NUCLEAR STRUCTURE ASPECTS OF
ATOMIC PARITY VIOLATION IN BARIUM

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The weak interaction between an atomic nucleus and the orbiting electrons is responsible for small parity mixings in the electron wave functions that give rise to atomic transitions forbidden between pure-parity states. The degree of the parity mixing, and thus the strength of the nominally forbidden atomic transitions, depends on the weak charge of the nucleus, driven mainly by the neutron distribution. We focus in this work on polarized electron elastic scattering by nuclei as a tool to extract information on the nuclear weak charge and radius needed to analyze atomic parity violation measurements. A set of Barium isotopes of interest for atomic parity violation experiments have been chosen in this work.

Key words: Parity-violating electron scattering. Nuclear structure. Atomic parity violation. Barium isotopes.

1. INTRODUCTION

Atomic parity violation arises from the exchange of weak neutral bosons $Z^0$ between a shell electron and the atomic nucleus, both carrying weak charge. The degree of violation is very sensitive to the neutron distribution within the nucleus, since the weak charge of neutrons is larger than the one of protons. Due to the action of the weak interaction, atomic transitions arise that would not be possible with parity conservation. By analysing these atomic transitions one can obtain relevant information on the electroweak interaction at low energies, as well as extract accurate values of Standard Model constants. To do so it is necessary to know the weak charge distribution of the atomic nucleus. Parity violation may help once again in reaching this goal by using polarized electron scattering by the nuclei under study. The idea of extracting nuclear structure information, especially on the neutron distribution, using parity violation in electron scattering was first proposed by Donnelly and collaborators [1]. Further developments in the same line were carried out on a

set of $N = Z$ nuclei in [2] with the focus on neutron distributions and on nuclear isospin mixing. The PREX experiment at Jefferson Laboratory has put this idea into practice to determine with high accuracy the neutron radius of $^{208}$Pb [3], based on theoretical calculations as for instance [4, 5]; new experiments are being considered on the same nucleus and on $^{48}$Ca (CREX). More recently efforts have been made to estimate the theoretical uncertainties in parity-violating observables in polarized electron scattering [6], which could be applied to the work presented here.

In this work we study stable Barium isotopes ($Z$=56) with an even number of neutrons ($A = 130, 132, 134, 136, 138$ and $140$). They all have zero spin ground states, thus avoiding electron-nucleus spin-dependent interactions and hyperfine structure effects. It is interesting to choose an element with large $Z$ since the parity-violating effects in atoms increase faster than $Z^3$ (see below). In order for these effects to show up the overlap between the atomic electron and the nuclear wave functions should be as large as possible, favouring the exchange of the short-ranged ($\approx 10^{-18}$ m) $Z^0$ bosons. Ionized Barium atoms, with atomic structure $\text{Ba}^+:[\text{Xe}]6s$, have one odd electron with zero orbital angular momentum, which has a large overlap with the nucleus.

1.1. ATOMIC PARITY VIOLATION

Atomic shell electrons interact with the atomic nucleus through both the electromagnetic and the neutral weak interactions. Let us consider an electric dipole transition between two atomic states of the same nominal parity, $\langle f|D_z|i\rangle$. The electric dipole selection rules forbid transitions between states with the same parity, but small parity mixings due to the weak neutral interaction between the shell electrons and the nucleus may prevent this transition amplitude from vanishing. Let us then suppose that the atomic states can be expressed as:

$$|a\rangle = |a^{(0)}\rangle + G_F|a^{(1)}\rangle, \quad (1)$$

where $|a^{(0)}\rangle$ is an eigenstate of the atomic Hamiltonian due to the electromagnetic interaction and $|a^{(1)}\rangle$ is the first-order correction due to the weak interaction, having opposite parity to $|a^{(0)}\rangle$. This perturbative expansion may be used to define the atomic parity-violating amplitude:

$$A_{PV} = \langle f^{(0)}|D_z|i^{(1)}\rangle + \langle f^{(1)}|D_z|i^{(0)}\rangle, \quad (2)$$

whose relative contribution is proportional to the weak coupling constant $G_F$. By expressing $|a^{(1)}\rangle$ in terms of the eigenstate basis $|n^{(0)}\rangle$ one gets

$$|a^{(1)}\rangle = \sum_n \frac{\langle n^{(0)}|\mathcal{H}_W|a^{(0)}\rangle}{E_n - E_a} |n^{(0)}\rangle, \quad (3)$$
where $\mathcal{H}_W$ is the weak interaction Hamiltonian between the nucleus and the electron and $E_a$ are the eigenvalues of the electromagnetic Hamiltonian. The amplitude then yields:

$$A_{PV} = \sum_n \frac{(f^{(0)}|D_z|n^{(0)})\langle n^{(0)}|\mathcal{H}_W|i^{(0)}\rangle}{E_i - E_n} + \frac{(f^{(0)}|\mathcal{H}_W|n^{(0)})\langle n^{(0)}|D_z|i^{(0)}\rangle}{E_f - E_n}.$$

