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Gauge invariant evaluation of nuclear polarization with the collective model

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The nuclear-polarization (NP) energies with the collective model commonly employed in the NP calculations for hydrogenlike heavy ions are found to have serious gauge violations when the ladder and cross diagrams only are taken into account. Using the equivalence of charge-current density with a schematic microscopic model, the NP energy shifts with the collective model are gauge invariantly evaluated for the $1s_{1/2}$ states in $^{208}_{82}\mathrm{Pb}^{81+}$ and $^{238}_{92}\mathrm{U}^{91+}$.

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High-precision Lamb-shift measurement on high-Z hydrogenlike atoms [1] spurred a renewed interest in the quantum electrodynamical (QED) calculation of electronic atoms. Comparison of theoretical results with experimental data allows sensitive tests of QED in strong electromagnetic fields [2,3]. In this context, the study of the nuclear-polarization (NP) effect becomes important because the NP effect, as a non-QED effect that depends on the model used to describe the nuclear dynamics, sets a limit to any high-precision test of QED.

A relativistic field-theoretical NP calculation was presented by Plunien and co-workers [4,5] utilizing the concept of effective photon propagators with nuclear-polarization insertions. They considered the Coulomb interaction only based on the argument that the relative magnitude of transverse interaction is of the order of $(v/c)^2$ and the velocity v associated with nuclear dynamics is mainly nonrelativistic.

The effect of the transverse interaction was studied in the Feynman gauge by Yamanaka *et al.* [7] with the same collective model used in Refs. [4–6] for nuclear excitations. They found that the transverse contribution is several times larger than the Coulomb contribution in heavy electronic atoms, before the contributions of the positive and negative energy states cancel. However, due to the nearly complete cancellation between them, the transverse effects become small and the net effect is destructive to the Coulomb contribution in both $1s_{1/2}$ states of $^{208}_{82}\mathrm{Pb}^{81+}$ and $^{238}_{92}\mathrm{U}^{91+}$. As a result, the total NP energy almost vanishes in $^{208}_{82}\mathrm{Pb}^{81+}$.

Recently, the NP effects for hydrogenlike and muonic $^{208}_{82}\mathrm{Pb}^{81+}$ were calculated in both the Feynman and Coulomb gauges, using a microscopic random phase approximation (RPA) to describe nuclear excitations [8,9]. It was found that, in the hydrogenlike atom, the NP effects due to the ladder and cross diagrams have serious gauge dependence and inclusion of the seagull diagram is indispensable to restore the gauge invariance [8]. In contrast, the magnitude of the seagull collection is a few percent effect in the muonic atom, although it improves the gauge invariance [9].

In the present paper, we report that the nuclear collective model employed for hydrogenlike ions in Refs. [4–7] also leads to a large violation of gauge invariance as far as the ladder and cross diagrams only are considered. Then it is shown, based on the equivalence of the transition density of the collective model and a microscopic nuclear model with a schematic interaction between nucleons, that the seagull corrections should also be calculated with the collective model in order to obtain gauge invariant NP results. The resulting gauge invariant NP energy shifts are given for the $1s_{1/2}$ states in $^{208}_{82}\mathrm{Pb}^{81+}$ and $^{238}_{92}\mathrm{U}^{91+}$.

For spherical nuclei, the Hamiltonian of the small amplitude vibration with multipolarity L is written as

$$H_L=\frac{1}{2}\left(\frac{1}{D_L}\sum_M \hat{\pi}^\dagger_{LM}\hat{\pi}_{LM}+C_L\sum_M \hat{\alpha}^\dagger_{LM}\hat{\alpha}_{LM}\right), \tag{1}$$

where $\hat{\pi}_{LM}$ are the canonically conjugate momenta to the collective coordinates $\hat{\alpha}_{LM}$. The lowest vibrational modes are expected to have density variations with no radial nodes, which may be referred to as shape oscillations. The corresponding charge density operator with the multipolarity L is written as

$$\hat{\rho}_L(t,\boldsymbol{r})=\rho_L(r)\sum_M Y^*_{LM}\hat{\alpha}_{LM}(t) \tag{2}$$

to the lowest order of $\hat{\alpha}^\dagger_{LM}(t)$.

