Hyperfine splitting of hydrogenlike atoms based on relativistic mean field theory

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We evaluate the hyperfine splitting of hydrogenlike ^{209}Bi and ^{207}Pb atoms based on a relativistic method for both the electron system and the nucleon system. The Bohr-Weisskopf (BW) effect is calculated with Lorentz covariant current. It is shown that the BW correction to the hyperfine splitting (HFS) is 0.58%–0.67% for $^{209}Bi^{82+}$ and 3.79%–4.00% for $^{207}Pb^{81+}$. It is also concluded that relativistic mean field theory reproduces the observed values of the HFS within the accuracy of 5% in $^{209}Bi^{82+}$ and 13% in $^{207}Pb^{81+}$.

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I. INTRODUCTION

Seeking the original quantum mechanical study for the hyperfine splitting (HFS), we need to trace back to Fermi in 1930 [1], in which he evaluated the HFS using given nuclear magnetic moment values. The finite nuclear magnetization effect of the HFS was studied by Bohr and Weisskopf [2]. Although this Bohr-Weisskopf (BW) effect as well as nuclear magnetic moments were expected to be probe of the nuclear structure, it was difficult to settle experimentally the pygmy energy shift due to the BW effect.

In the last decade, however, some rigorous splitting energies in hydrogenlike atoms have been reported from the laser spectroscopic measurements [3,4]. These high-precision experiments have evoked the corresponding HFS calculations as well as the higher-order quantum electrodynamics (QED) corrections, and have been compared with many theoretical calculations using the nuclear models such as "dynamic proton model" (DPM) by Labzowsky *et al.* [5] and "dynamic correction model" by Tomaselli *et al.* [6,7], and so on [8–12]. Also, recently, the nuclear polarization effect on the HFS was reported by Nefiodov *et al.* [13]. In the above theoretical studies except DPM, however, the relativistic formalism was only used for the electron, while nonrelativistic formalism was used for the nucleus.

In the present study, we calculate the HFS of hydrogenlike atom $^{207}Pb^{81+}$ and $^{209}Bi^{82+}$ in the relativistic formalism. In this formalism, we evaluate the first-order perturbation energy of the HFS [14,15] by using not only Lorentz covariant current of electron but also that of nucleons. In DPM the anomalous magnetic moment in the nuclear current is not considered, while it is included in our calculations. In the relativistic calculation of nuclei, single-particle states of nucleons are usually given by relativistic mean field (RMF) calculation which has succeeded in reproducing the single-particle properties and *ls* splitting, and so on [16–19]. The aim of this paper is to clarify whether RMF gives good description for the HFS and to determine the correction factor of the BW effect (ϵ).

As for the electron, we solve Dirac equation for electron in the Coulomb field generated from the charge distribution calculated by RMF. This finite size (FS) effect is sometimes called as the "Breit-Schawlow effect" [20–23]. The FS effect calculated in our model is compared with those in the other studies.

In Sec. II, RMF theory for nuclei and the relativistic formalism for one electron are reviewed. The explicit form of the HFS is given. Numerical results of the HFS and the BW effect are given in Sec. III. Finally, we give our summary and conclusion in Sec. IV.

II. FORMALISM

A. Calculation of hyperfine splitting

The interaction Hamiltonian is written as

$$\mathcal{H}_I = e\hat{j}_e^{\mu}\hat{A}_{\mu} + e\hat{J}_N^{\mu}\hat{A}_{\mu}, \tag{1}$$

where $\hat{j}_e^{\mu}$ and $\hat{J}_N^{\mu}$ are Lorentz covariant current operators for the electron and the nucleus, respectively,

$$\hat{j}_e^{\mu} = \hat{\bar{\psi}}_e\gamma^{\mu}\hat{\psi}_e, \tag{2}$$

$$\hat{J}_N^{\mu} = \frac{1+\tau_3}{2}\hat{\bar{\psi}}_N\gamma^{\mu}\hat{\psi}_N + \frac{\lambda}{2M}\partial_{\nu}\left(\hat{\bar{\psi}}_N\sigma^{\mu\nu}\hat{\psi}_N\right), \tag{3}$$

where

$$\sigma^{\mu\nu} = \frac{i}{2}[\gamma^{\mu},\gamma^{\nu}], \tag{4}$$

$\hat{\psi}_e$ and $\hat{\bar{\psi}}_e$ are the electron field operators, $\hat{\psi}_N$ and $\hat{\bar{\psi}}_N$ are the nucleon field operators, and λ is the static anomalous mag-

