

Nuclear Matrix Elements for Tests of Fundamental Symmetries

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The nuclear matrix elements for the momentum quadrupole operator and nucleon spin operator are important for interpretation of precision atomic physics experiments that search for violations of Lorentz and CPT symmetry and for new spin-dependent forces. We use the configuration-interaction nuclear shell model and self-consistent mean field theory to calculate the relevant matrix elements in ²¹Ne, ¹³¹Xe, and ²⁰¹Hg. We find that the spin expectation values in these nuclei are dominated by the odd neutron, while the quadrupole moment of the nucleon momentum, M , has comparable neutron and proton contributions. These are the first microscopic calculations of the nuclear matrix elements for the momentum quadrupole tensor that go beyond the single-particle estimate. We show that they are strongly suppressed by the many-body correlations, in contrast to the well known enhancement of the spatial quadrupole nuclear matrix elements.

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Several types of precision low energy tests of the Standard Model use nuclear-spin-polarized atoms to achieve very high sensitivity by relying on long nuclear spin coherence times that are possible with atoms in ¹S₀ ground state, such as ³He, ²¹Ne, ¹²⁹Xe, ¹³¹Xe, ¹⁹⁹Hg and ²⁰¹Hg. Such tests include searches for violation of Lorentz and CPT symmetry [1], [2], [3], and for new spin-dependent forces mediated by light particles, such as an axion [4], [5], [6], [7], [8], [9].

The interpretation and comparison of these experiments requires knowledge of nuclear matrix elements responsible for new interactions beyond the Standard Model. A number of simple models have been used to estimate the relevant nuclear matrix elements [10], [11], [12], but no detailed nuclear structure calculations have been performed so far for this purpose. This can be contrasted with a large number of nuclear structure calculations performed to estimate the scattering cross-sections for dark matter particles [13], [14], [15] and rates for neutrinoless double-beta decay [16].

The nuclear matrix elements relevant in searches for violations of Lorentz symmetry within the Standard Model Extension (SME) are derived in [10]. Here we focus on matrix elements that generate couplings to CPT-odd b_μ and CPT-even $c_{\mu\nu}$ terms in the SME Lagrangian for fermions:

$$\mathcal{L} = \frac{1}{2} i \bar{\psi} (\gamma_\nu + c_{\mu\nu} \gamma^\mu) \overleftrightarrow{\partial}^\nu \psi - \bar{\psi} (m + b_\mu \gamma_5 \gamma^\mu) \psi. \quad (1)$$

For non-relativistic nucleon motion they generates an en-

ergy shift

$$\mathcal{H} = -2b_j S_j - (c_{jk} + c_{00} \delta_{jk}/2) p_j p_k / m, \quad (2)$$

where S_j is the spin operator, p_j is the momentum operator, and m is the mass of the fermion. Traditionally, Lorentz violation effects and spin-dependent forces have been analyzed separately at the level of neutrons and protons under the assumption that they are independent. This provides a way to roughly classify the experiments without making assumptions about a microscopic theory that would likely generate comparable effects in neutrons and protons. For particles that are on average at rest, only the spherical rank-2 components of the tensor $p_i p_j$ give a finite energy shift. Using Wigner-Eckart theorem, they can be expressed in terms of the matrix elements of the quadrupole tensor operator $\hat{M} = 2p_z^2 - p_x^2 - p_y^2$,

$$M = \langle I, I | \hat{M} | I, I \rangle = \langle I, I | 2p_z^2 - p_x^2 - p_y^2 | I, I \rangle, \quad (3)$$

for a nucleus with spin I . So far in the analyses of the Lorentz-violation experiments the matrix elements of the nucleon spin $\langle S_p \rangle$ $\langle S_n \rangle$ have been calculated using either a single-valence nucleon wavefunction [10] or phenomenological models that adjust the spin expectation values using experimental values of the nuclear magnetic moments [17], [11]. For the quadrupole momentum matrix elements, only the single-particle wavefunctions has been used [10].

In this letter we perform the first many-body calculations of the momentum quadrupole moment M ,

for several nuclei that can be used in precision low-energy tests of the Standard Model. We find that the contributions of protons and neutrons are comparable. Therefore, Lorentz symmetry tests relying on momentum quadrupole moments constrain both neutron and proton effects with similar sensitivity. We show that the core-polarization mechanism that is well known to enhance the spatial quadrupole moment Q has the effect of reducing the M values compared to values obtained in the valence shell-model space. We also show results for the expectation of spin operators. In contrast to the quadrupole moments, the matrix elements for the spin operators for these nuclei with an odd-neutron are dominated by the neutron contribution. Thus, the experimental limits relying on spin expectation values primarily constrain neutron contributions. We also point out these atomic experiments can constrain Lorentz violation in the purely electromagnetic sector due to the quadrupole anisotropy of the nuclear Coulomb potential in the presence of Lorentz violation effects [18], [19], but quantitative calculations for these nuclear matrix elements remain to be obtained.