The liquid drop model of Bohr (BM) [10] is a simple model of such a shape oscillation obtained by considering deformation of the nuclear radius parameter while leaving the surface diffuseness independent of an angle,

$$R(\Omega)=R_0\left[1+\sum_{LM}\alpha_{LM}Y^*_{LM}(\Omega)\right], \tag{3}$$

where R_0 is the nuclear radius parameter of the ground state. The radial charge density of BM is given by

$$\rho_L(r)=-R_0\frac{d}{dr}\varrho_0(\boldsymbol{r}), \tag{4}$$

where $\varrho_0(\boldsymbol{r})$ is a charge distribution with spherical symmetry.

If we assume that under distortion, an element of mass moves from $\boldsymbol{r}_0$ to $\boldsymbol{r}$ without alteration of the volume it occu-

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pies, i.e., the nucleus is composed of an inhomogeneous incompressible fluid, a harmonic vibration of an originally spherical surface $r=r_0$ in the nucleus is given by

$$r(\Omega)=r_0\left[1+\sum_{LM}\left(\frac{r_0}{R_0}\right)^{L-2}\alpha_{LM}Y^*_{LM}(\Omega)\right]. \quad (5)$$

For this model we obtain

$$\rho_L(r)=-\frac{1}{R_0^{L-2}}r^{L-1}\frac{d}{dr}\varrho_0(\boldsymbol{r}). \quad (6)$$

This version will be hereafter referred to as the Tassie model (TM) [11]. In Eqs. (4) and (6), $\varrho_0(\boldsymbol{r})$ is usually taken to be equal to the ground-state charge distribution.

In either case, the motion of nuclear matter is assumed to be incompressible and irrotational, hence the velocity field $\boldsymbol{v}(t,\boldsymbol{r})$ is given by a velocity potential as $\boldsymbol{v}(t,\boldsymbol{r})=\boldsymbol{\nabla}\Phi(t,\boldsymbol{r})$. This implies the nuclear current defined by $\boldsymbol{J}(\boldsymbol{r})=\varrho_0(r)\boldsymbol{v}(r)$ yields the transition multipole density of current operator

$$\hat{\boldsymbol{J}}_L(t,\boldsymbol{r})=J_{LL-1}(r)\sum_M \boldsymbol{Y}^*_{LL-1M}\hat{\alpha}_{LM}(t). \quad (7)$$

Note that the $J_{LL+1}(r)$ part does not appear in the transition density of current operator given by Eq. (7).

Therefore, in this kind of collective model, the continuity equation of charge gives

$$i\Delta E_L\rho_L(r)+\sqrt{\frac{L}{2L+1}}\left(\frac{d}{dr}-\frac{L-1}{r}\right)J_{LL-1}(r)=0, \quad (8)$$

where ΔE_L is the excitation energy of the surface oscillation. Hence the transition density of current is given by

$$J_{LL-1}(r)=i\Delta E_L\sqrt{\frac{2L+1}{L}}r^{L-1}\int_r^\infty x^{1-L}\rho_L(x)dx \quad (9)$$

in terms of the transition density of charge. If we assume the uniform charge distribution $\varrho_0(r)=\varrho_0\Theta(R_0-r)$, we obtain, for both BM and TM,

$$\rho_L(r)=\langle J_f\|r^LY_L\|J_i\rangle\frac{1}{R_0^{L+2}}\delta(R_0-r), \quad (10)$$

$$J_{LL-1}(r)=\langle J_f\|r^LY_L\|J_i\rangle i\Delta E_L\sqrt{\frac{2L+1}{L}}\frac{r^{L-1}}{R_0^{2L+1}}\Theta(R_0-r). \quad (11)$$

The transition densities given by Eqs. (10) and (11) have been employed in the previous NP calculations for $L\geqslant 1$ [4–7]. It should be mentioned that, although the surface oscillation applies to the case of the multipolarity $L\geqslant 2$, Eqs. (10) and (11) with $L=1$ give the transition densities of the giant dipole resonance given by the Goldhaber-Teller model describing the relative motion of neutrons and protons [12]. For the monopole vibration, it is also possible to construct corresponding charge and current densities [4,7].