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TABLE I. rms charge radii for nuclei constructed by RMF with NLC. All values are in femtometer.

	^{209}Bi	^{207}Pb
Calculation	5.566	5.559
Expt.[a]	5.519	5.497

[a]Reference [24].

netic moment for nucleons: $\lambda=1.793\mu_N$ for proton and $\lambda=-1.913\mu_N$ for neutron.

We evaluate the HFS using the first-order perturbation based on S-matrix method [14,15]. The HFS is written as

$$\Delta E_{\rm HFS} = e^2\langle IjFM|j_e^s(\boldsymbol{x_1})D_{st}(\boldsymbol{x_1},\boldsymbol{x_2};0)J_N^t(\boldsymbol{x_2})|IjFM\rangle|_{F=I-j}^{F=I+j}$$
$$= e^2\sum_{L\eta}\frac{1}{\hat{L}^2}(-1)^{L+1-\eta}\Delta W(I\eta Fj;Ij)\int r^2drR^2dR\frac{r'^L_<}{r'^{L+1}_>}$$
$$\times(-1)^\eta\langle j\|[Y_L\otimes j_e]^\eta\|j\rangle\langle I\|[Y_L\otimes J_N]^\eta\|I\rangle, \tag{5}$$

where $\hat{L}=\sqrt{2L+1}$, I is the total angular momentum of the nucleus, and j is the total angular momentum of the electron, $j=1/2$ for $(1s_{1/2})$. $F=I\oplus j$ is the total angular momentum and M is its z component. In Eq. (5),

$$\Delta W(I\eta Fj;Ij) = W(I\eta I+jj;Ij) - W(I\eta I-jj;Ij), \tag{6}$$

where W is the Racah coefficient. The transverse part of photon propagator is

$$D_{st}(\boldsymbol{x_1},\boldsymbol{x_2};0) = \frac{\delta_{st}}{4\pi|\boldsymbol{x_1}-\boldsymbol{x_2}|}, \tag{7}$$

where subscripts s and t run from 1 to 3.

Substituting $j=1/2$ in Eq. (5), the matrix elements in Eq. (5) vanish unless $\eta=L=1$ due to the electron current property. The reduced matrix for nucleus can be separated into the Dirac part $\mathcal{J}_D(R)$ and the anomalous part $\mathcal{J}_A(R)$, so that the HFS is represented as follows:

$$\Delta E_{\rm HFS} = \frac{e^2}{3}\Delta W\left(I\eta F\frac{1}{2};I\frac{1}{2}\right)\int r^2drR^2dR\frac{r'_<}{r'^2_>}\mathcal{J}_e(r)$$
$$\times[\mathcal{J}_D(R)+\mathcal{J}_A(R)]. \tag{8}$$

The electron part $\mathcal{J}_e(r)$ and the Dirac part and the anomalous part for nucleus are, respectively,

$$\mathcal{J}_e(r) = 2g(r)f(r)\left\langle 0\tfrac{1}{2}\tfrac{1}{2}\right\|[Y_1\otimes\sigma]^1\left\|1\tfrac{1}{2}\tfrac{1}{2}\right\rangle, \tag{9}$$

$$\mathcal{J}_D(R) = -2u(R)v(R)\frac{1+\tau_3}{2}\left\langle l\frac{1}{2}I\right\|[Y_1\otimes\sigma]^1\left\|\bar{l}\frac{1}{2}I\right\rangle, \tag{10}$$