Our main finding is that momentum anisotropy is greatly suppressed by many-body correlations in the nuclear wave function. This will be seen in the two many-body treatments presented here, namely the configuration interaction (CI) method including core polarization effects, and in the self-consistent mean-field model (SCMF) with a commonly used energy density functional. The qualitative effect can be seen easily with a very simple density-functional model which generalizes the harmonic oscillator model of Bohr and Mottelson [20]. We take the energy functional as

$$E = \langle \Psi | \frac{p^2}{2m} | \Psi \rangle + \int d^3r \mathcal{V}[\rho(r)], \quad (4)$$

where \mathcal{V} is an interaction-energy functional depending only on the local density $\rho(r) = \langle \Psi | a_r^\dagger a_r | \Psi \rangle$. Consider the change in energy when the wave function is changed by the scaling transformation $\Psi'(r_1, r_2) = \Psi(r'_1, r'_2)$ where $r' = (x', y', z') = (xe^{-\varepsilon}, ye^{-\varepsilon}, ze^{2\varepsilon})$. The interaction energy remains the same with the new wave function because the Jacobian for the transformation of variables is unity, ie. $d^3r = d^3r'$. The kinetic term does change, depending on ε as

$$\frac{1}{2m} \langle p^2 \rangle^\varepsilon = \frac{1}{2m} (\langle p_x^2 \rangle e^\varepsilon + \langle p_y^2 \rangle e^\varepsilon + \langle p_z^2 \rangle e^{-2\varepsilon}). \quad (5)$$

The energy is minimum in ground state implying $d\langle T \rangle^\varepsilon / d\varepsilon = 0$. Carrying out the algebra, one finds that the derivative vanishes only if $2\langle p_z^2 \rangle - \langle p_x^2 \rangle - \langle p_y^2 \rangle = 0$.

The best current limits on quadrupole Lorentz violation effects currently come from the nucleus ^{21}Ne [3], which we now discuss. The pure single-particle model would treat this as a $d_{3/2}$ neutron, since the nucleus has an odd neutron number and spin-parity $3/2^+$. The moments for the electric quadrupole operator Q , the momentum anisotropy operator M , the angular momentum

operators S, L , and the magnetic moment μ are shown on the first line of Table I. The second line shows the moments found from the CI method that includes the full sd -shell with a Hamiltonian that has been globally validated on properties of nuclei in that mass region [21]. One sees that the full sd -shell calculation reproduces the experiment magnetic moment, but falls short by a factor of 2 on the quadrupole moment. The single-particle model is not even qualitatively correct. The problem with quadrupole moment in the sd -shell calculation is that it omits an important contribution from the polarization of the orbitals by the deformed field. These may be treated perturbatively as excitations to higher orbitals of the same parity, and in practice they are treated as effective charge factors in the valence-shell calculations. Thus the quadrupole moments are calculated as

$$Q_p = Q_p^{sd}(1 + \delta_{pp}) + Q_n^{sd}\delta_{np},$$

and

$$Q_n = Q_n^{sd}(1 + \delta_{nn}) + Q_p^{sd}\delta_{pn}. \quad (6)$$

where δ_{vc} are the corrections due to the polarization of the core nucleons (c) by the valence nucleons (v). For $N \sim Z$ one can use $\delta_{pp} = \delta_{nn} = \delta_p$ and $\delta_{pn} = \delta_{np} = \delta_n$. Values of $\delta_{pp} = \delta_{nn} = 0.35$ and $\delta_{np} = \delta_{pn} = 0.45$ are the effective charge parameters appropriate for sd -shell E2 observables [21]. The resulting quadrupole moments are shown on the third line of Table I.

The same polarization physics applies for the momentum anisotropy operator, but with the opposite sign of the effective charge. This may be easily seen from the perturbative formula for the polarization contribution to the moment of an operator \mathcal{O} . In an obvious notation,

$$\delta\mathcal{O} = \sum_{p,h} \langle p | V | h \rangle \frac{1}{E_p - E_h} \langle p | \mathcal{O} | h \rangle, \quad (7)$$

where p, h are particle and hole orbitals. For harmonic oscillator orbitals p and h two major shells apart ($\Delta N = 2$ where $N = 2n + \ell$), and the matrix elements of the operators \hat{Q} and \hat{M} are related by

$$\langle p | \hat{Q} | h \rangle = -\frac{1}{m^2\omega_0^2} \langle p | \hat{M} | h \rangle. \quad (8)$$

where ω_0 is the oscillator frequency. Applying the above effective charges with the opposite sign, we obtain the values for the M matrix elements shown on third row of Table I.

