Polarization associated with the coupling to isoscalar dipole compression mode

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(Received 28 February 2000; published 24 July 2000)

The effect of core polarization on isoscalar dipole one-particle moments due to the coupling with isoscalar giant dipole resonance (compression mode) is estimated. Numerical calculations with the core nucleus $^{208}_{82}Pb_{126}$ show that a small enhancement of one-particle moments is obtained, of which the magnitude depends sensitively on relevant one-particle orbitals. The results are important for a microscopic understanding of the electric dipole moments (Schiff moments) measured for nuclei in this mass region.

PACS number(s): 21.10.Re, 21.60.Jz, 23.20.Js, 27.80.+w

The most precise limit on the electric dipole moment of the ground state of an isolated atomic system is the value of $d<1.3\times10^{-27}$ e cm obtained for the ground state of ^{199}Hg [1]. A nonzero value for this electric dipole moment can only occur through interactions which violate both parity conservation and time-reversal symmetry. The limit on the atomic dipole moment sets limits on the hadronic, semileptonic, and purely leptonic *P*-odd and *T*-odd weak interactions. The hadronic part associated with the electric dipole moment of the ^{199}Hg nucleus manifests itself through the Schiff moment which is the first nonzero term in the expansion of the nuclear electromagnetic potential after including the screening of the atomic electrons [2,3]. The Schiff moment can be interpreted in terms of the *P*-odd and *T*-odd quark-quark interaction only when the nuclear structure and nucleon structure aspects are understood. A limit which is not so precise as in the case of ^{199}Hg has also been obtained for the dipole moment of the ^{203,205}Tl atom [4]. The nuclear structure aspects of these Schiff moments has to date only been based upon qualitative models [5].

The purpose of this paper is to initiate a microscopic approach to the calculation of these Schiff moments within the framework of the nuclear shell model. In particular, in this paper we study the core-polarization corrections to the single-particle Schiff moments. The operator for the Schiff moment is [3]

$$S=\frac{1}{10}\sqrt{\frac{4\pi}{3}}\sum_{i}^{A} e_i\left(r_i^3-\frac{5}{3}\langle r^2\rangle r_i\right)Y_{1\mu}(\hat{r}_i), \qquad (1)$$

where e_i is e for a proton and zero for a neutron. We calculate the effective charges (core polarizations) associated with the coupling of single-hole states in ^{208}Pb to the collective excitation of the isoscalar giant dipole resonance (compression mode), which is an excitation closely connected with the Schiff operator. This is an important element in the full many-body calculation for ^{199}Hg and other nuclei around ^{208}Pb. ^{199}Hg, for example, would be treated as two proton holes and seven neutron holes in a closed-shell configuration for ^{208}Pb. The many-body aspects of this calculation will require a large-basis shell model calculation. With these wave functions the many-particle Schiff moment can be reduced to a linear combination of the single-particle Schiff moments considered here. Such many-body calculations for ^{205}Tl were discussed in Ref. [6] where the $3s_{1/2}$ proton single-particle contribution was found to dominate. The calculations for ^{199}Hg have not yet been carried out, but we expect that the $3p_{1/2}$, $3p_{3/2}$, and $2f_{5/2}$ neutron orbitals will be the most important terms for the Schiff moment.

The weak interaction between nucleons enters in a similar way as for the anapole moments [6]. For example, the Schiff moment for the $3p_{1/2}$ neutron-hole state is related to the weak interaction mixing of $ns_{1/2}$ neutron states. In this case the matrix elements $\langle ns_{1/2}|S|3p_{1/2}\rangle$ are zero (since the neutron charge is zero) and all of the contribution will come from the core polarization of the protons in the core. For the proton-hole states, $3s_{1/2}$, for example, the Schiff moment will arise both from the valence proton matrix elements $\langle np_{1/2}|S|3s_{1/2}\rangle$ and from core polarization. In the many-particle calculations for ^{199}Hg and ^{206}Tl, one will also need to include matrix elements of the type $\langle nd_{3/2}|S|3p_{1/2}\rangle$ and $\langle np_{3/2}|S|3s_{1/2}\rangle$.