$$\mathcal{J}_A(R) = \frac{\lambda}{2M}\left[\sqrt{\frac{2}{3}}\frac{d}{dR}\mathcal{J}_{A1}(R) + \frac{1}{\sqrt{3}}\left(\frac{d}{dR}+\frac{3}{R}\right)\mathcal{J}_{A2}(R)\right], \tag{11}$$

where

$$\mathcal{J}_{A1}(R) = u(R)^2\left\langle l\tfrac{1}{2}I\right\|[Y_0\otimes\sigma]^1\left\|l\tfrac{1}{2}I\right\rangle$$
$$-v(R)^2\left\langle \bar{l}\tfrac{1}{2}I\right\|[Y_0\otimes\sigma]^1\left\|\bar{l}\tfrac{1}{2}I\right\rangle, \tag{12}$$

$$\mathcal{J}_{A2}(R) = u(R)^2\left\langle l\tfrac{1}{2}I\right\|[Y_2\otimes\sigma]^1\left\|l\tfrac{1}{2}I\right\rangle$$
$$-v(R)^2\left\langle \bar{l}\tfrac{1}{2}I\right\|[Y_2\otimes\sigma]^1\left\|\bar{l}\tfrac{1}{2}I\right\rangle, \tag{13}$$

where l $(\bar{l})$ stands for the orbital angular momentum of the upper (lower) component of the nucleon field. $u(R)[v(R)]$ is the upper [lower] component of the nucleon field, normalized as $\int dRR^2[u(R)^2+v(R)^2]=1$. Like the nucleon system, $g(r)[f(r)]$ is the upper [lower] component of the electronic field and normalized as $\int drr^2[g(r)^2+f(r)^2]=1$.

B. Wave functions

For single-particle states of nucleons, we start from the effective Lagrangian with nonlinear interaction of the form

$$\mathcal{L} = \bar{\psi}\left[i\gamma^\mu\partial_\mu - g_v\gamma^\mu V_\mu - \frac{\tau_3}{2}g_\rho\gamma^\mu b_\mu - \frac{1+\tau_3}{2}e\gamma^\mu A_\mu\right.$$
$$\left. - (M-g_s\phi)\right]\psi + \frac{1}{2}[\partial_\mu\phi\partial^\mu\phi - m_s^2\phi^2] + \frac{1}{3}g_2\phi^3 - \frac{1}{4}g_3\phi^4$$
$$-\left[\frac{1}{4}(\partial_\mu V_\nu - \partial_\nu V_\mu)(\partial^\mu V^\nu - \partial^\nu V^\mu) - \frac{1}{2}m_v^2V_\mu V^\mu\right]$$
$$-\left[\frac{1}{4}(\partial_\mu b_\nu - \partial_\nu b_\mu)(\partial^\mu b^\nu - \partial^\nu b^\mu) - \frac{1}{2}m_\rho^2 b_\mu b^\mu\right]$$
$$-\frac{1}{4}(\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial^\mu A^\nu - \partial^\nu A^\mu). \tag{14}$$

The field of nucleons is denoted by ψ with mass M, and ϕ, V^μ, b^μ, and A^μ are fields of σ, ω, ρ meson, and photon, respectively. The Lagrangian parameters are the meson masses m_s, m_v, and m_ρ; the corresponding coupling constants

TABLE II. Properties of the $1s_{1/2}$ electron in the RMF with NLC.

	^{209}Bi^{82+}		^{209}Bi^{81+}	
	Point	RMF	Point	RMF
Binding energy (MeV)	−0.104394	−0.104319	−0.101582	−0.101515
rms radius (fm)	972.50	973.19	987.96	988.60
Magnetic moment (μ_B)	0.8567	0.8569	0.8603	0.8605

g_s, g_v, and g_ρ; and the nonlinear coupling constants g_2 and g_3. We use units with $c=\hbar=1$ and $e^2=4\pi\alpha$, where α is the fine structure constant, i.e., 1/137.036 04. Here γ^μ is 4×4 gamma matrix and the third component of isospin τ_3 is 1 for proton and −1 for neutron.