In general, the charge conservation relation between the charge and current densities is necessary but not sufficient for the gauge invariance of the NP calculation. Unfortunately, it is practically impossible to construct a model that incorporates gauge invariance explicitly in terms of the collective variables of the model. However, it is possible to evaluate the NP energy gauge invariantly with the above collective model as is shown below.

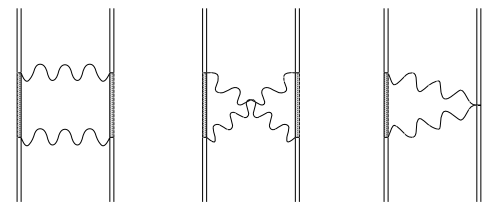

FIG. 1. Diagrams contributing to nuclear polarization in lowest order. (a) ladder, (b) cross, and (c) seagull diagrams.

The NP calculations with the collective model assume that a single giant resonance with spin multipolarity L saturates the energy-weighted $B(EL)$ strength for each isospin. In this respect, let us recall the fact that the transition densities of charge to the sum-rule saturated levels are given in terms of the ground-state charge density [13]. This can be seen as follows. For a pair of single-particle operators $g(\boldsymbol{r})=g(r)Y_{LM}(\Omega)$ and $f(\boldsymbol{r})=f(r)Y_{LM}(\Omega)$, the energy-weighted sum rule can be generalized to

$$\frac{1}{2J_i+1}\sum_n (E_n-E_i)[\langle J_n\|g(r)Y_L\|J_i\rangle^*\langle J_n\|f(r)Y_L\|J_i\rangle]$$
$$=\frac{2L+1}{4\pi}\frac{h^2}{2M}\int r^2dr\varrho_0(r)\left[g'(r)f'(r)+\frac{L(L+1)}{r^2}g(r)f(r)\right], \quad (12)$$

where $\varrho_0(r)$ is the charge distribution of the ground state normalized as $\int r^2dr\varrho_0(r)=Z$ [14]. When a single excited state $|J_fM_f\rangle$ saturates the $B(EL)$ strength, $|J_fM_f\rangle \propto r^LY_{LM}|J_iM_i\rangle$, the transition density of charge to this state is derived from the sum-rule relation (12) model independently and is given by

$$\varrho_{fi}(r)=-\frac{1}{2L+1}\frac{\langle J_f\|r^LY_L\|J_i\rangle}{\langle J_i|r^{2L-2}|J_i\rangle}r^{L-1}\frac{d}{dr}\varrho_0(r). \quad (13)$$

If the charge distribution of the ground state is assumed to be a uniform distribution with a radius R_0, this becomes identical with the transition density of the collective model given by Eq. (10).

On the other hand, it is well known that the schematic RPA with a separable interaction,

$$V_S(\boldsymbol{r}_i,\boldsymbol{r}_j)=\kappa_L\sum_M r_i^LY_{LM}(\Omega_i)r_j^LY^*_{LM}(\Omega_j), \quad (14)$$

for particle-hole excitations $|mi^{-1}\rangle$ with a degenerate particle-hole excitation energy ϵ gives a collective state $|LM\rangle$, which exhausts the energy-weighted sum rule for the single-particle operator r^LY_{LM},

$$\Delta E_L|\langle LM|r^LY_{LM}|0\rangle|^2=\epsilon\sum_{mi}|\langle m|r^LY_{LM}|i\rangle|^2, \quad (15)$$

TABLE I. Nuclear-polarization correction (meV) to the $1s_{1/2}$ state of $^{208}_{82}Pb^{81+}$. NP denotes the correction due to the whole of the Coulomb and transverse interactions. CNP the correction only due to the Coulomb interaction. Energy shifts in the parentheses are due to seagull contribution.

	Present work					Ref. [7]	Ref. [6]
L^π	Feynman (NP)		Coulomb (NP)		CNP	NP	CNP
0^+	−3.3	(−0.2)	−3.3	(+0.0)	−3.3	−6.6	−3.3
1^-	−22.1	(−42.3)	−21.5	(−7.3)	−17.0	+16.3	−17.6
2^+	−5.8	(+0.3)	−5.8	(+0.6)	−5.8	−7.0	−5.8
3^-	−2.7	(+0.2)	−2.8	(+0.2)	−2.9	−2.9	−2.6
4^+	−1.0	(+0.1)	−1.0	(+0.1)	−1.1		
5^-	−0.5	(+0.1)	−0.6	(+0.0)	−0.6		
total	−35.4	(−41.8)	−35.0	(−6.4)	−30.7	−0.2	−29.3

