Estimate of Contribution from $P - D$ Mixing in Atomic PNC

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Abstract

We investigate possible contributions to future atomic parity nonconservation (PNC) experiments from parity admixtures between single-electron atomic states with total angular momentum $j = 3/2$. We develop new formalism for studying these admixtures between atomic $p$ and $d$ states, which enter only when finite nuclear size effects are considered and have been neglected in the literature to date. We use analytic approximations to provide an order-of-magnitude estimate of the contribution from these admixtures, and identify a dimensionless ratio which sets the scale of the correction. Using realistic numerical wavefunctions in Ba$^+$ we confirm the results of our analytic expressions, and conclude quantitatively that these novel admixtures are likely to be negligible in essentially all cases.
INTRODUCTION

In recent years, precision experiments measuring parity nonconservation (PNC) in atomic transitions have developed into low-energy tests of the Standard Model which complement high energy collider experiments. PNC effects in atomic transitions arise due to neutral-weak interactions between electrons and the nucleus. Atomic PNC experiments are sensitive to the radiatively corrected weak charge of the nucleus, $Q_w$, which has been calculated to one-loop in the Standard Model and is given at tree level by $Q_w^0 = -N + Z(1 - 4\sin^2\theta_w)$. Because radiative corrections enter into low- and high-energy observables differently, these precision atomic PNC experiments provide a search for possible physics beyond the Standard Model which is complementary to more conventional accelerator based searches.

It is well known that the experimental observable must be corrected for finite nuclear size when compared to the Standard Model prediction due to variation of the atomic electron wavefunctions over the extent of the nucleus. It has been shown that the transition amplitude between initial and final atomic states can be formally factorized to separate nuclear and atomic physics contributions. The nuclear structure correction to atomic PNC is non-negligible (about 4% in $^{133}$Cs) and grows as $(Z\alpha)^2$, but is reliably calculable. Differences between neutron and proton distributions modify this slightly.

The most precise atomic PNC experiment to date involves parity admixtures of initial and final states with total angular momentum $j = 1/2$, but there are several other PNC measurements which have either been performed or are currently in progress looking for PNC effects in transitions involving $j = 3/2$ final states. To date, all calculations in the literature consider only contributions from parity admixtures between $S_{1/2}$ and $P_{1/2}$ states because the $D_{3/2}$ state has vanishing amplitude and derivative at the origin. In principle, there could be an additive contribution to the PNC transition amplitude arising from opposite parity admixtures to the $j = 3/2$ final state which is induced by a finite sized nucleus. Motivated by the scale of the finite nuclear size correction to $s - p$ mixing amplitudes, we have quantified the effect of $p - d$ mixing when finite nuclear size effects are taken into account.

We begin this work by developing formalism necessary for studying parity admixtures
between $P_{3/2}$ and $D_{3/2}$ states in future atomic PNC experiments. We define a dimensionless ratio which sets the scale of the additive contribution due to $p-d$ mixing relative to the dominant $s-p$ mixing term. We then use approximate analytic calculations to provide an order-of-magnitude estimate of this ratio. Using realistic numerical wavefunctions, we confirm our analytic estimates in Ba$^+$, one of the atomic systems in which PNC effects involving a final $D$-state may be measured [12].

**FORMALISM**

The parity violating electron-nucleon interaction is dominated by exchange of $Z^0$-bosons and can be written in terms of vector and axial-vector currents for electrons and nucleons:

$$H_{PNC} = A_e V_N + V_e A_N.$$ (1)

The second term depends on the orientation of the nuclear spin and usually amounts to at most a few percent of the first, in part because the vector electron-$Z^0$ coupling is small compared its axial-vector counterpart. Additional suppression arises because the nuclear spin-dependent currents do not add coherently like the vector nucleon currents, which are independent of the spin of the nucleus. The nuclear spin independent (NSID) piece of the interaction is proportional to $Q_w$ and can be isolated experimentally by averaging over hyperfine states in the transition, so henceforth we neglect the second term in Eq. 1.