In the zeroth-order perturbative expansion, one proton particle state (^{209}Bi) and one neutron hole state (^{207}Pb) are given by

$$|^{209}\mathrm{Bi}\rangle = \hat{a}^\dagger_{1h_{9/2}}|^{208}\mathrm{Pb}\rangle, \tag{15}$$

$$|^{207}\mathrm{Pb}\rangle = \hat{b}_{3p_{1/2}}|^{208}\mathrm{Pb}\rangle, \tag{16}$$

where $|^{208}\mathrm{Pb}\rangle$ is the core ground state wave function and $\hat{a}^\dagger(\hat{b})$ creates a proton (neutron) valence particle (hole). The charge density is defined in Ref. [16] as

$$\rho_c(\boldsymbol{R}) = \int d\boldsymbol{x}'\rho_{sn}(\boldsymbol{x}-\boldsymbol{x}')\rho_p(\boldsymbol{x}'), \tag{17}$$

$$\rho_{sn}(\boldsymbol{y}) = \frac{\mu^3}{8\pi}\exp(-\mu|\boldsymbol{y}|), \tag{18}$$

$$\mu = \sqrt{0.71} \quad (\mathrm{GeV}). \tag{19}$$

Here, the proton density $\rho_p(\boldsymbol{R})$ is constructed from RMF and normalized to the charge number Z; $\int d\boldsymbol{R}\rho_p(\boldsymbol{R})=Z$. Table I shows root mean square charge radii of ^{209}Bi and ^{207}Pb nuclei calculated by this method. Properties of electron in the RMF with NLC are shown in Table II. The binding energy of electron of the RMF in $^{207}\mathrm{Pb}^{81+}$ nearly agrees with the results −0.10151464 MeV and −0.10151435 MeV in Ref. [25]. The two-parameter Fermi model in Ref. [24], also used in Refs. [5–8,10], gives −0.104 320 MeV for $^{209}\mathrm{Bi}^{82+}$ and −0.101 515 MeV for $^{207}\mathrm{Pb}^{81+}$, which completely agree with the results of the RMF in Table II. This indicates the validity of the charge distribution obtained by Eqs. (17)–(19) with the proton density $\rho_p(\boldsymbol{R})$ constructed from the RMF.

III. RESULTS AND DISCUSSION

The model parameters for Lagrangian (14) we have used are given in Table III. The results of the HFS for $^{209}\mathrm{Bi}^{82+}$ and $^{207}\mathrm{Pb}^{81+}$are shown in Table IV for different parameter sets.

In $^{209}\mathrm{Bi}^{82+}$, we find that the nonlinear models NL-SH, NL3, and NLC are close to the experimental value compared with the linear model HS. In particular, the NLC result of 5.292 eV agrees very well with the experimental value of 5.0840 eV. On the other hand, in $^{207}\mathrm{Pb}^{81+}$, all of the parameter sets give similar results, namely, the parameter dependence among them is less than 1.0%. This different behavior of dependence on the parameter sets is explained as follows. Neglecting the BW effect, i.e., $r'_<=R, r'_>=r$, in Eq. (8), the HFS is approximately written as

TABLE III. Model parameters in the relativistic mean field calculations.

	HS[a]	NL-SH[b]	NL3[c]	NLC[d]
M (MeV)	939.0	939.0	939.0	939.0
m_s (MeV)	520.0	526.059	508.194	500.8
m_v (MeV)	783.0	783.0	782.501	783.0
m_ρ (MeV)	770.0	763.0	763.0	770.0
g_s	10.47	10.4444	10.217	9.7524
g_v	13.80	12.945	12.868	12.2037
g_ρ	8.076	8.766	8.948	8.6597
g_2 (fm^{-1})		−6.9099	−10.431	−12.67
g_3		−15.8337	−28.885	−33.33