Because of the large transition moments associated with collective excitations, the particle-vibration coupling gives rise to important modifications in the effective one-particle moments. It is known that the static polarization effect produced by an attractive coupling is generally in phase with the single-particle moment, while a repulsive coupling implies opposite phase for the polarization effect and the single-particle moment. In the case of electric quadrupole transitions we have sufficient experimental informations on the properties of isoscalar and isovector shape-oscillation giant resonances (namely, $\Delta N\approx2$ excitations). Consequently, the modifications coming from the coupling to both low ($\Delta N\approx0$) and high ($\Delta N\approx2$) excitations have been well studied. For example, see Ref. [7].

In the present paper we estimate the polarization due to the coupling with the isoscalar dipole compression mode. The observation of isoscalar compression giant dipole resonance in ^{208}Pb is reported in Ref. [8], though the extracted total strength consumed by the observed peak at $E_x=22.5$ MeV may contain some ambiguity. In the self-consistent Hartree-Fock (HF) plus RPA calculations of ^{208}Pb a broad peak is obtained around $E_x=25$ MeV for both the SGII and SkM* interaction. It is known that the peak posi-

0556-2813/2000/62(2)/024318(5)/$15.00

tion depends appreciably on the compressibility of the Skyrme interaction employed. In the calculations of Refs. [9,10] in which the continuum effect is properly treated, the energy of the broad peak shifts downward by about 2.5 MeV due to the RPA correlation. In lighter nuclei the calculated distribution of isoscalar compression dipole strength becomes much wider. Consequently, it is difficult to identify the peak position or a corresponding collective mode [10].

To our knowledge, the polarization effect due to the coupling to any compression modes was never examined, presumably because it is not of practical interests. The best-studied compression mode is certainly the isoscalar monopole compression mode. Though the isoscalar monopole giant resonance is experimentally identified in various mass region of nuclei [11], the modification of one-particle moments associated with the coupling to the giant resonance can hardly be pinned down using presently available experiments. In contrast, the modification of isoscalar dipole matrix elements between $\Delta N \approx 1$ one-particle orbitals associated with the coupling to isoscalar dipole giant resonance (compression mode and $\Delta N \approx 3$ excitations) can be of practical interests in connection with the Schiff moment described above. Moreover, it would be interesting to try to find the one-particle dipole strength by varying nuclear reactions with different energies of various incident particles, since the population of excitation modes with a radial node in transition densities may have a sensitive dependence on reactions.

The isoscalar dipole transition operator is written as

$$D_{\mu}^{\lambda=1,\tau=0} = \sum_i r_i^3 Y_{1\mu}(\hat{r}_i). \tag{2}$$

In the self-consistent HF plus RPA calculation the isoscalar dipole strength coming from the center of mass motion appears at zero excitation energy and, thus, should be completely separated from excitations of physical significance. However, in actual numerical calculations there always remains very small spurious component in the nonzero excitation-energy region, which in turn contributes considerably to the calculated matrix element of the operator (2), see Ref. [10]. One way to avoid obtaining the spurious (center of mass) excitation strength is to use

$$\delta\rho_{tr}(r) = \rho_{tr}(r) - \varepsilon \frac{d\rho_0(r)}{dr} \tag{3}$$

as the radial transition density instead of the originally calculated $\rho_{tr}(r)$. In expression (3) the constant ε is determined so that the transition density (3) will give vanishing spurious excitation strength. This procedure is equivalent to evaluating the strength function of the operator

$$\overline{D}_{\mu}^{\lambda=1,\tau=0} = \sum_i^A (r_i^3 - \eta r_i) Y_{1\mu}(\hat{r}_i), \tag{4}$$

where $\eta = \frac{5}{3}\langle r^2 \rangle$, using the original transition density $\rho_{tr}(r)$. We note that the $\overline{D}$ operator has the same structure as the Schiff moment operator in Eq. (1). The energy weighted sum rule for the operator (4) is obtained as

$$\sum_k \hbar\omega_k |\langle k|\overline{D}_{\mu}^{\lambda=1,\tau=0}|0\rangle|^2 = \frac{A\hbar^2}{8\pi M}\left(11\langle r^4\rangle - \frac{25}{3}\langle r^2\rangle^2\right). \tag{5}$$

