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NUCLEAR MAGNETIC QUADRUPOLE MOMENTS IN SINGLE-PARTICLE APPROXIMATION

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НОВОСИБИРСК

Nuclear Magnetic Quadrupole Moments in Single-Particle Approximation

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Abstract

Static magnetic quadrupole moment of a nucleus, induced by T- and P-odd nucleon-nucleon interaction, is investigated in the single-particle approximation. Models are considered allowing for analytical solution. The problem is also treated numerically in a Woods-Saxon potential with spin-orbit interaction. The stability of results is discussed.

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1. Magnetic quadrupole moment is a static characteristic of a quantum system which is forbidden by P- and T-invariance. Nuclear magnetic quadrupole moment (NMQM) can be induced both by the nucleon electric dipole moment[1] and by P- and T-odd nuclear forces[2]. The interest to NMQM is due to the experimental searches for P- and T-odd effects in atoms and molecules (see, e.g., book[3]).

The manifestation of electric dipole moment (EDM), which also violates P- and T-invariance, in atomic and molecular phenomena is strongly hampered by the electrostatic screening. In a stationary system of nonrelativistic pointlike particles interacting via Coulomb forces such a screening of average electric field acting on any paricle is complete. Therefore, in such a system for a particle EDM there is nothing to interact with, which means that this EDM just cannot be observed [4, 5].

The nuclear dipole moment becomes observable however due to the finite size of a nucleus, more exactly, due to different distribution of its charge and EDM [6]. One more way to transfer nuclear P- and T-violation to an atom or molecule is via NMQM [1]. It demands of course nuclei with spin $I > 1/2$. Besides, the NMQM induces P- and T-odd effects only in atoms (molecules) with unpaired electron angular momenta since it interacts directly with magnetic field of the electrons. However, when operative, the NMQM is much more effective for circumventing the electrostatic shielding in atoms and molecules [1, 2, 3].

It has been shown in Ref.[2] that the NMQM induced by the P- and T-odd internucleon interaction can be much larger than that due to the nucleon EDM. In that paper the quadrupole moments, induced by that interaction,

were evaluated in a simple model where the profile of nuclear density was assumed to coincide with that of nuclear potential. In the present article we calculate NMQM within a more accurate approach. Namely, we use a realistic description of the nuclear density; the nucleon wave functions and Green's functions are obtained with Woods-Saxon potential which includes the spin-orbit interaction. We include also the contribution of the current generated by the spin-orbit interaction; contrary to naive expectations, this contribution does exist for an outer neutron, but does not for an outer proton. One more model admitting a closed analytical solution is considered, that of the oscillator potential. We restrict throughout the present paper to the single-particle approximation, that of a valence nucleon above a spherically-symmetric core.

This approach was recently used by us [7] for treatment of nuclear anapole moments, P-odd, but T-even characteristic.

2. Let us begin with discussing the T-and P-odd nucleon-nucleon potential. In the local limit and to first order in the nucleon velocities p/m it can be written as follows (see, e.g., book [3])

$$W_2 = \frac{G}{\sqrt{2}}\frac{1}{2m}\sum_{a,b}\Big((\xi_{ab}\vec{\sigma}_a - \xi_{ba}\vec{\sigma}_b)\cdot\vec{\nabla}\delta(\vec{r}_a-\vec{r}_b)+ \\ + \xi'_{ab}\,[\vec{\sigma}_a\times\vec{\sigma}_b]\cdot\{(\vec{p}_a-\vec{p}_b),\delta(\vec{r}_a-\vec{r}_b)\}\Big) \qquad (1)$$

where the notation $\{\quad,\quad\}$ means anticommutator. The dimensionless constants ξ characterize the magnitude of the interaction in units of the Fermi weak interaction constant $G = 10^{-5}/m^2$ and are supplied with subscripts in order to distinguish between protons and neutrons.