One cannot apply the CI method to most heavy nuclei due to the large size of the model space. However, self-consistent mean field theory has proven to be quite reliable for calculating matrix elements of one-body operators such as Q in deformed nuclei [22]. Before presenting those results for heavy nuclei of interest, we apply the theory to ^{21}Ne . Here we use the Hartree-Fock-

Bogoliubov method [23], [24], with the Gogny D1S interaction [25]. The odd-particle orbital is blocked and time-odd fields are taken into account in the self-consistent process. Axial symmetry is preserved so that the different mean field configurations can be labeled with the K quantum number of deformed nuclei. Reflection symmetry is allowed to be broken, but in the five isotopes treated here parity remains a good quantum number. For ^{21}Ne $I = 3/2^+$, the calculation gives a prolate deformed state with Nilsson quantum numbers $[N n_z \Lambda] = [211]$ and $\beta_2=0.40$. The matrix elements are first obtained in terms of the intrinsic deformations Q^i

$$Q_p^i = \langle i | (3r_z^2 - r^2)_p | i \rangle = 43.2 \text{ fm}^2, \quad (9)$$

$$Q_n^i = \langle i | (3r_z^2 - r^2)_n | i \rangle = 48.7 \text{ fm}^2, \quad (10)$$

$$M_p^i = \langle i | (3p_z^2 - p^2)_p | i \rangle = 0.335 (\hbar/\text{fm})^2, \quad (11)$$

and

$$M_n^i = \langle i | (3p_z^2 - p^2)_n | i \rangle = 0.506 (\hbar/\text{fm})^2. \quad (12)$$

Then they are projected onto the laboratory frame by

$$Q = \frac{[3K^2 - I(I+1)]}{(I+1)(2I+3)} Q^i. \quad (13)$$

For ^{21}Ne with $K = I = 3/2$, $Q = Q^i/5$, and

$$Q_p = \langle I, I | (3r_z^2 - r^2)_p | I, I \rangle = 8.6 \text{ fm}^2, \quad (14)$$

$$Q_n = \langle I, I | (3r_z^2 - r^2)_n | I, I \rangle = 9.7 \text{ fm}^2, \quad (15)$$

$$M_p = \langle I, I | (3p_z^2 - p^2)_p | I, I \rangle = 0.067 (\hbar/\text{fm})^2, \quad (16)$$

and

$$M_n = \langle I, I | (3p_z^2 - p^2)_n | I, I \rangle = 0.101 (\hbar/\text{fm})^2. \quad (17)$$

The results are shown in the last line of Table I. The conversion between $(\hbar/\text{fm})^2$ and the units of m MeV is

$$(\hbar/\text{fm})^2 = m(197)^2/(938) \text{ MeV} = 41.4 m \text{ MeV}, \quad (18)$$

where m is the nucleon mass. (The X matrix elements given [3] are related to M by $M/\sqrt{6}$) The SCMF agrees well with the CI method for Q , and it also shows a large suppression of M . The agreement between the CI method and SCMF is encouraging given that the methods of calculation and Hamiltonians are entirely different. For the quadrupole momentum matrix elements we recommend using the deformed-model results since this model takes into account the quadrupole excitations self consistently, whereas the shell-model results based on effective charges first-order in perturbation theory. The

magnetic moment is not so well reproduced, but it at least has the correct sign, unlike the pure single-particle model. In [3], a $0d_{3/2}$ single particle neutron wavefunction was used, but they also used a low value for the nucleon kinetic energy, which gives $M_n = -4m$ MeV. Thus, the more accurate value for the neutron quadrupole momentum operator is similar in magnitude, but has opposite sign from the estimate used in [3] and the more complete theory introduced a proton matrix element of similar size to the neutron.

Table II shows the results for the SCMF theory in the heavy nuclei of interest, ^{131}Xe and ^{201}Hg . These nuclei are very soft with respect to β . The best procedure in this case is to choose a value for β that reproduces the experimental Q moment. The SCMF results are compared with the extreme single-particle model obtained in a spherical basis with the Skx Skyrme interaction [26]. In the single-particle model, $(M/Q) = 2m \langle T \rangle / \langle r^2 \rangle$ where $\langle T \rangle$ is the kinetic energy. One sees that the single-particle model does not provide useful guidance for the individual moments Q and M .

In Table I we also show the calculated spin matrix elements for ^{21}Ne obtained with the free nucleon operators for the spin and orbital g-factors. The sd model gives good agreement for the experimental magnetic moment of ^{21}Ne . The SCMF value is too large compared to experiment because the spin-polarization is not included. We also calculated the spin matrix elements in the heavy nuclei using the SCMF theory shown in Table II. Again the SCMF is too large compared to experiment due to the lack of spin-polarization. For the spin matrix elements it is preferable to use results based on CI methods [14], [27], [15].