[a]Reference [16].
[b]Reference [17].
[c]Reference [18].
[d]Reference [19].

$$\Delta E_{\mathrm{FS}} = i\frac{\alpha}{M}\sqrt{\frac{2\pi}{3}}\sqrt{\frac{(2I+1)(I+1)}{I}}\Delta W(I\eta Fj;Ij) \times \mu_I\int dr\mathcal{J}_e(r), \tag{20}$$

where the nuclear magnetic moment μ_I is given by

$$\mu_I = \langle I|\hat{\mu}_z|I\rangle/\frac{|e|}{2M} = -iM\sqrt{\frac{8\pi}{3}}\frac{1}{\hat{I}}\langle II10|II\rangle \times \int R^3 dR[\mathcal{J}_D(R)+\mathcal{J}_A(R)]. \tag{21}$$

Nuclear magnetic moments for each parameter set are shown in Table V [27]. Similar to the HFS, the nonlinear models also give different nuclear magnetic moments for ^{209}Bi and similar ones for ^{207}Pb. The difference comes from the fact that the Dirac part of the nuclear magnetic moments depends on the effective mass and is proportional to M/M^*; the effective mass is different for the different parameter sets. For ^{209}Bi, therefore, several parameter sets give different values of the nuclear magnetic moments and the HFS. On the contrary, the anomalous part of nuclear magnetic moments is reduced to the following form:

TABLE IV. HFS calculated with different parameter sets. All values are in eV.

	$^{209}\mathrm{Bi}^{82+}$	$^{207}\mathrm{Pb}^{81+}$
HS	6.349	1.383
NL-SH	5.776	1.378
NL3	5.664	1.375
NLC	5.292	1.371
Expt.	5.0840[a]	1.2166[b]

[a]Reference [3].
[b]Reference [4].

TABLE V. Nuclear magnetic moments in μ_N and the effective mass for nuclear matter.

	^{209}Bi	^{207}Pb	M^*/M
HS	5.0641	0.6726	0.541
NL-SH	4.6082	0.6693	0.597
NL3	4.5187	0.6683	0.595
NLC	4.2230	0.6661	0.63
Expt. (corrected)[a]	4.1106	0.59258	

[a]Reference [27].

$$\mu_{IA} = \begin{cases} -\dfrac{\lambda I}{I+1}\left[1+\dfrac{1}{I}\int dRR^2\upsilon(R)^2\right] & (k>0\text{: spin down}) \\ \lambda\left[1-\dfrac{1}{I+1}\int dRR^2\upsilon(R)^2\right] & (k<0\text{: spin up}). \end{cases} \tag{22}$$

Since the nuclear current of ^{207}Pb consists of only the anomalous part $\mathcal{J}_A$ and the integral on the square of the lower component is negligible compared with the unity, we find from Eq. (22) that the value of the nuclear magnetic moments of ^{207}Pb is approximately constant. In short, the anomalous part of the nuclear magnetic moments is independent of the wave functions. For ^{207}Pb, hence, the value of the nuclear magnetic moments and the HFS are independent of the parameters of the RMF models.

In Table VI, we show the energy difference due to the FS and the BW effects for each parameter set, and compare them with those of the previous works. The BW correction factor ϵ is defined as $\epsilon = 1-\Delta E_{\text{tot}}/\Delta E_{\text{BS}}$ in Ref. [28]. In the present paper, we set $\Delta E_{\text{BS}} = \Delta E_{\text{FS}}$ as the energy including the FS effect, and $\Delta E_{\text{tot}} = \Delta E_{\text{HFS}}$. The HFS energy for point nucleus obtained by substituting $\mathcal{J}_e^P(r)$ for $\mathcal{J}_e(r)$ in Eq. (20),

$$\mathcal{J}_e^{\text{P}}(r) = 2g_0(r)f_0(r)\left\langle 0\tfrac{1}{2}\tfrac{1}{2}\right\|[Y_1\otimes\sigma]^1\left\|1\tfrac{1}{2}\tfrac{1}{2}\right\rangle, \tag{23}$$

is denoted by ΔE_{P} and energy differences δE_{FS} and δE_{BW} are defined by

$$\delta E_{\text{FS}} = \Delta E_{\text{P}} - \Delta E_{\text{FS}}, \tag{24}$$

$$\delta E_{\text{BW}} = \Delta E_{\text{FS}} - \Delta E_{\text{tot}}, \tag{25}$$

where $g_0(r)$ $[f_0(r)]$ is the upper [lower] component of the electron field for point nucleus.