After averaging this expression over the core nucleons we obtain the P- and T-odd mean field potential for an outer nucleon

$$W(\vec{r}) = \frac{G}{\sqrt{2}}\frac{\xi_a}{2m}\vec{\sigma}\cdot\vec{\nabla}\rho(r)\ . \qquad (2)$$

Here $\rho(r)$ is the density of the core nucleons normalized by the condition $\int d\vec{r}\rho(r) = A$ $(A \gg 1)$;

$$\xi_a = \xi_{ap}\frac{Z}{A} + \xi_{an}\frac{N}{A}\ ,$$

the subscript a takes the values p and n for an outer proton and neutron, respectively.

Let us note that, as distinct from the case of the P-odd, T-even interaction, no contact current is generated here in the single-particle approximation,

even if one starts from the two-body interaction (1). Indeed, it is only the last term in (1), dependent on ξ'_{ab}, which contributes to the contact current operator

$$\hat{\vec{j}}_c = \frac{i}{2}\sum_a\{[W_2, e_a\vec{r}_a], \delta(\vec{r}-\vec{r}_a)\}. \qquad (3)$$

However, even this contribution vanishes obviously after averaging over the core nucleons.

Now, the correction $\delta\Psi$ to the valence nucleon wave function generated by the interaction (2) is a solution of the equation

$$(\hat{H}_0 - E)\delta\Psi(\vec{r}) = -W(\vec{r})\Psi(\vec{r}) \qquad (4)$$

where $\hat{H}_0$ and $\Psi(\vec{r})$ are the unperturbed mean field Hamiltonian and the unperturbed nucleon wave function. To begin with, let us discuss a simple model where the profiles of the nuclear density and the central mean field potential coincide:

$$\rho(r) = -\frac{\rho_0}{U_0}U(r),$$

and the spin-orbit potential is absent [2].

Eq.(4) transforms here as follows:

$$(\hat{H}_0 - E)\delta\Psi(\vec{r}) = -\imath\frac{G}{\sqrt{2}}\frac{\xi}{2m}\frac{\rho_0}{U_0}[\hat{H}_0\,,\,\vec{\sigma}\cdot\hat{\vec{p}}]\Psi(\vec{r}), \qquad (5)$$

which gives

$$\delta\Psi(\vec{r}) = -\imath\frac{G}{\sqrt{2}}\frac{\xi}{2m}\frac{\rho_0}{U_0}(\vec{\sigma}\cdot\hat{\vec{p}})\Psi(\vec{r}) = \\ = -\frac{G}{\sqrt{2}}\frac{\xi}{2m}\frac{\rho_0}{U_0}(\vec{\sigma}\cdot\vec{n})\Omega_{Ilm}(\vec{n})\left(\frac{dR(r)}{dr} + \frac{1+K}{r}R(r)\right). \qquad (6)$$

Here Ω_{Ilm} is a spherical spinor, $R(r)$ is the unperturbed radial wave function of a nucleon, and $K = (l-I)(2I+1)$.

Even in a more general case, beyond this model, it is convenient to define the correction $\delta R(r)$ to radial wave function by the following relation:

$$\delta\Psi(\vec{r}) = -\frac{G}{\sqrt{2}}\xi\,\rho_0\,(\vec{\sigma}\cdot\vec{n})\Omega_{Ilm}(\vec{n})\delta R(r). \qquad (7)$$

The correction $\delta R(r)$ can be calculated using two independent solutions of the radial Schrödinger equation $u_1(r)$ and $u_2(r)$, regular at the origin and at the infinity, respectively. These solutions are normalized to the unit Wronskian:

$$u_1\frac{du_2}{dr} - \frac{du_1}{dr}u_2 = 1.$$

This correction is

$$\delta R(r) = -\frac{u_{1,Il'}}{r}\int_r^\infty dr'\, u_{2,Il'}(r')\frac{df(r')}{dr'}u_0(r') -$$

$$-\frac{u_{2,Il'}}{r}\int_0^r dr'\, u_{1,Il'}(r')\frac{df(r')}{dr'}u_0(r'), \qquad (8)$$

where $l' = 2I - l$, $u_0(r) = rR(r)$ and $f(r)$ is a density profile $f(r) = \rho(r)/\rho_0$.

