PHYSICAL REVIEW A VOLUME 58, NUMBER 1 JULY 1998

Nuclear-spin-dependent parity-nonconserving transitions in Ba^+ and Ra^+

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(Received 22 January 1998)

An experiment to observe parity nonconservation using the $|5p^6 6s\rangle_{1/2} \rightarrow |5p^6 5d\rangle_{3/2}$ transition in Ba^+ has been proposed [N. Fortson, Phys. Rev. Lett., **70**, 2383 (1993)]. We have carried out relativistic configuration-interaction calculations to explore whether the $|5p^6 6s\rangle_{1/2} \rightarrow |5p^6 5d\rangle_{5/2}$ and $|6p^6 7s\rangle_{1/2} \rightarrow |6p^6 6d\rangle_{5/2}$ transitions in Ba^+ and Ra^+ respectively are good candidates for carrying out similiar experiments to measure the nuclear anapole moment. Our results suggest that Ra^+ might be a good candidate for such an experiment. [S1050-2947(98)51007-4]

PACS number(s): 32.10.Dk, 32.80.Ys, 32.90.+a

I. INTRODUCTION

The dominant contribution to parity nonconservation (PNC) in atoms comes from the neutral weak current interaction between nucleons and electrons [1]. This interaction is of two types: one of which is nuclear spin independent (NSI) and the other nuclear spin dependent (NSD) [2]. Parity-nonconserving weak interactions between nucleons can lead to a nuclear anapole moment, which in turn can interact with the electrons in an atom via the electromagnetic interaction [2]. The Hamiltonian describing this interaction is NSD in character. There are therefore two sources—the neutral weak current and the nuclear anapole moment that give rise to NSD parity-nonconserving interactions in an atom. Although it is not possible to experimentally distinguish between these two effects, it is known from theoretical considerations that the contribution of the latter to PNC in heavy atoms is much larger than that of the former [2].

PNC arising from the NSI neutral weak current interaction has been observed in several atoms during the last two decades [3]. However, it is only very recently that PNC induced by the NSD interactions was observed for the first time, and this led to a definitive measurement of the nuclear anapole moment [4]. This experiment was carried out for the $6s \rightarrow 7s$ transition in atomic cesium. Experiments of this type based on sophisticated optical techniques in combination with calculations of PNC induced by the NSD interactions can provide a unique opportunity for studying hadronic weak interactions that can give rise to nuclear PNC [5]. It is therefore important to consider atomic systems that can be used for carrying out PNC experiments to observe NSD effects.

Fortson has proposed an experiment to measure PNC in the $6s \rightarrow 5d_{3/2}$ transition in Ba^+ using the techniques of laser cooling and ion trapping [6], which is sensitive to both the NSI and NSD interactions. It may also be possible to do a similar PNC experiment on the $6s \rightarrow 5d_{5/2}$ transition in Ba^+. This transition has an important advantage—it is only sensitive to the NSD effect and is therefore a very direct way of measuring the nuclear anapole moment. With this approach one does not have to disentangle the NSD effect from its much larger NSI counterpart. The preceding remarks also apply to the $7s \rightarrow 6d_{5/2}$ transition in Ra^+. The lasers required for these two experiments are available (see Fig. 1). Indeed, several high-precision experiments on laser-cooled and trapped Ba^+ have been carried out [7], and a PNC experiment for the $6s \rightarrow 5d_{3/2}$ transition is presently underway [8]. The possibility of performing a similar PNC experiment for the $7s \rightarrow 6d_{5/2}$ transition in Ra^+ is being presently explored [9]. In this paper, we calculate the parity-nonconserving NSD electric dipole transition amplitudes for the aforementioned transition in $^{137}Ba^+$ and $^{227}Ra^+$.

II. METHOD OF CALCULATION

We use the relativistic configuration-interaction (CI) method [10] to carry out our calculations. If H_0 is the unperturbed atomic Hamiltonian and $|\Psi_0\rangle$ is the atomic state function, then

$$H_0|\Psi_0\rangle = E_0|\Psi_0\rangle. \tag{1}$$

Treating the NSD parity-nonconserving interaction as a first-order perturbation results in changing a state of definite parity to a state of mixed parity:

$$|\Psi_i^0\rangle \rightarrow |\Psi_i^0\rangle + |\Psi_i^1\rangle, \tag{2}$$

$$|\Psi_f^0\rangle \rightarrow |\Psi_f^0\rangle + |\Psi_f^1\rangle. \tag{3}$$

The electric dipole transition amplitude corresponding to the mixed parity initial and final states is