where ΔE_L is the excitation energy of $|LM\rangle$ [15]. If the ground state is assumed to be a filled major shell of the harmonic oscillator potential

$$H_{HO}=\frac{1}{2M_N}\boldsymbol{p}^2+\frac{M_N\omega^2}{2}\boldsymbol{r}^2, \tag{16}$$

the particle-hole excitation energy ϵ is taken to be $1\hbar\omega$ for 1^- and $2\hbar\omega$ for 0^+ and 2^+. The corresponding collective states exhaust the energy-weighted sum rules, because the transition strengths vanish outside these p-h excitation spaces. Therefore, the transition densities of charge to the collective states of this fictitious nucleus are given by Eq. (13). When the ground-state charge density is approximated by a uniform charge density, the transition density of charge becomes identical with that of the collective model employed in NP calculations for hydrogenlike atoms. However, the gauge invariant electromagnetic interaction of this schematic microscopic model is given by the minimal substitution $\boldsymbol{p}_i \rightarrow \boldsymbol{p}_i - e_i\boldsymbol{A}$ to the Hamiltonian $H=H_{HO}+V_S$. Hence the lowest-order contributions to NP with this model are given by the three Feynman diagrams in Fig. 1, where two photons are exchanged between a bound electron and a nucleus. The nuclear vertices are understood to have no diagonal matrix elements for the ladder and cross diagrams, and no nuclear intermediate states for the seagull diagram. It is well known that the NP results with this model is gauge invariant provided these three diagrams are taken into account. Although $J_{LL+1}(r)$ current density appears in this model, $J_{LL-1}(r)$ dominates in the transition to the collective state.

Thus we can conclude that the gauge invariance of the collective model is also guaranteed with the charge-current density satisfying the continuity equation (8), provided the contributions from the three diagrams are taken into account. In the actual NP calculations [4–7] with the collective model, the assumption that each nuclear intermediate state saturates the sum rule is not strictly obeyed, because the observed nuclear data are used for the low-lying states. However, since the gauge violation is serious only in the dipole giant resonance, this does not invalidate our arguments as is confirmed by the numerical results in the following.

The formulas to calculate the NP energy shifts due to the three diagrams of Fig. 1 were given in Ref. [8] for arbitrary nuclear models. In the present NP calculations of the $1s_{1/2}$ states in hydrogenlike $^{208}_{82}Pb$ and $^{238}_{92}U$, the parameters of the collective model are the same as those given in Refs. [6,7]. The same low-lying states and giant resonances are taken into account. In addition, the contributions from the 4^- and 5^- giant resonances are also calculated in order to see the effects of higher multipoles neglected previously. The $B(EL)$ values are adjusted to the observed values for low-lying states and the $B(EL)$ are estimated through the energy-weighted sum rule for giant resonances. It should be noted that the seagull correction is given in terms of the ground-state charge density, and the correction with the collective model also can be calculated for both $^{208}_{82}Pb$ and $^{238}_{92}U$ using the same formulas given in Ref. [8].

Tables I and II show the results for the $1s_{1/2}$ states in $^{208}_{82}Pb^{81+}$ and $^{238}_{92}U^{91+}$, where the sum of the contributions from the three diagrams of Fig. 1 is given for each multipole. The second and the third columns are the results including the transverse effects in the Feynman and Coulomb gauges, respectively. The values in the parentheses are the contributions from the seagull diagram. The NP energy shifts due to the ladder and crossed diagrams only are obtained by subtraction of the seagull contributions given in the parentheses. The fourth column gives the results of the present Coulomb

TABLE II. Nuclear-polarization correction (meV) to the $1s_{1/2}$ state of $^{238}_{92}U^{91+}$. The notations are the same as in Table I.

