) nonrelativistic or 54 relativistic configurations calculation clearly shows that the effect of electron correlation on \(E_{1PNC}\) 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]

\[ H_{ee} = \sum_k \alpha_k \frac{4\pi}{2k+1} \sum_{\eta=-1}^k Y^\eta_k(\theta_1, \phi_1) Y^\eta_k(\theta_2, \phi_2) \frac{\mu^k}{r^\eta}, \]

where \(\alpha_k\)’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\(_i\)\) and \(1P\(_i\)\) experimental energies is indeed very good for this case and we obtain \(E_{1PNC} = -0.768 \times 10^{-11}iea_0Q_W\). The contribution of the \(6s6p(1P_i)\) state is \(-0.895 \times 10^{-11}iea_0Q_W\). Our result is in reasonable agreement with De Mille’s estimate of \(|\text{Im} E_{1PNC}| = 1.1(4) \times 10^{-11}iea_0\) [1], which takes into consideration only the dominant contribution to \(E_{1PNC}\), which comes from the 6p5d configuration, which strongly mixes with the 6s6p configuration in the \(1P_i\) 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.

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