In practice, it is very difficult to obtain a reliable estimate of the polarization by using the result of the self-consistent RPA calculations of isoscalar dipole compression modes. This is because the spurious (center of mass) excitation strength at nonzero excitation-energy appears due to a numerical inaccuracy and, consequently, the corresponding radial transition density does not exactly have the r dependence of the second term of Eq. (3). Also, a small lower-lying strength, which is spurious, may contribute appreciably to the polarization. We note that no appreciable amount of isoscalar compression dipole strength has ever been observed in the low excitation-energy region of ^{208}Pb.

Thus, in the present work we use a more schematic model simulating the result of HF plus RPA calculations. A Woods-Saxon potential is constructed, of which the one-particle level scheme is similar to that of the HF calculation with the SkM* interaction. Then, assuming that the whole strength (5) is consumed by one collective mode at a given $\hbar\omega$, we construct the RPA wave function and evaluate the polarization effect on isoscalar dipole one-particle moments. The particle-vibration coupling is written as

$$H_{\rm PV} = c h(r) \sum_{\mu} Y_{\lambda\mu}^* \alpha_{\lambda\mu}, \tag{6}$$

where the constant c is later determined so that the RPA solution at $\hbar\omega$ consumes the sum-rule strength. The form factor $h(r)$ is written as

$$h(r) = \left(10r + 3r^2 \frac{\partial}{\partial r} - \frac{5}{3}\langle r^2\rangle \frac{\partial}{\partial r}\right)\rho_0(r) \tag{7}$$

which except for a small correction term is obtained [12,9] from the assumption of the presence of only one collective mode that consumes the whole sum-rule strength.

The RPA amplitude of the hole $(n_h j_h l_h)$ and particle (jl) configuration is obtained by solving the inhomogeneous differential equation

$$\begin{aligned} &\frac{d^2\varphi_j}{dr^2} - \frac{l(l+1)}{r^2}\varphi_j + \frac{2m}{\hbar^2}[E - V_0(r)]\varphi_j \\ &= \frac{2m}{\hbar^2} c \langle n=1|\alpha|n=0\rangle \langle j_h \| Y_1 \| j\rangle h(r)\phi_{j_h} \\ &\quad - \frac{2m}{\hbar^2}\sum_{\epsilon_j \langle \epsilon_F} \phi_j \langle (j j_h)_1^{-1}|H_{\rm PV}|n=1\rangle, \end{aligned} \tag{8}$$

where

$$r R_{j_h}(r) \equiv \phi_{j_h}(r), \quad r X_j^{(j_h)}(r) \equiv \varphi_j(r), \quad \text{and} \quad r Y_j^{(j_h)}(r) \equiv \varphi_j(r) \tag{9}$$

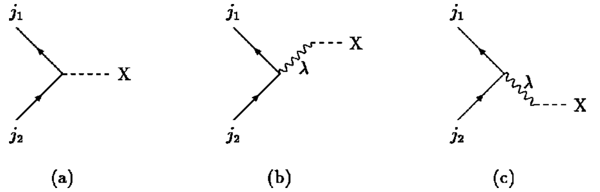

FIG. 1. Core-polarization effect on one-particle operators. The dashed line with a cross mark expresses the external field in Eq. (4), while the wavy line denotes the isoscalar dipole ($\lambda=1$) compression vibration. The one-particle matrix element is expressed in (a), while the diagrams in (b) and (c) represent the core-polarization effect which renormalizes the one-particle bare operator in (a).