Due to the small effective momentum transfer associated with atomic PNC observables, the three-vector part of the nuclear current in the first term of Eq. 1 is highly suppressed relative to the charge ($\mu = 0$) component. Keeping only the dominant charge component, we have [11, 10, 11]

$$\langle i | H_{PNC,1} | j \rangle = \frac{G_F}{\sqrt{2}} \int d^3 r \psi^\dagger_{ei}(r) \gamma^5 \psi_{ej}(r) \rho_w(r)$$

$$= \frac{G_F}{\sqrt{2}} C_{ij}(Z) N q_p Q^{\exp}_w.$$ (2)

Here $G_F$ is the Fermi constant, $\rho_w$ is the weak nuclear charge density, $C_{ij}(Z)$ depends on the full multi-electron wavefunction, and contains atomic structure effects including many-body correlations for a point nucleus calculation; $N \equiv \overline{\psi}_{ei}(0)\gamma^5 \psi_{ej}(0)$ is a normalization factor for the single-electron axial transition matrix element evaluated at the origin; $q_p$ is the correction factor for finite nuclear size. The remaining factor, $Q^{\exp}_w$, is the experimentally
determined weak neutral charge of the nucleus which is compared directly with the Standard Model prediction. The factorization in the second line of Eq. 3 can be used because the PNC matrix elements only depend on the electronic wavefunctions over the extent of the nucleus where binding energies can be neglected with respect to the Coulomb potential. Therefore, apart from an overall normalization factor, all of the axial electronic matrix elements which contribute are essentially identical.

Of the atomic PNC experiments involving $j = 3/2$ final states, the proposed measurement [12] of PNC in a single trapped Ba$^+$ ion is the theoretically simplest, since it involves a single valence electron outside of a tightly closed shell. The others involve at least two valence electrons, leading to additional considerations such as configuration mixing which must ultimately be taken into account. In the proposed Ba$^+$ experiment, atomic PNC effects will be measured by studying the allowed $\hat{E}2$ transition between the $6S_{1/2}$ ground state and the $5D_{3/2}$ excited state. This transition has a small additional PNC-induced $\hat{E}1$ amplitude given by [12]:

$$
\mathcal{E}_{m'm}^{\text{PNC}} = \langle 5D_{3/2}, m' | \hat{E}1 | 6S_{1/2}, m \rangle
\approx \sum_{n,m''} \frac{\langle 5D_{3/2}, m' | \hat{E}1 | nP_{1/2}, m'' \rangle \langle nP_{1/2}, m'' | H_{\text{PNC},1} | 6S_{1/2}, m \rangle}{W_{6S_{1/2}} - W_{nP_{1/2}}}
+ \sum_{n,m''} \frac{\langle 5D_{3/2}, m' | H_{\text{PNC},1} | nP_{3/2}, m'' \rangle \langle nP_{3/2}, m'' | \hat{E}1 | 6S_{1/2}, m \rangle}{W_{5D_{3/2}} - W_{nP_{3/2}}}
\equiv \mathcal{E}_{s-p}^{\text{PNC}} + \mathcal{E}_{p-d}^{\text{PNC}},
$$

(3)

where $\mathcal{E}_{s-p}^{\text{PNC}}$ and $\mathcal{E}_{p-d}^{\text{PNC}}$ carry implicit dependence on $m'$, $m$. The $\Delta j = 0$ selection rule for matrix elements of $H_{\text{PNC},1}$ has already been explicitly used in determining the intermediate states present in the sums in this expression [9, 10, 11]. Here we have separated the PNC-induced transition amplitude into contributions arising from parity admixtures of the initial $s$-state ($\mathcal{E}_{s-p}^{\text{PNC}}$) and the final $d$-state ($\mathcal{E}_{p-d}^{\text{PNC}}$).

In initial estimates of the size of the PNC-induced amplitude for the Ba$^+$ and similar experiments [2, 12, 13] only amplitudes arising from $s - p$ mixing were included, with the assumption that $p$ and $d$ states are not mixed by $H_{\text{PNC},1}$. For a point-like nucleus this is an exact description of the system (to first order in $H_{\text{PNC},1}$). When finite nuclear size effects are included, however, the validity of neglecting contributions from $p - d$ mixing is less clear. As discussed in Refs. [9, 10, 11, 14], the neutral weak interaction is a contact interaction
between nucleons and the transition electron in atomic PNC. Therefore the matrix elements of $H_{\text{PNC,1}}$ depend on electronic wavefunctions evaluated over the extent of the nucleus. Upper- and lower-component Dirac radial wavefunctions vanish as $r \to 0$ for $j \geq 3/2$, so all PNC matrix elements in the second sum in Eq. 3 vanish identically for a point nucleus. For a finite-sized nucleus the first term in Eq. 3 still dominates, but it has already been shown in Refs. [10, 11] that finite nuclear size effects can modify $E_{\text{PNC}}^{s-p}$ at the $5 - 10\%$-level, depending on $Z$. We now investigate the conditions under which $E_{\text{PNC}}^{p-d}$ might contribute at levels approaching the finite nuclear size correction to $E_{\text{PNC}}^{s-p}$ in Eq. 3.