The magnetic quadrupole moment operator $\hat{M}_{ij}$ is defined by analogy with the electric quadrupole one $\hat{Q}_{ij}$, via the interaction with the corresponding field gradient:

$$\hat{H}_Q = -\frac{1}{6}\hat{Q}_{ij}\nabla_i E_j, \qquad (9)$$

$$\hat{H}_M = -\frac{1}{6}\hat{M}_{ij}\nabla_i B_j.$$

The symmetric tensor $\hat{M}_{ij}$ is related in the following way to the current density $\hat{J}_n$:

$$\hat{M}_{ij} = \int d\vec{r}(r_i\epsilon_{jmn} + r_j\epsilon_{imn})r_m\hat{J}_n. \qquad (10)$$

For a valence nucleon this operator can be presented as[2, 3]

$$M_{ij} = \frac{e}{2m}\left(3\mu(r_i\sigma_j + r_j\sigma_i - \frac{2}{3}\delta_{ij}(\vec{\sigma}\cdot\vec{r})) + 2q(r_i l_j + r_j l_i)\right), \qquad (11)$$

where μ is the nucleon magnetic moment, and q equals 1 for a proton and 0 for neutron.

With the usual definition

$$M = \langle Im = I|M_{zz}|Im = I\rangle$$

one obtains after taking expectation value over angular variables

$$M = \frac{G}{\sqrt{2}}\xi\,\rho_0\,\frac{e}{m}(\mu - q)\frac{2I-1}{I+1}(\delta R|r|R). \qquad (12)$$

The radial matrix element here is

$$(\delta R|r|R) = \int_0^\infty r^2 dr\,\delta R(r) r R(r). \qquad (13)$$

For the simple model described above (6) the matrix element can be calculated analytically with the following result

$$(\delta R|r|R) = \frac{K - 1/2}{2mU_0}. \qquad (14)$$

One more model allowing for an exact analytical result for MQM is that of the oscillator potential. Here it is convenient to start from expression (13) for the matrix element. Separating the tensor structure in (2), (11) one obtains

$$(\delta R|r|R) = -\frac{1}{4m}\sum_n \frac{\langle 0|f'(\vec{\sigma}\cdot\vec{n})|n\rangle\langle n|\vec{\sigma}\cdot\vec{r}|0\rangle + \langle 0|\vec{\sigma}\cdot\vec{r}|n\rangle\langle n|f'(\vec{\sigma}\cdot\vec{n})|0\rangle}{E_0 - E_n}. \qquad (15)$$

For a harmonic oscillator

$$(\vec{\sigma}\cdot\vec{r}) = \frac{i}{m\omega^2}[(\vec{\sigma}\cdot\vec{p}), H].$$

Substituting this identity into (15) and using the completeness relation, we find

$$(\delta R|r|R) = -\frac{i}{4m^2\omega^2}\langle 0|[f'(\vec{\sigma}\cdot\vec{n}), \vec{\sigma}\cdot\vec{p}]|0\rangle.$$

Taking again expectation value over angular variables, we obtain

$$(\delta R|r|R) = \frac{1}{4m\omega^2}\langle f'' - \frac{2K}{r}f'\rangle. \qquad (16)$$