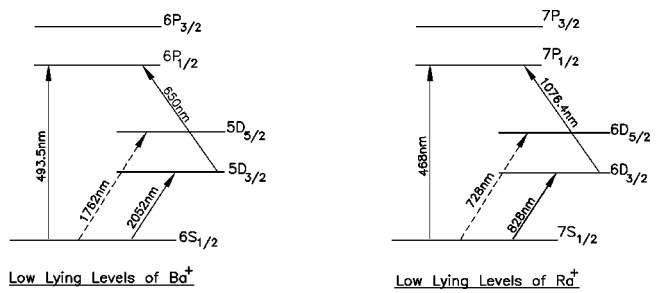

FIG. 1. Energy levels for Ba^+ and Ra^+.

$$\mathcal{A}(E_1^{NSD}) = \sum_I \frac{\langle \Psi_f^0 | D | \Psi_I^0 \rangle \langle \Psi_I^0 | H_{PNC}^{NSD} | \Psi_I^0 \rangle}{E_i^0 - E_i^0} + \sum_I \frac{\langle \Psi_f^0 | H_{PNC}^{NSD} | \Psi_I^0 \rangle \langle \Psi_I^0 | D | \Psi_i^0 \rangle}{E_f^0 - E_I^0}, \quad (4)$$

where

$$H_{PNC}^{NSD} = \frac{G_F}{2\sqrt{2}} \sum_e \vec{\alpha}^e \cdot \vec{\mu_W} \rho(r_e). \quad (5)$$

$\vec{\mu_W} = \mu_W \vec{I}$ can be considered as a weak moment arising from the nuclear anapole moment and nucleon (axial vector) –electron (vector) neutral weak current interaction. $\vec{I}$ is the nuclear spin, $\rho(r_e)$ is the normalized nucleon number density, G_F is the Fermi coupling constant, and $\vec{\alpha}$ is the Dirac matrix.

The parity of Ψ_I is opposite to that of Ψ_i and Ψ_f, as H_{PNC} and D are odd under parity. The atomic states Ψ_i, Ψ_f, and Ψ_I can be expressed as a linear combination of configuration state functions (CSF's) of the same angular momentum and parity, which are built out of an appropriate set of single-particle orbitals. The diagonalization of the atomic Hamiltonian in the space spanned by all the configurations yields its eigenvalues and eigenvectors, which are, respectively, the energies and the configuration mixing coefficients of the atomic states.

The reduced matrix element of $\mathcal{A}(E_1^{NSD})$ is of the form [11]

$$\mathcal{M}(E_{1\,red}^{NSD}) = \frac{G_F \mu_W}{2\sqrt{2}} \frac{(-1)}{\sqrt{3}} [k, F_i, F_f, 1]^{1/2} \frac{\langle I || \hat{I} || I \rangle}{I} \begin{Bmatrix} I & I & 1 \\ J_i & J_f & k \\ F_i & F_f & 1 \end{Bmatrix} \tilde{T}^k(f,i), \quad (6)$$

where

$$\tilde{T}^k(f,i) = \sum_I (-1)^{k+J_i+J_f} [k]^{1/2} \begin{Bmatrix} 1 & 1 & k \\ J_i & J_f & J_I \end{Bmatrix} \frac{\langle \Psi_f || D || \Psi_I \rangle \langle \Psi_I || H_{PNC}^{NSD} || \Psi_i \rangle}{E_i - E_I} + (-1)^k \frac{\langle \Psi_f || H_{PNC}^{NSD} || \Psi_I \rangle \langle \Psi_I || D || \Psi_i \rangle}{E_f - E_I}. \quad (7)$$

Here $|\Psi\rangle$ refers to atomic state functions.

III. DISCUSSION AND RESULTS

We calculate the PNC electric dipole transition amplitude between the states $5p^6 6s_{1/2}$ and $5p^6 5d_{5/2}$ for Ba^+. In the present calculation we treat $1s^2 2s^2 \ldots 5p^6$ as the $(N-1)$ occupied electrons, and the outermost orbital $6s$ is considered as the valence orbital. The virtual orbitals considered for the calculation are $7s$, $8s$, $6d$, $7d$, $6p$, $7p$, and $8p$. In the case of Ra^+ the PNC electric dipole transition amplitude is calculated between the states $6p^6 7s_{1/2}$ and $6p^6 6d_{5/2}$. We treat $1s^2 2s^2 \ldots .6p^6$ as the $(N-1)$ occupied electrons and the outermost orbital $7s$ is considered as the valence orbital. The virtual orbitals considered for the calculation are $8s$, $9s$, $7d$, $8d$, $7p$, $8p$, and $9p$. The GRASP multiconfiguration Dirac-Fock code [12] was used to generate virtual V_{N-1} orbitals.