(4)

The matrix element of the weak Hamiltonian can be expressed as [7, 8]:

$$\langle a^{(0)}|\mathcal{H}_W|b^{(0)} \rangle = \frac{G_F}{2\sqrt{2}} C_{ab} R_p^{2\gamma - 2} Q_W(N,Z),$$

(5)

with $\gamma = \sqrt{1 - (\alpha Z)^2}$, where $G_F$ is the Fermi coupling constant, $C_{ab}$ is a factor dependent on the atomic wave functions of states $|a\rangle$ and $|b\rangle$ and $R_p$ is the mean square radius of the protons within the nucleus. The nuclear weak charge is defined as:

$$Q_W = 2\beta_V \int \rho_n(r) [N\psi_{e_s}^\dagger \gamma_5 \psi_{ep}^\dagger] d^3r + 2\beta_V Z \int \rho_p(r) [N\psi_{e_s}^\dagger \gamma_5 \psi_{ep}^\dagger] d^3r,$$

(6)

where $\rho(r)$ are nucleon density distributions. This expression derives from the non-relativistic approximation to the weak neutral interaction Hamiltonian and keeps just the term which increases with the number of nucleons and is independent of the nucleon spins (whose contributions average to a small value or vanish). The initial and final orbital electron wave functions $\psi$ have been taken here as s- and p-waves, with normalization factor $N = \psi_{e_s}^\dagger (0) \gamma_5 \psi_{ep} (0)$. The nucleon vector weak charges $\beta_V$ will be defined later on (Eq. 14) in terms of the Weinberg angle.

The amplitude $A_{PV}$ depends on atomic as well as on nuclear properties. The former can be cancelled out by considering ratios of amplitudes between different isotopes, which differ only in the number of neutrons and therefore the factor $C_{ab}$ is approximately equal (ignoring isotopic corrections). This ratio can be written as:

$$\mathcal{R} = \frac{A_{PV}}{A_{PV}^0} = \frac{Q_W}{Q_{W}^0} \left(\frac{R_p}{R_p^0}\right)^{2\gamma - 2}.$$  

(7)

From Eqs. 7, 6 and 14 (see below) one can express, for instance, the Weinberg angle in terms of the ratio of atomic parity violation amplitudes for different isotopes $\mathcal{R}$, of the charge radii $R_p$ and of the nucleon density distributions $\rho$. A first approximation to the error in extracting the Weinberg angle in this manner (assuming a spherical nucleus with constant densities) can be shown to depend only on the nuclear structure and to decrease as the mass difference between the isotopes considered in the ratio increases. Barium is very well suited for this study because it has up to 10 isotopes with half-lives long enough to perform experiments aimed to measure atomic parity violation. In addition, the Ba$^+$ ion has one odd electron with
quantum numbers $L = 0$ and $S = 1/2$ ($^2S_{1/2}$ in standard notation). An advantage of the alkaline-like atoms is that the fine structure does not show up since the orbital angular momentum is zero.

From what has just been said it is clear that accurate knowledge of nuclear properties is needed to analyze atomic parity violation data. It is worth noticing that atomic parity violation effects are sensitive to the atomic nucleus structure at small momentum transfer values. As a rough estimate, the odd electron in Ba$^+$, with an almost negligible binding energy of 10 eV, feels the extremely short-ranged weak interaction of the nucleus when it is at least on its surface, carrying a kinetic energy $T \sim -V = Z\alpha/R$ where $V$ is the potential energy in the nuclear Coulomb field, $\alpha$ is the corresponding coupling constant, $R$ is the nuclear radius ($\sim 5$ fm, see below), and $Z$ is the total nuclear charge (56, non screened at this distance). With these conditions one has $p \sim T \sim 16$ MeV, and the momentum transfer (see next subsection) is $q \leq 2p \sim 32$ MeV on the nuclear surface (larger upper bounds may apply deeper into the nucleus). Other estimations of the momentum transfer in atomic parity violation can be found in [9]. As a general rule, atomic parity violation effects increase as $Z^3$ since the parity mixing depends on $q^2 \sim Z^2$, according to the previous arguments, and the weak charge of the nucleus itself depends mainly on the number of neutrons, which is of the order of $Z$.