3. Expression (11) for the MQM corresponds to the contribution of the convection and the spin electromagnetic current densities. In this section we discuss one more contribution to MQM, that originating from the momentum dependence of the spin-orbit two-nucleon forces. In the single-particle approximation this current density is [7]

$$\vec{j}^p_{ls} = eU^{pn}_{ls}\rho_0\frac{N}{A}\frac{df(r)}{dr}\vec{\sigma}\times\vec{n} \qquad (17)$$

for a valence proton and

$$\vec{j}^n_{ls} = -eU^{pn}_{ls}\frac{Z}{A}\rho_0 f(r)\,\vec{\nabla}\times\left(\psi^\dagger(\vec{r})\vec{\sigma}\psi(\vec{r})\right) \qquad (18)$$

for a valence neutron. Here U^{pn}_{ls} is the constant entering two-body proton-neutron spin-orbit treated in the contact limit:

$$U_{ls} = \frac{1}{2}\sum_{pn} U^{pn}_{ls}\,(\vec{p}_p - \vec{p}_n)\cdot(\vec{\sigma}_p + \vec{\sigma}_n)\times\vec{\nabla}\delta(\vec{r}_p - \vec{r}_n). \qquad (19)$$

The proton-proton spin-orbit interaction does not contribute to the current density in the zero-range limit we use.

The direct calculation shows that, contrary to naive expectations, the proton spin-orbit current (17) does not contribute to the static NMQM. However, for an outer neutron the corresponding correction does not vanish. It equals

$$M_{ls}^{n} = -2\frac{G}{\sqrt{2}}\xi\,\rho_0^2\,eU_{ls}^{np}\frac{Z}{A}\frac{2I-1}{I+1}(\delta R|rf(r)|R). \qquad (20)$$

4. We are ready now for a more realistic single-particle calculation. This numerical treatment is based on the Woods-Saxon potential including spin-orbit interaction and on a realistic description of nuclear density. The profiles of both density and the central part of nuclear potential are described by a Fermi-type function

$$f(r) = \frac{1}{1+exp(\frac{r-R}{a})}, \qquad (21)$$

The total single-particle potential $U(\vec{r})$ is chosen in a standard Woods-Saxon form

$$U(\vec{r}) = U_0 f(r) + U_{ls}\frac{1}{r}\frac{df(r)}{dr}(\vec{l}\vec{\sigma}) + U_C(r), \qquad (22)$$

where $U_C(r)$ is the Coulomb potential of a uniformly charged sphere.

We use the values of the density parameters from book [8]:

$$R = 1.11\,A^{1/3}\,fm; \quad a = 0.54\,fm \quad \rho_0 = 0.17\,fm^{-3}. \qquad (23)$$

The Woods-Saxon potential is parametrized as in [9]:

$$R = R_{ls} = 1.24A^{1/3}\,fm, \quad a = a_{ls} = 0.63\,fm,$$
$$U_0 = (-53.3 \pm 33.6\frac{N-Z}{A})\,MeV, \quad U_{ls} = -0.263\,(1+2\frac{N-Z}{A})\,U_0 \qquad (24)$$

The spin-orbit interaction constant as fitted in Ref. [10] is:

$$U_{ls}^{pn} = 134.3\,MeV\cdot fm^5. \qquad (25)$$

The correction $\delta R(r)$ calculated in this way is plotted in Fig.1 together with the model function (6). Obviously, the latter is a reasonably good approximation to the correction δR, as calculated numerically in the more realistic approach.