Writing each atomic state as a sum of CSF's, we incorporate contributions to Ψ_i, Ψ_I, and Ψ_f from different configurations. Here we generate different CSF's from a given set of occupied and valence orbitals, taking into consideration certain types of correlation effects. We have taken into

TABLE I. $\mathcal{M}(E_{1\,red}^{NSD})$ for Ba^+ and Ra^+ in units of $iea_0\mu_W \times 10^{-12}$. Note, $I = 3/2$.

Ion	Configurations	$F_f=3$ to $F_i=2$	$F_f=2$ to $F_i=2$	$F_f=2$ to $F_i=1$	$F_f=1$ to $F_i=2$	$F_f=1$ to $F_i=1$
	$\|5p^6 6s\rangle_{1/2}, \|5p^6 5d\rangle_{5/2}, \|5p^6 6p\rangle_{3/2}, \|5p^5 6s 5d\rangle_{3/2}$	−0.080	−0.045	−0.045	−0.013	−0.029
	previous $+\|5p^5 6s 6p\rangle_{1/2}, \|5p^5 6s 6p\rangle_{5/2}$	−0.068	−0.038	−0.038	−0.011	−0.025
	previous $+\|5p^5 5d 6p\rangle_{1/2}, \|5p^5 5d 6p\rangle_{5/2}$	−0.055	−0.031	−0.031	−0.010	−0.020
Ba^+	previous $+\|5p^5 6s^2\rangle_{3/2}, \|5p^5 5d^2\rangle_{3/2}, \|5p^5 6p^2\rangle_{3/2}$	−0.052	−0.029	−0.029	−0.009	−0.019
	previous $+\|5s5p^6 6s^2\rangle_{1/2}, \|5s5p^6 5d^2\rangle_{1/2}, \|5s5p^6 5d^2\rangle_{5/2}$	−0.046	−0.026	−0.026	−0.008	−0.017
	previous $+\|5s5p^6 6p^2\rangle_{1/2}, \|5s5p^6 6p^2\rangle_{5/2}$, $\|5s5p^6 5d 6p\rangle_{3/2}, \|5s5p^6 6s 6p\rangle_{3/2}$	−0.070	−0.039	−0.039	−0.011	−0.0255
	$\|6p^6 7s\rangle_{1/2}, \|6p^6 6d\rangle_{5/2}, \|6p^6 7p\rangle_{3/2}, \|6p^5 7s 6d\rangle_{3/2}$	−0.989	−0.553	−0.553	−0.161	−0.362
	previous $+\|6p^5 7s 7p\rangle_{1/2}, \|6p^5 7s 7p\rangle_{5/2}$	−0.57	−0.319	−0.319	−0.093	−0.209
Ra^+	previous $+\|6p^5 6d 7p\rangle_{1/2}, \|6p^5 6d 7p\rangle_{5/2}$	−0.45	−0.233	−0.233	−0.070	−0.166
	previous $+\|6p^5 7s^2\rangle_{3/2}, \|6p^5 6d^2\rangle_{3/2}, \|6p^5 7p^2\rangle_{3/2}$	−0.417	−0.233	−0.233	−0.068	−0.153
	previous $+\|6s6p^6 7s^2\rangle_{1/2}, \|6s6p^6 6d^2\rangle_{1/2}, \|6s6p^6 6d^2\rangle_{5/2}$	−0.378	−0.211	−0.211	−0.062	−0.138
	previous $+\|6s6p^6 7p^2\rangle_{1/2}, \|6s6p^6 7p^2\rangle_{5/2}$, $\|6s6p^6 6d 7p\rangle_{3/2}, \|6s6p^6 7s 7p\rangle_{3/2}$	−0.615	−0.344	−0.344	−0.100	−0.225

TABLE II. $\mathcal{M}(E_{1\,red}^{NSD})$ for Ba^+ and Ra^+ in units of $iea_0\mu_W \times 10^{-12}$ for the complete calculation.

Ions	$F_f=3$ to $F_i=2$	$F_f=2$ to $F_i=2$	$F_f=2$ to $F_i=1$	$F_f=1$ to $F_i=2$	$F_f=1$ to $F_i=1$
Ba^+	-0.082	-0.046	-0.046	-0.0134	-0.030
Ra^+	-0.635	-0.355	-0.355	-0.104	-0.232

consideration the core-valence correlation wherein the $5p$ and $6s$ orbitals for Ba^+ are excited to other virtual orbitals. In the case of Ra^+ $6p$ and $7s$ orbitals are excited to other virtual orbitals. We have also considered single excitations from the core and the valence orbitals; such excitations having odd parity are extremely important for PNC. The core-core correlation excitation of two core orbitals to valence and/or virtual orbitals is not taken into consideration.