Since $E_{s-p}$ is the dominant piece it must be calculated quite accurately, including overall normalizations which require sophisticated atomic many-body calculations [7, 8]. In order to study the contribution from $p - d$ mixing, we factor out this dominant term, leaving a small dimensionless correction factor which we estimate roughly:

$$E_{m/m'}^{\text{PNC}} = E_{s-p}^{\text{PNC}} \left[ 1 + \mathcal{R}_{p-d} \right], \tag{4}$$

where

$$\mathcal{R}_{p-d} = \frac{E_{p-d}^{\text{PNC}}}{E_{s-p}^{\text{PNC}}}. \tag{5}$$

Formally, this ratio involves sums over transition matrix elements of $H_{\text{PNC,1}}$ and $E1$ operators between full many-electron atomic states including correlation effects, the calculation of which is beyond the scope of the present work. Since our goal is an order-of-magnitude estimate for the correction, however, we approximate the transition matrix elements using single-electron atomic states of nominally good parity. We expect this to be a reasonable approximation for Ba$^+$ because the transition involves a single valence electron outside of a tightly bound core. Using the solutions to the Dirac central potential problem with definite parity [15], we perform the angular integration explicitly [14], reducing these single-electron matrix elements to expressions containing simple radial integrals. We then express the PNC matrix elements as

$$\langle nP_{1/2}, m'' | H_{\text{PNC}} | 6S_{1/2}, m \rangle \equiv -i \delta_{m''m} \frac{G_F}{2\sqrt{2} I_{\text{PNC}}} \mathcal{T}_{n\pi l \pi s}^{\text{PNC}}, \tag{6}$$

$$\langle 5D_{3/2}, m' | H_{\text{PNC}} | nP_{3/2}, m'' \rangle \equiv -i \delta_{m'm''} \frac{G_F}{2\sqrt{2} I_{\text{PNC}}} \mathcal{T}_{5dnp}^{\text{PNC}}, \tag{7}$$
and the $\hat{E}1$ matrix elements as (taking the $z$-component for simplicity)

$$
\langle 5D_{3/2}, m'|\hat{E}1_z|nP_{1/2}, m'' \rangle \equiv i \frac{2\sqrt{2}}{3} e^\delta_{m'm''} T_{5dnp}^{E1} nP_{1/2}, m''
$$

(8)

$$
\langle nP_{3/2}, m''|\hat{E}1_z|6S_{1/2}, m \rangle \equiv i \frac{2\sqrt{2}}{3} e^\delta_{m'm''} T_{np6s}^{E1} nP_{3/2}, m''
$$

(9)

With these simplifications applied to Eqs. \[ \text{3} \] and \[ \text{4} \], our correction factor arising from $p - d$ mixing can be written

$$
\mathcal{R}_{p-d} = \frac{\sum_n T_{5dnp}^{PNC} T_{np6s}^{E1} / (W_{5D_{3/2}} - W_{nP_{1/2}})}{\sum_n T_{3dnp}^{E1} T_{np6s}^{PNC} / (W_{6S_{1/2}} - W_{nP_{1/2}})}.
$$

(10)

In these expressions we find it convenient to define transition radial integrals, $I_{n_1n_2l_1n_2l_2}$, because phases, numerical constants, and all dependence on magnetic quantum numbers cancel in the ratio.