and $E=\pm\hbar\omega+\epsilon_{j_h}$ for forward- and backward-going amplitudes $X_j^{(j_h)}(r)$ and $Y_j^{(j_h)}(r)$ [13,14]. In Eq. (8) the phonon number of the isoscalar giant dipole resonance (compression mode) is expressed by n, while the potential $V_0(r)$ consists of the Woods-Saxon and spin-orbit potential plus Coulomb potential in case of protons. The second term on the right-hand side of Eq. (8) is needed to fulfill the requirement that the solution φ_j should be orthogonal to single-particle wave functions ϕ_j of all occupied orbits with the angular momentum j. The solution $\varphi_j(r)$ is constructed so as to have the proper asymptotic behavior corresponding to the sign and value of E. Solving the inhomogeneous equation for all possible (jl) in connection with all occupied orbits $(n_h j_h l_h)$, we sum up the solution and obtain the radial transition density as

$$\rho_{tr}(r)=\sum_{p,h}\frac{1}{\sqrt{3}}\langle j\|Y_1\|j_h\rangle[X_j^{(j_h)}(r)+Y_j^{(j_h)}(r)]R_{j_h}(r). \tag{10}$$

The reduced transition probability is calculated as

$$B(0^+\rightarrow 1^-)=3\left[\int_0^\infty r^3\rho_{tr}(r)r^2\,dr\right]^2. \tag{11}$$

We note that in our RPA calculation all excitations of the particles in the ground state, which can contribute to the compression giant dipole resonance, are included and there is no truncation of the configuration space.

The core polarization effect on one-particle moments is expressed by Fig. 1, in which the wavy line denotes the isoscalar dipole ($\lambda=1$) compression vibration. The polarizability χ is the ratio of the contribution by Figs. 1(b) and 1(c) to the one by Fig. 1(a), and expressed by [see the analogous expression (6-218) in Ref. [7]]

$$\chi=-\frac{\langle j_1|h(r)|j_2\rangle}{\langle j_1|r^3-\frac{5}{3}\langle r^2\rangle r|j_2\rangle}\frac{c\langle n=1|\alpha|n=0\rangle}{\sqrt{3}}$$
$$\times|\langle n=1|\overline{D}_\mu^{\lambda=1,\tau=0}|n=0\rangle|$$
$$\times\frac{2}{\hbar\omega}\frac{(\hbar\omega)^2}{(\hbar\omega)^2-(\epsilon_{j_1}-\epsilon_{j_2})^2}. \tag{12}$$

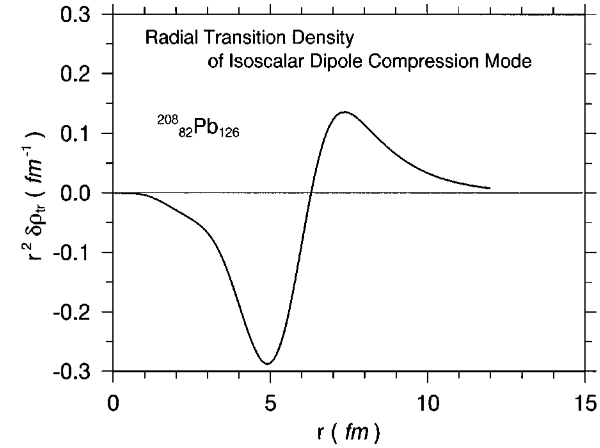

FIG. 2. Calculated radial transition density (3) of the isoscalar dipole compression vibration of ${}^{208}_{82}\mathrm{Pb}_{126}$ as a function of radial coordinate.

In the present case only one phonon exhausts the whole sum rule. Writing expression (12) as

$$\chi\equiv\chi_0\frac{(\hbar\omega)^2}{(\hbar\omega)^2-(\epsilon_{j_1}-\epsilon_{j_2})^2}, \tag{13}$$

the quantity χ_0 is called as static polarizability.