Contributions from the low-lying configurations of Ba^+, i.e., the configurations arising out of single and double excitations from $5p$ and $6s$ to $6p$ and $5d$ are tabulated in Table I. The addition of $|5p^66p\rangle_{3/2}$ alone as the intermediate CSF does not contribute to the parity-nonconserving electric dipole reduced matrix element because of vanishing PNC matrix elements. But due to the addition of $|5p^56s5d\rangle_{3/2}$ the contribution becomes nonzero because of the mixing between those two CSF's. Also from the table it is clear that the CSF's $|5p^56s6p\rangle_{1/2,5/2}$ and $|5p^55d6p\rangle_{1/2,5/2}$ make important contributions. By adding excitations from the $5s$ core to the above the value turns out to be $-0.070\ iea_0\mu_W \times 10^{-12}$. This is also tabulated in Table I.

An important reason for the difference between the values for the above two cases for Ba^+ given in Table I is the nonvanishing PNC and electric dipole matrix elements between the valence-core correlation CSF $|5s5p^66p^2\rangle$ and the intermediate CSF $|5s5p^66s6p\rangle_{3/2}$. The interplay between other correlation and electric dipole / PNC effects involving configuration with $5d$ orbitals also contributes to this difference.

Contributions from the low-lying configurations of Ra^+, i.e., the configurations arising out of single and double excitations from $6s$, $6p$, and $7s$ orbitals to $7p$ and $6d$ orbitals are tabulated in Table I. The contribution of the excitations from the $6s$ core in Ra^+ follows the same trend as in the case of Ba^+. This is also tabulated in Table I. From the calculation using the low-lying configurations it is clear that the mixing of the CSF's $|6p^67p\rangle_{3/2}$ and $|6p^57s6d\rangle_{3/2}$ leads to a nonzero contribution. Also from the table it can be seen that $|6p^57s7p\rangle_{1/2,5/2}$, $|6p^56d7p\rangle_{1/2,5/2}$, $|6s6p^67p^2\rangle_{1/2,5/2}$, $|6s6p^66d7p\rangle_{3/2}$, and $|6s6p^67s7p\rangle_{3/2}$ make important contributions.

Contributions from the configurations arising out of single and double excitations from $5s$, $5p$ and $6s$ to $7s$, $8s$, $5d$, $6d$, $7d$, $6p$, $7p$, and $8p$ for Ba^+ and $6s$, $6p$, and $7s$ to $8s$, $9s$, $6d$, $7d$, $8d$, $7p$, $8p$, and $9p$ for Ra^+ are tabulated in Table II. The calculation using the above orbitals leads to 774 relativistic configurations. Comparing with the result in Table I, we find that the dominant contributions come from the low-lying configurations.

The final results given in Table II for the NSD contribution to PNC for the transitions $|5p^66s\rangle_{1/2}\rightarrow|5p^65d\rangle_{5/2}$ and $|6p^67s\rangle_{1/2}\rightarrow|5p^66d\rangle_{5/2}$ in Ba^+ and Ra^+, respectively, can now be compared with our earlier calculation [10] for the NSD contribution for Ba^+, for the transition $|5p^66s\rangle_{1/2}\rightarrow|5p^65d\rangle_{3/2}$ for the case $F_f=3$ to $F_i=2$. The NSD contribution for the $s_{1/2}\rightarrow d_{5/2}$ transition in Ba^+ is eight times smaller than that for the $s_{1/2}\rightarrow d_{3/2}$ transition, but worth pursuing since there is no masking by the NSI contribution. For Ra^+, the NSD contribution for the $s_{1/2}\rightarrow d_{5/2}$ transition is about the same as the NSD contribution in Ba^+ for the $s_{1/2}\rightarrow d_{3/2}$ transition, making Ra^+ an attractive choice for a clean measurement of the nuclear anapole moment. Our group is studying the feasibility of this experiment. Comparing the present calculations with the NSD calculation done for Cs for the transition $|5p^66s\rangle_{1/2}\rightarrow|5p^67s\rangle_{1/2}$ for $F_f=4$ to $F_i=3$ we find that while the NSD contribution in Ba^+ is roughly ten times smaller, for Ra^+ it is only one and one-half times smaller.

IV. CONCLUSION

We have calculated the parity-nonconserving electric dipole transition amplitudes for $|5p^66s\rangle_{1/2}\rightarrow|5p^65d\rangle_{5/2}$ and $|6p^67s\rangle_{1/2}\rightarrow|6p^66d\rangle_{5/2}$ in Ba^+ and Ra^+, respectively, using the relativistic configuration-interaction method. Low-lying configurations were found to be important in the present calculations. The relatively large size of the NSD electric dipole transition amplitude for Ra^+ makes it more favorable than Ba^+ from an experimental point of view. It is indeed worthwhile to carry out detailed feasibility studies to observe the nuclear anapole moments in these two ions.

ACKNOWLEDGMENT

We are grateful to Professor Norval Fortson for valuable discussions.

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