We now turn to evaluating the transition radial integrals of interest. In terms of single-electron radial wavefunctions, the integrals arising from the matrix elements of $H_{PNC,1}$ take the form

$$
I_{np6s}^{PNC} = \int dr \rho_w(r) \left[ G_{np1/2}(r)F_{6s1/2}(r) - F_{np1/2}(r)G_{6s1/2}(r) \right]
$$

(11)

$$
I_{5dnp}^{E1} = \int dr \rho_w(r) \left[ G_{5d3/2}(r)F_{5p3/2}(r) - F_{5d3/2}(r)G_{5p3/2}(r) \right].
$$

(12)

These integrals constitute the finite nuclear size corrections to the $s - p$ and $p - d$ mixing contributions to atomic PNC, with the weak charge density of the nucleus ($\rho_w = -N\rho_n + Z(1 - 4\sin^2 \theta_w)\rho_p$) integrated against a radial folding function. These expressions contain essentially all dependence of $\mathcal{R}_{p-d}$ on nuclear physics. The transition radial integrals arising from the $\hat{E}1$ matrix elements are given by

$$
I_{5dnp}^{E1} = \int dr F_{5d3/2}(r)G_{np1/2}(r)
$$

(13)

$$
I_{np6s}^{E1} = -\int dr G_{np3/2}(r)F_{6s1/2}(r).
$$

(14)

The parity-allowed $\hat{E}1$ transition strengths and energy denominators present in the ratio, $\mathcal{R}_{p-d}$, are generally of similar orders of magnitude [14, 17]. Therefore we expect the scale of the correction due to $p - d$ mixing to be set by the PNC transition matrix elements. We now look for analytic approximations to the transition radial integrals in Eqs. [14] and [12].
APPROXIMATE ANALYTIC RESULTS

Although the integrals in Eqs. 11 and 12 formally extend over all space, the weak charge density only contributes appreciably for \( r \lesssim 10 \text{ fm} \). Therefore the PNC transition radial integrals can be estimated reliably by considering the form of the electron wavefunctions in the vicinity of the nucleus. In this region the electronic potential is dominated by the nuclear Coulomb potential, with screening and correlation effects negligible [9]. Also, the electronic binding energies can be safely neglected with respect to the potential in the vicinity of the nucleus, as discussed in Refs. [11, 14]. Using power series solutions of the Dirac radial equations [15] under these minimal assumptions, we find that the PNC transition radial integrals can be expressed as

\[
\mathcal{I}_{np6s}^{\text{PNC}} \simeq \frac{1}{4\pi} A_{np_{1/2}} A_{6s_{1/2}} \left\{ -N \left[ 1 - \frac{2}{9} \phi_0 (\phi_0 - 2m_e) \langle r^2 \rangle_n + \cdots \right] 
+ Z (1 - 4 \sin^2 \theta_w) \left[ 1 - \frac{2}{9} \phi_0 (\phi_0 - 2m_e) \langle r^2 \rangle_p + \cdots \right] \right\},
\]

\[
\mathcal{I}_{5dnp}^{\text{PNC}} \simeq \frac{1}{4\pi} A_{5d_{3/2}} A_{np_{3/2}} \left\{ -N \langle r^2 \rangle_n + Z (1 - 4 \sin^2 \theta_w) \langle r^2 \rangle_p + \cdots \right\}.
\]

In obtaining these results we have expanded the realistic nuclear Coulomb potential in a Taylor series about the origin, \( V(r) \simeq \phi_0 + \phi_2 r^2 + \cdots \). Here \( \phi_0 \) is the leading term in the expansion of the potential, and \( A_{nljm} \) is the coefficient of the leading term in a power series expansion of the normalized single-electron wavefunction, \( |nljm, m\rangle \). We note that the quantities in square brackets in Eq. 15 are the finite nuclear size corrections defined in Refs. [1, 10, 11], and that the \( p - d \) transition radial integrals, \( \mathcal{I}_{5dnp}^{\text{PNC}} \), vanish for a point nucleus as expected.

Because we are looking for an order-of-magnitude estimate of \( R_{p-d} \), details like the \( \sim 5\% \) finite nuclear size correction to \( \mathcal{I}_{np6s}^{\text{PNC}} \) and possible differences in neutron and proton mean-square radii are unimportant at this stage. We further simplify the PNC transition radial integrals by setting the finite nuclear size correction equal to unity in Eq. 15 and replacing \( \langle r^2 \rangle_n \) and \( \langle r^2 \rangle_p \) in Eq. 16 with the nucleon mean-square radius \( \langle r^2 \rangle_N \). With these approximations we find

\[
\mathcal{I}_{np6s}^{\text{PNC}} \approx \frac{1}{4\pi} A_{np_{1/2}} A_{6s_{1/2}} \left\{ -N + Z (1 - 4 \sin^2 \theta_w) \right\}
\]