1.2. ELECTRON SCATTERING BY NUCLEI

We focus in this work on polarized electron elastic scattering by nuclei as a tool to extract information on the nuclear weak charge and radius. The incident electron kinetic energy in natural units is $\epsilon = \sqrt{m_e^2 + p^2} - m_e \approx p$ where the approximation is possible because the electron momentum $p$ is much larger than its mass $m_e$. The energy transfer in the process, due to the nuclear recoil, can be written as $\omega = \sqrt{M^2 + q^2} - M$, which is negligible since the nuclear mass is very large, and the momentum transfer is $q \approx 2\epsilon \sin(\theta/2)$.

In Born Approximation (first order) one photon and one $Z^0$ are exchanged in this process. The weak interaction is hidden by the electromagnetic one unless a parity-violating observable is measured. One of them is the parity-violating asymmetry:

$$A = \frac{d\sigma^+ - d\sigma^-}{d\sigma^+ + d\sigma^-},$$

where $d\sigma^+$ is the cross-section of electrons polarized parallel to their momenta and $d\sigma^-$ is the cross-section of the electrons polarized antiparallel to their momenta.

In plane wave Born approximation (PWBA), i.e. ignoring the distortion of the incoming and outgoing electron wave functions due to the nuclear Coulomb field,
the asymmetry can be written as:
\[ A = \frac{G_F Q^2}{2\pi \alpha \sqrt{2}} \frac{W^{PV}}{W^{PC}} , \]  
(9)
where \( G_F \) and \( \alpha \) are the coupling constants of the weak and of the electromagnetic interaction respectively, and \( Q \) is the four-momentum transfer. \( W^{PC} \) and \( W^{PV} \) are the parity-conserving and the parity-violating responses, respectively.

In this work, as in previous ones [2, 5], we use nuclear targets with \( J^\pi = 0^+ \) ground states, for which the responses ratio can be written as:
\[ \frac{W^{PV}}{W^{PC}} = \frac{2e_A}{F_{C0}(q)} , \]  
(10)
where \( F_{C0} \) is the Coulomb-type monopole electromagnetic form factor of the nucleus and \( \tilde{F}_{C0} \) is the Coulomb-type monopole weak neutral form factor of the nucleus. In terms of the proton and neutron form factors, the asymmetry can be written as:
\[ A = \frac{G_F Q^2}{2\pi \alpha \sqrt{2}} 2e_A \left[ \frac{\tilde{G}_{E_n} F_{n}^0 N + \tilde{G}_{E_p} F_{p}^0 Z}{G_{E_n} F_{n}^0 N + G_{E_p} F_{p}^0 Z} \right] , \]  
(11)
where \( e_A \) is the axial weak charge of the electron (the nucleon weak form factors \( \tilde{G} \) contain the vector weak charges of the nucleons, see below). The proton and neutron form factors are defined as:
\[ F_{n}^0(q) = \frac{1}{Z} \int d^3r j_0(qr) \rho_n(r) ; \quad F_{p}^0(q) = \frac{1}{N} \int d^3r j_0(qr) \rho_p(r) , \]  
(12)
In Eq. 11 the electric-type electromagnetic, \( G_E \), and weak neutral, \( \tilde{G}_E \), nucleon form factors are related by:
\[ \tilde{G}_{E_p} = \beta^p_V G_{E_p} + \beta^n_V G_{E_n} ; \quad \tilde{G}_{E_n} = \beta^p_V G_{E_p} + \beta^n_V G_{E_n} , \]  
(13)
where the parameters \( \beta^p_V \) and \( \beta^n_V \) are obtained as a direct sum of the parameters corresponding to the constituent quarks, and are related to the Weinberg angle:
\[ \beta^p_V = 0.5 - 2\sin^2 \theta_W ; \quad \beta^n_V = -0.5 \]  
(14)
Neglecting the electric neutron form factor, \( G_{E_n} \), the asymmetry can be approximately written as:
\[ A \approx \frac{G_F Q^2 e_A \beta^n_V N}{\pi \alpha \sqrt{2}} \left[ F_{n}^0 \frac{Z}{F_{p}^0} + \beta^p_V \frac{Z}{N} \right] , \]  
(15)
where the second of the terms in the square brackets is also small. Therefore the asymmetry is approximately proportional to the ratio of the form factor of neutrons and the form factor of protons within the nucleus.
2. RESULTS

The goal of this work is to compute the PV asymmetry in electron-nucleus scattering defined in Eq. (8) for a chain of Barium isotopes of interest in atomic parity violation experiments. They are even-even isotopes with mass numbers between 130 and 140, which show a relatively simple atomic structure and a large nuclear charge.