We also point out that tests of Lorentz violation effects in nuclei are sensitive to Lorentz violation in the purely electromagnetic sector. As was discussed recently [19], certain types of Lorentz violation in electromagnetism can be described as a quadrupole distortion of the normally spherically-symmetric Coulomb potential for a point charge [18]. To get an order of magnitude estimate for this effect we imagine that the electric quadrupole moment of ^{21}Ne is created by a proton orbiting a spherically symmetric nuclear core, assuming that there is no Lorentz violation in the strong interactions. In this picture Lorentz violation in the electromagnetic sector will result in a quadrupolar anisotropy of the Coulomb potential of the core, which will then interact with the proton quadrupole moment. The expected energy shift is on the order of proton Coulomb energy times the Coulomb potential quadrupole anisotropy, described by the electromagnetic Lorentz-violation parameter $\tilde{\kappa}_{e-}^{jk}$ [18]. The valence nucleon Coulomb energy is on the order of 1 MeV, while the energy resolution of the recent experiment with ^{21}Ne is on the order of 10^{-23} eV, indicating that the coefficients $\tilde{\kappa}_{e-}^{jk}$ can be constrained at the level of 10^{-29} , many orders of magnitude smaller than recent [19] and

TABLE I: Quadrupole and spin matrix elements for ^{21}Ne . CP is the addition of the core-polarization correction.

	I^π	model	Q_{exp} $e \text{ fm}^2$	Q_p fm^2	Q_n fm^2	M_p $m \text{ MeV}$	M_n $m \text{ MeV}$	$\langle S_{zp} \rangle$	$\langle S_{zn} \rangle$	$\langle L_{zp} \rangle$	$\langle L_{zn} \rangle$	μ	μ_{exp}
^{21}Ne	$3/2^+$	$0d_{3/2}$	10.3(8)	0	-4.5	0	-18.2	0	-0.3	0	1.8	1.148	-0.662
^{21}Ne	$3/2^+$	CI sd	“	5.4	6.4	21.9	25.9	0.022	0.292	0.243	0.942	-0.720	“
^{21}Ne	$3/2^+$	CI sd with CP	“	10.2	11.0	2.7	7.0	0.022	0.292	0.243	0.942	-0.720	“
^{21}Ne	$3/2^+$	SCMF	“	8.6	9.7	2.8	4.2	-0.037	0.410	0.037	1.090	-1.737	“

TABLE II: Quadrupole and spin matrix elements for heavy nuclei.

	I^π	model	β_2	Q_{exp} $e \text{ fm}^2$	Q_p fm^2	Q_n fm^2	M_p $m \text{ MeV}$	M_n $m \text{ MeV}$	$\langle S_{zp} \rangle$	$\langle S_{zn} \rangle$	$\langle L_{zp} \rangle$	$\langle L_{zn} \rangle$	μ	μ_{exp}
^{131}Xe	$3/2^+$	$1d_{3/2}$		-11.7(6)	0	-10.0	0	-17.7	0	-0.3	0	1.8	1.148	0.692
^{131}Xe	$3/2^+$	SCMF	-0.033	“	-11.6	-13.6	-4.7	5.17	0.011	-0.202	-0.011	1.702	0.822	“
^{201}Hg	$3/2^-$	$2p_{3/2}$		38.7(10)	0	-11.9	0	-18.6	0	0.5	0	1.0	-1.913	-0.560
^{201}Hg	$3/2^-$	SCMF	0.064	“	38.7	58.4	-20.5	1.5	-0.027	0.423	0.027	1.077	-1.742	“

proposed [28] experiments using Yb ions. We leave detailed analysis of this effect to a future publication.

In summary, we present the first detailed nuclear shell model calculation of the matrix elements relevant for low-energy tests of Lorentz invariance involving polarized nuclear spins. We find that spin matrix elements are dominated by the valence nucleon, while momentum anisotropy matrix elements are comparable for protons and neutron and are strongly suppressed. The present analysis for ^{21}Ne reaffirms the limits on Lorentz violation established in [3]. Further analysis of nuclear matrix elements can set new stringent limits from existing experiments on Lorentz violation for other fermion coefficients in SME [10], beyond those listed in Eq. (1), as well as Lorentz violation in the electromagnetic sector.

As this paper was prepared for publication, we became aware of a new analysis of the momentum quadrupole operator [29]. They also relate the momentum quadrupole operator to the electric quadrupole moment but using only a phenomenological model and without considering core-polarization corrections and the change in its sign between Q and M . As the result, their estimate of the momentum quadrupole operator in ^{21}Ne is nearly 20 times larger, which is not supported by our more detailed analysis. After we shared an early version of our paper with the author, a revised version was submitted [30] giving results for ^{21}Ne that are close to ours.

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