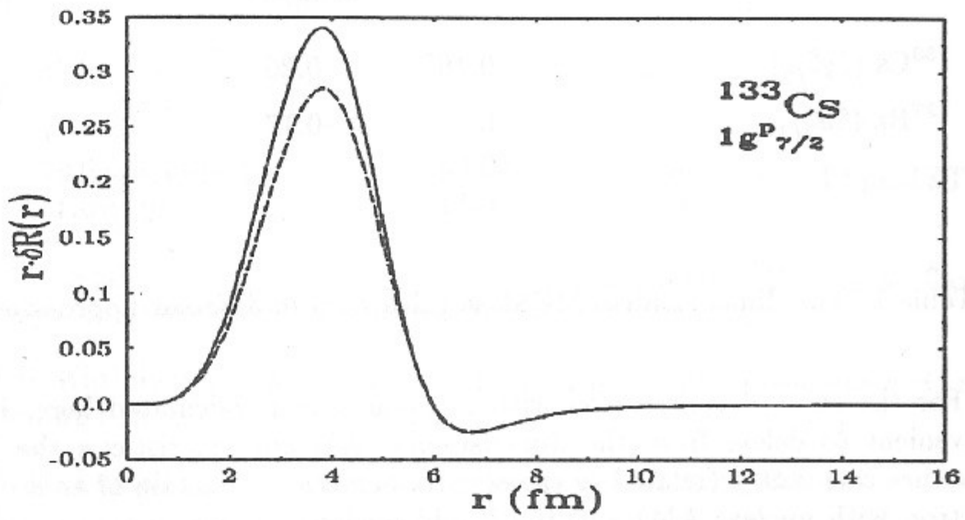

Figure 1. The correction $\delta R(r)$ for ^{137}Cs. Dashed line is the model function (6). Full line is δR in the Woods-Saxon potential.

Our results are conveniently presented in terms of the dimensionless constant τ related to the NMQM as follows

$$M = \frac{G}{\sqrt{2}}\xi\,\frac{2I-1}{2I+2}\,e\,\tau. \qquad (26)$$

This constant itself consists in general of two contributions:

$$\tau = \tau_0 + \tau_{ls},$$
$$\tau_0 = \frac{\rho_0}{m_p}(\mu - q)\,2(\delta R|r|R), \qquad (27)$$
$$\tau_{ls}^{n} = -4U_{ls}^{np}\frac{Z}{A}\rho_0^2(\delta R|rf(r)|R), \qquad (28)$$
$$\tau_{ls}^{p} = 0.$$

The values of τ calculated for two neighbouring nuclei, with odd Z and odd N respectively, are presented in Table 1.

5. In conclusion let us compare the results obtained for the NMQM, generated by P- and T-odd potential, with those for the nuclear anapole moment (AM), generated by P-violating, but T-even potential. In particular, we wish to compare the stability of nuclear single-particle calculations for those two moments, T-odd and T-even.

Nucleus		$\rho = -U\rho_0/U_0$	Harmonic oscillator	Woods-Saxon
^{133}Cs $(1g^p_{7/2})$	$\tau = \tau_0$	0.16	0.26	0.18
^{137}Ba $(2d^n_{3/2})$	τ_0	−0.09	−0.17	−0.12
	τ_{ls}	−0.02		−0.02
	τ	−0.11		−0.14

Table 1: The dimensionless MQM as calculated in different approaches

For the sake of comparison with the constant τ calculated here, it is convenient to delete from the dimensionless AM characteristic κ the fine structure constant α (related to the electromagnetic interaction of an atomic electron with nuclear AM) and the P-odd nucleon-nucleon constant g (the T-even analogue of the constant ξ used here). The typical value of this AM characteristic is[11, 3, 7]

$$\frac{\kappa}{\alpha g} \simeq \frac{\mu}{mr_0} A^{2/3}, \tag{29}$$

where $r_0 = 1.2fm$.

As to τ, its typical value is

$$\tau \simeq \mu K 4m^2 U_0 r_0^3. \tag{30}$$

The ratio of those two factors, i.e., of the T-odd effect to T-even one,

$$\frac{K}{4mU_0 r_0^2} A^{-2/3} \simeq 0.15\, K\, A^{-2/3} \tag{31}$$

is very small. The origin of the AM enhancement $\sim A^{2/3}$ can be traced back to the AM dependence on the geometrical cross-section of nucleus, this is a bulk nucleus effect [11, 3, 7]. As to the NMQM, its magnitude depends completely on the nuclear boundary (see eqs.(2), (16)).

It results not only in the relative suppression of the T-odd effect. The value of NMQM is more sensitive to the details of the nuclear model than that of AM, it is less stable.

However reliable theoretical predictions both for AM and NMQM can be obtained only when the single-particle calculations will be supplemented by a serious treatment of many-body effects.

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