The ground state structure of the nuclei under study here has been obtained from a self-consistent Hartree-Fock mean field calculation using Skyrme nucleon-nucleon interactions, including pairing correlations within BCS approximation. The single particle wave functions are expressed in a cylindrical harmonic oscillator basis with length and deformation parameters optimized to minimize the nuclear energies.

Figure 1 shows the energy-deformation curves of the nuclei under study, obtained from a Skyrme (SLy4) Hartree-Fock calculation with BCS pairing. Only one of the isotopes in the chain is spherical, $^{138}$Ba, influenced by the magicity of the neutron number ($N = 82$). The other isotopes are prolate in their ground state, and some of them ($A = 130, 132, 134$) show another equilibrium deformation as an excited configuration.

![Energy-deformation curves of the Barium isotopes](image)

Fig. 1 – Energy-deformation curves of the Barium isotopes under study from a Skyrme (SLy4) Hartree-Fock calculation with BCS pairing. The deformation parameter $\beta$ is proportional to the quadrupole moment.

The spherical densities of protons and neutrons are relevant to compute the nuclear weak charge as defined in Eq. 6. As the number of neutrons increases within the isotopic chain, the corresponding central density of neutrons also increases and the one of protons decreases. They are shown in Fig. 2. In Figure 3 we show the corresponding weak charge densities, defined as $\rho_W = 2\beta^6_{\nu}\rho_n + 2\beta^6_{\nu}\rho_p$. Finally, in Fig. 4 the proton and neutron form factors of these isotopes, defined in Eq. 12, are plotted. These results are necessary steps towards the calculation of the parity-violating asymmetries in electron scattering by those nuclear targets.
Coming to the polarized electron scattering by the nuclei under study and the corresponding parity-violating asymmetries, they are shown in Figure 5. Transfer momentum dependence is contained in the form factors as well as in the factor $Q^2$. The zeros in the plots correspond to values of $q$ where the neutron form factor vanishes, whereas the divergences correspond to values of $q$ where the proton form factor vanishes. This behavior arises due to the Plane Wave Approximation used in the calculation. The divergences are smeared out if the distortion of the electron wave function due to the nuclear Coulomb field is taken into account [2].

As a final step we analyze the dependence of our results on the details of the nuclear structure calculation. As an example, we show in Figure 6 the PV asymmetries
Fig. 4 – Proton (red) and neutron (black) form factors in the ground state of the isotopes under study from a Skyrme (SLy4) HF+BCS calculation.

Fig. 5 – Parity-violating asymmetry in electron scattering by Barium isotopes from a Skyrme (SLy4) HF+BCS calculation.

in polarized electron scattering for the three different Skyrme forces, which appear to be very small. In Figure 7 we plot the nucleon densities of $^{130}$Ba for three different Skyrme forces. The surface thickness can be defined as the distance between the radius at which the nuclear density is a 75% of the central value and the radius where it drops to a 25% of the central value. The calculated surface thickness varies less than a 20% for different Skyrme forces, which is an uncertainty small enough so as not to spoil the desired 1% precision in the mean square radius of neutrons that can be extracted from the asymmetry measurements using the theoretical nucleon distribution. The calculated proton and neutron root mean square radii are plotted in Fig. 8
for three Skyrme forces, differing less than 1%; theoretical (SLy4) and experimental data for charge rms radii are also shown.

Fig. 6 – Parity-violating asymmetries in electron scattering by $^{130}$Ba nuclei for three different Skyrme parametrizations: SLy4 (solid line), Sk3 (dashed line) and SGII (dotted line).

Fig. 7 – Neutron (black line) and proton (red line) densities of $^{130}$Ba from a HF+BCS calculation with three different Skyrme parametrizations: SGII (dotted line), Sk3 (dashed line), SLy4 (solid line).
Fig. 8 – Root mean square radii of neutrons and of protons for Barium isotopes from a HF+BCS calculation using three different Skyrme parametrizations: SLy4 (circle), Sk3 (triangle) and SGII (square). Charge rms radii are also shown, both theoretical SLy4 (plus) and experimental [10] (cross).

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