\[
\mathcal{I}_{5dnp}^{\text{PNC}} \approx \frac{1}{4\pi} A_{5d_{3/2}} A_{np_{3/2}} \left\{ -N + Z (1 - 4 \sin^2 \theta_w) \right\} \langle r^2 \rangle_N.
\]
It is important to note that the $A_{nlj}$’s in Eqs. 15 and 16 are dimensionful constants, and that the constants for $j = 1/2$ and $j = 3/2$ have different units. Both $T_{np6s}^{PNC}$ and $T_{5dnp}^{PNC}$ arise from matrix elements of the same operator, $H_{PNC,1}$, so the ratio must be dimensionless. This expansion of the integrals for small $r$ shows, therefore, that the ratio $(A_{5d3/2}^n A_{np1/2})/(A_{n2p1/2}^n A_{6s1/2})$ should have dimension $[L]^{-2}$, where $L$ is a length scale relevant to the normalization of atomic bound state wavefunctions.

This dependence on a characteristic atomic length scale is indicative of the fundamental difference between estimating contributions from $p - d$ mixing and studying the sensitivity of the Boulder $^{133}$Cs experiment to the spatial neutron distribution [1, 4]. In the Boulder experiment [1], only parity admixtures between $s$ and $p$ states are present, so a formal factorization of the transition amplitude (Eq. 2) is possible. This factorization gives separate multiplicative factors dependent on contributions from nuclear and atomic physics which can be calculated independently. In evaluating $R_{p-d}$ no such factorization is possible, so we must estimate the normalization constants $A_{nlj}$. Plugging Eqs. 17 into our expression for the $p - d$ mixing correction factor, Eq. 10, we now have

$$R_{p-d} \approx \frac{A_{5d3/2}^n \langle r^2 \rangle_N}{A_{6s1/2}^n} \frac{\sum_n A_{np3/2}^n T_{np6s}^{E1}}{\sum_n A_{np1/2}^n T_{5dnp}^{E1}/(W_{5D3/2} - W_{nP3/2})}/\frac{\sum_n A_{np1/2}^n T_{5dnp}^{E1}/(W_{6S1/2} - W_{nP1/2})}. \tag{18}$$

Here, the sums in numerator and denominator should be of similar orders of magnitude [16, 17], so we expect that the overall scale of the correction factor will be given by the ratio out in front. We will confirm this expectation numerically for Ba$^+$ in the next section.

In order to estimate the coefficients $A_{nlj}$ in Eqs. 15 and 16, normalized electronic wavefunctions satisfying the condition $\int_0^\infty (G_{nlj}^2 + F_{nlj}^2) = 1$ must be constructed and expanded for small $r$. Hence, calculation of the normalization coefficients at the origin requires knowledge of the electron wavefunctions over atomic distance scales where shielding and correlation effects become important. Such calculations are beyond the scope of the present work. We note, however, that our correction factor $R_{p-d}$ will depend on the ratio of $\langle r^2 \rangle_N$ to the relevant atomic length scale, and that all atoms are roughly the same size. We therefore first look to hydrogenic electron wavefunctions for analytic expressions to estimate the $A_{nlj}$ and study the dependence on the characteristic parameters of the problem. Fractional deviations between (upper-component) relativistic and nonrelativistic radial wavefunctions are generally of order $(Z\alpha)^2$, except where one of the wavefunctions has a node [18]. We therefore look at the normalization of nonrelativistic hydrogenic wavefunctions at the origin for order-
of-magnitude estimates of the $A_{nlj}$'s. The coefficient of the leading term in an expansion of the nonrelativistic hydrogenic wavefunction as $r \to 0$ is given by [14, 19]

$$C_{nl} = \left( \frac{2Z}{na_0} \right)^{3/2+l} \frac{(n + l)!}{2n(n - l - 1)!} \frac{1}{(2l + 1)!},$$

(19)

where $a_0$, the Bohr radius, gives the length scale relevant to atomic wavefunction normalizations. Replacing the $A_{nlj}$'s in Eq. 18 by the nonrelativistic $C_{nl}$'s we find

$$R_{p-d} \simeq 0.04 \frac{Z^2 \langle r^2 \rangle_N}{a_0^2} \sum_n \frac{C_{np} T_{np6s}^{E1}/(W_{5D3/2} - W_{n3p/2})}{\sum_n C_{np} T_{5dnp}^{E1}/(W_{6S1/2} - W_{n1p/2})} \sim 1 \times 10^{-6} \sum_n \frac{C_{np} T_{np6s}^{E1}/(W_{5D3/2} - W_{n3p/2})}{\sum_n C_{np} T_{5dnp}^{E1}/(W_{6S1/2} - W_{n1p/2})},$$