In the self-consistent HF plus RPA calculation with the SkM* interaction [10] of ${}^{208}\mathrm{Pb}$ the lowest $\Delta N\approx 3$ unperturbed particle-hole (p-h) excitations, in which the particle state is either a bound or resonant state, start slightly above $E_x=27\,\mathrm{MeV}$, while the peak of the calculated RPA strength appears at $E_x=25\,\mathrm{MeV}$. It is difficult to obtain parameters of a Woods-Saxon potential, which produces both the p-h excitation energies and root-mean-square radius that are similar to the result of the HF calculation. We make a compromise by taking the Woods-Saxon parameters; radius parameter $r=r_c=1.18\,\mathrm{fm}$, diffuseness $a=0.60\,\mathrm{fm}$, and spin-orbit potential parameter $\lambda=32$. See, for example, Ref. [15] for parameters of Woods-Saxon potentials. The p-h excitations in this Woods-Saxon potential start at 25.7 MeV, while the calcu-

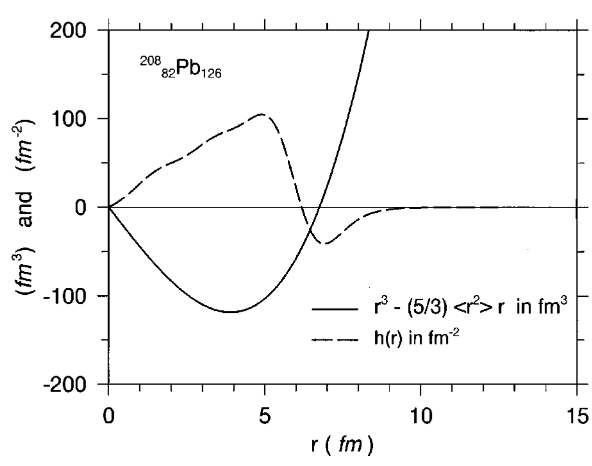

FIG. 3. Radial dependence of the operators appearing in the numerator and denominator of Eq. (14) in the case of ${}^{208}_{82}\mathrm{Pb}_{126}$.

TABLE I. Calculated static polarizability χ_0 in Eq. (13), the ratio (14), and the radial matrix elements of the operators, r^3 and $r^3-\frac{5}{3}\langle r^2\rangle r$, for some selected neutron and proton orbitals in ${}^{208}_{82}\mathrm{Pb}_{126}$.

	$n_1 j_1$	$n_2 j_2$	$\lvert\langle j_1\lvert r^3\rvert j_2\rangle\rvert$ in fm^3	$\lvert\langle j_1\lvert r^3-\frac{5}{3}\langle r^2\rangle r\rvert j_2\rangle\rvert$ in fm^3	Ratio in Eq. (14) in fm^{-5}	χ_0
Neutron	$4s_{1/2}$	$3p_{1/2}$	234	66.5	−0.062	0.015
	$3s_{1/2}$	$3p_{1/2}$	168	20.3	−0.83	0.21
	$2s_{1/2}$	$3p_{1/2}$	64	46.1	−0.78	0.20
	$1s_{1/2}$	$3p_{1/2}$	12	8.7	−1.52	0.38
	$3d_{3/2}$	$3p_{1/2}$	250	32.3	+0.43	−0.11
	$2d_{3/2}$	$3p_{1/2}$	140	15.3	−0.61	0.15
Proton	$3p_{1/2}$	$3s_{1/2}$	153	30.3	−0.67	0.17
	$2p_{1/2}$	$3s_{1/2}$	108	13.3	−0.44	0.11
	$1p_{1/2}$	$3s_{1/2}$	35	29.3	−0.85	0.21
	$3p_{3/2}$	$3s_{1/2}$	150	26.9	−0.67	0.17
	$2p_{3/2}$	$3s_{1/2}$	115	16.3	−0.48	0.12