	Present work					Ref. [7]	Ref. [6]
L^π	Feynman (NP)		Coulomb (NP)		CNP	NP	CNP
0^+	−9.3	(−0.4)	−9.3	(+0.0)	−9.3	−21.5	−9.5
1^-	−54.3	(−65.7)	−52.5	(−3.9)	−41.6	−3.8	−42.4
2^+	−131.6	(+0.0)	−131.7	(+1.6)	−131.6	−148.2	−138.9
3^-	−6.5	(+0.3)	−6.5	(+0.4)	−6.7	−7.3	−6.8
4^+	−2.0	(+0.2)	−2.0	(+0.2)	−2.1		
5^-	−1.0	(+0.1)	−1.0	(+0.1)	−1.1		
total	−204.7	(−65.5)	−203.0	(−1.6)	−192.4	−180.8	−197.6

nuclear polarization (CNP). The last two columns are the results of the previous calculations.

The results with the collective model, as with the microscopic RPA model [8], also lead to large violations of gauge invariance if ladder and crossed diagram contributions only are considered. The seagull corrections are considerable in the 1^- contributions for both of $^{208}_{82}\mathrm{Pb}^{81+}$ and $^{238}_{92}\mathrm{U}^{91+}$. Note that, in the limit of point nucleus, which is not unrealistic even for heavy hydrogenlike ions, the seagull collection occurs only in the dipole mode which involves the current density $J_{10}(r)$.

In $^{208}_{82}\mathrm{Pb}^{81+}$, the sum of contributions from the low-lying states is about 10% of the total result and the NP energy is mainly determined by the giant resonance contributions. The most dominant contribution comes from the giant dipole resonance, where a large violation of gauge invariance occurs if the seagull contributions in the parentheses are neglected: -22 meV becomes $+20$ meV and -14 meV in the Feynman and Coulomb gauges, respectively. The total NP energy of $^{208}_{82}\mathrm{Pb}^{81+}$ is $-35.0(-35.4)$ meV in the collective model compared with $-38.2(-37.0)$ meV in the microscopic model [8] for the Coulomb (Feynman) gauge. The transverse NP effects are less than 20% of the CNP and similar in both models. The agreement of the two models provides stability of the prediction of the NP effects with respect to the choice of the nuclear models.

In $^{238}_{92}\mathrm{U}^{91+}$, the total NP energy is $-205(-203)$ meV for the Coulomb (Feynman) gauge. The dominant contribution comes from the lowest 2^+ with a large $B(E2)$ value. Since the transition density of current given by Eq. (11) is proportional to the excitation energy, the transverse contribution of the lowest 2^+ is negligible due to its exceptionally small excitation energy $\Delta E_2 = 44.9$ keV. Apart from this large Coulomb contribution, the results show similar tendencies as in $^{208}_{82}\mathrm{Pb}^{81+}$. Namely, contributions from the low-lying states are small compared with contributions form the giant resonances, and a large gauge violation occurs in the giant dipole resonance when the seagull contribution is omitted.

The fifth column of Tables I and II gives the previous results in the Feynman gauge without seagull contributions. The differences between the two results in the Feynman gauge without seagull contributions come: from the accuracy of numerical integration over the continuum threshold region of electron intermediate states and from the differences of the electron wave functions. Here we have used wave functions in a finite charge distribution, while [7] employs point Coulomb solutions. Without the seagull correction, however, the Feynman gauge gives an erroneous estimate of NP, although numerical calculation in this gauge is easier than in the Coulomb gauge. The results of Ref. [7] should be corrected by the present gauge invariant estimates. On the other hand, the CNP results of Ref. [6] in the last column agree with the gauge invariant total NP results within a margin of error of about 20%. Hence, the Coulomb contributions in the Coulomb gauge with the collective model provide the correct order of magnitude of the total NP corrections in both nuclei.

To summarize, the NP energy shifts with the collective model are estimated gauge invariantly by inclusion of the seagull contribution. The gauge invariance is satisfied to a few percent levels in both $^{208}_{82}\mathrm{Pb}^{81+}$ and $^{238}_{92}\mathrm{U}^{91+}$ for each of the multipole separately. The net transverse effect is about 14–15% of the Coulomb energy shift in $^{208}_{82}\mathrm{Pb}^{81+}$. This should be compared with the transverse effect of the $1s_{1/2}$ state in muonic $^{208}_{82}\mathrm{Pb}$, which is about 6% of the Coulomb effect [9]. In $^{238}_{92}\mathrm{U}^{91+}$, it is reduced to about 6% of the Coulomb effect due to the dominant Coulomb contribution from the lowest 2^+ state.

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