(20)

(using $Z = 56$ and $\langle r^2 \rangle_N^{1/2} = 4.84$ fm for Ba$^+$. Based on this rough estimate, it appears that the ratio of nuclear to atomic length scales predicted by the analytic approximations serves as the primary suppression factor in considering $p - d$ mixing. Thus far we have made general arguments that the scale of $R_{p-d}$ should be set by the ratio of PNC radial integrals in Eq. 10 without estimating the $\hat{E}1$ radial integrals or energy denominators. Physically, we know that $\hat{E}1$ transition strengths and binding energies for the states of interest here are generally within an order of magnitude of one another [16, 17]. Theoretically, these quantities cannot be reliably estimated in the context of our approximations because they depend on long range atomic physics. In the next section we use realistic numerical wavefunctions [17] to evaluate all quantities in Eq. 10 as a check of our approximate analytic results.

**NUMERICAL RESULTS**

The calculations presented in the previous section are instructive in quantifying the mechanism of suppression for parity admixtures of atomic states with $j \geq 3/2$, but are admittedly crude. We now wish to test the validity of the order-of-magnitude estimate as well as investigate whether the energy denominators and $\hat{E}1$ transition radial integrals which we have not yet addressed might give rise to enhancements to $R_{p-d}$. We have obtained realistic binding energies and atomic radial wavefunctions for Ba$^+$, calculated in a relativistic Dirac-Hartree-Fock model [17]. Using these tabulated wavefunctions, we have performed the transition radial integrals in Eqs. 11 through 14 numerically. The sums in both numerator and denominator of Eq. 10 are dominated by the $n = 6$ admixed states, but we have included
contributions from $n = 7, 8$ as well. This calculation yields $R_{p-d} \approx 4 \times 10^{-6}$, in good agreement with our crude but analytic estimate.

In order to study this numerical check on our approximate analytic calculation, we have fit the relativistic numerical wavefunctions to polynomials near the origin and extracted the coefficients of the leading terms of the upper- and lower-components. Overall wavefunction normalizations are not fixed by power series solutions near the origin, but the ratio of leading term normalizations of upper- and lower-component wavefunctions is uniquely determined by the value of the potential at the origin. Comparing this ratio estimated from the fitted numerical wavefunctions and from power series solutions for relativistic hydrogenic wavefunctions assuming that the total potential at the origin is dominated by the nuclear Coulomb potential, we find that the two methods agree to better than 5%. As an additional check, we assume that $R_{p-d}$ is dominated by the $n = 6$ term and estimate $I_{6dp}/I_{6ps}$ as simplified in Eqs. using both nonrelativistic and fitted coefficients. The nonrelativistic hydrogenic estimate gives $1 \cdot 10^{-6}$, while the estimate from fitting numerical wavefunctions gives $0.6 \cdot 10^{-6}$. These numerical checks indicate that our crude analytic approximate results are in reasonable agreement with a more detailed, full calculation requiring many-electron atomic wavefunctions including the effects of correlations and shielding.

CONCLUSIONS

These calculations indicate that neglecting possible $p - d$ mixing contributions to atomic PNC amplitudes which involve $j = 3/2$ initial or final states is an exceedingly good approximation. We have demonstrated that errors from neglecting $p - d$ mixing effects are well below other sub-1% effects which have been neglected to date, including contributions from the three-vector nucleon currents, radiative corrections such as one-photon one-$Z^0$ exchange box diagrams, and parity violating electron-electron interactions. While we have focused on the simplest atomic system proposed for experiment, Ba$^+$, we expect this result to be applicable to more complex systems like Ytterbium because the scale of the correction is proportional to $Z^2\langle r^2 \rangle_N/a_0^2$ in all cases. The most likely source of significant enhancement of the $p - d$ mixing term would be an exceedingly small energy difference between the the admixed $p$ and $d$ states in a heavy atom, which would depend sensitively on the particular atomic system.
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