lated root-mean-square radius of ^{208}Pb is 5.23 fm, which is smaller than the HF value, 5.55 fm. If one uses the ‘‘standard’’ parameters [7] of Woods-Saxon potential which produce the observed root-mean-square radius or the HF one, the p-h excitations with $\Delta N \approx 3$ start at 22.1 MeV. Since the reported energy of the giant resonance is 22.5 MeV, the unperturbed p-h excitation energies of 22.1 MeV are too low. We estimate the polarizability assuming that the whole sum-rule strength is consumed by an RPA solution at $\hbar\omega = 23.5$ MeV, which is pushed down by 2.2 MeV compared with the lowest-lying $\Delta N \approx 3$ p-h excitations. We have checked that the value of polarizability estimated in the present note is rather insensitive to the details of Woods-Saxon parameters, as far as the energy shift by the RPA correlation is taken to be slightly larger than 2 MeV.

In Fig. 2 we show the calculated radial transition density, while in Fig. 3 the radial dependence of the operators appearing in the numerator and denominator of the first factor in Eq. (12)

$$\frac{\langle j_1|h(r)|j_2\rangle}{\langle j_1|r^3-(5/3)\langle r^2\rangle r|j_2\rangle} \tag{14}$$

is plotted. In Table I the calculated static polarizability, the ratio (14), and matrix elements of r^3 and $r^3-\frac{5}{3}\langle r^2\rangle r$ are given for some selected neutron and proton orbitals. The dynamical factor, namely the second factor in expression (13), may make the actual polarizability χ larger than the static polarizability χ_0 by a factor of 1.1–1.3 for the $\Delta N \approx 1$ pairs of orbitals in Table I. For the operator for the Schiff moment (1) the effective charge, which includes the polarization charge estimated in the present note, becomes

$$e_{eff}=\begin{cases}\left(1+\dfrac{Z}{A}\chi\right)e & \text{for protons,}\\[2ex] \dfrac{Z}{A}\chi e & \text{for neutrons.}\end{cases} \tag{15}$$

The calculated polarizability is small, but it depends strongly on the combination of particle orbitals because of the presence of radial node in the relevant operators as exhibited in Fig. 3. Both matrix elements appearing in Eq. (14) are often the result of cancellation between the contributions from the inside and outside of the nucleus. For example, for the neutron ($4s_{1/2}$, $3p_{1/2}$) pair the sign of the total matrix elements is the same as that of the contribution from the outside, while for the proton ($2p_{1/2}$, $3s_{1/2}$) pair it is the same as that from the inside.

We note that in the RPA calculation most components contribute coherently to the isoscalar giant dipole resonance (compression mode), while a few components, for example the neutron $(n_h=3, l_h=1)\rightarrow(l=2)$ excitations such as $3p_{1/2}\rightarrow d_{5/2}$ and $3p_{1/2}\rightarrow d_{3/2}$, make a destructive contribution. The static polarizability calculated in the related neutron pairs of orbitals, such as $3p_{3/2}\rightarrow 3d_{5/2}$ and $3p_{1/2}\rightarrow 3d_{3/2}$, has a negative sign. The fact that a few components do not make a coherent contribution to the giant resonance shows that the present compression mode is not really an ideal collective mode.

In conclusion, we have estimated the modification of one-particle isoscalar dipole moments due to the coupling with the isoscalar giant dipole resonance (compression mode). Corresponding to the attractive particle-vibration coupling, the renormalization is in phase with most of one-particle moments. The magnitude is small, however, it depends sensitively on particle orbitals involved. As discussed in the Introduction, the type of matrix elements studied in this paper are required for a microscopic calculation of the electric dipole moments of nuclei around ^{208}Pb in order to extract information of the P odd and T odd strength of the hadronic weak interaction from the very precise limits which have been determined experimentally.

B.A.B. was supported by NSF Grant No. PHY-9605207.

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