Comparing δE_{BW} and ϵ with those of the previous works, our results are smaller than the previous works in ^{209}Bi^{82+}, while they are near the results of Refs. [10] [without spin orbit (SO)] and [12] in ^{207}Pb^{81+}. The empirical value ϵ_{emp} is estimated by

$$\epsilon_{\text{emp}} = 1-(\Delta E_{\text{expt}}-\Delta E_{\text{QED}})/\Delta E_{\text{FS}}^{\text{expt}}, \tag{26}$$

where ΔE_{QED} is -0.0298 eV for ^{209}Bi^{82+} [10,29,30] and -0.0073 eV for ^{207}Pb^{81+} [29]. $\Delta E_{\text{FS}}^{\text{expt}}$ is given by inserting the experimental value of nuclear magnetic moments into Eq. (20) instead of the calculated value μ_I. Then ϵ_{emp} is 0.0150 for ^{209}Bi^{82+} and 0.0413 for ^{207}Pb^{81+}. Compared to the empirical values, our results are smaller for ^{209}Bi^{82+} and similar for ^{207}Pb^{81+}.

The ratio of the FS effect to ΔE_{P} agrees among the results with different parameter sets in the present work and is the same as the previous works.

IV. CONCLUSION

We have calculated the HFS for ^{209}Bi^{82+} and ^{207}Bi^{81+} from RMF with the linear and the nonlinear models by using the Lorentz covariant current. For electron, we use Dirac equations with the Coulomb potential calculated from RMF.

The nonlinear model with NLC reproduces nuclear magnetic moments as well as the HFS better than those with the other parameter sets in ^{209}Bi^{82+}. On the contrary, in ^{207}Pb^{81+}, parameter dependence is not noticeable for both nuclear magnetic moments and the HFS.

TABLE VI. The BW effect and the FS effect for each parameter set. δE are all in eV and values in parentheses are the ratios to ΔE_P in percentage.

	^{209}Bi^{82+}			^{207}Pb^{81+}		
	δE_{FS}	δE_{BW}	ϵ	δE_{FS}	δE_{BW}	ϵ
HS	0.791 (11.01)	0.048 (0.67)	0.0075	0.168 (10.41)	0.065 (4.00)	0.0447
NL-SH	0.724 (11.07)	0.041 (0.62)	0.0070	0.168 (10.47)	0.062 (3.84)	0.0429
NL3	0.711 (11.08)	0.040 (0.62)	0.0070	0.168 (10.48)	0.062 (3.88)	0.0433
NLC	0.667 (11.13)	0.035 (0.58)	0.0066	0.168 (10.52)	0.061 (3.79)	0.0423
Ref. [5]		0.0678	0.0131			
Ref. [10] (no SO)			0.0133	0.1498 (10.49)	0.0536 (3.75)	0.0419
Ref. [10] (SO)	0.6464 (11.11)	0.0610 (1.05)	0.0118			
Ref. [12]			0.0131			0.0429
Ref. [7]	0.6473 (11.08)		0.0210	0.1470 (10.50)		0.0289
Ref. [11]		0.050	0.0095		0.045	0.0353

TABLE VII. Parameters of the Gaussian bases for the nucleon system and the electron system.

	a_1	β	n
Nucleon	0.8034	25	24
Electron	6.367	942.31	50

Our calculation gives close values of the BW effect for these parameter sets: ϵ is 0.006–0.008 for $^{209}Bi^{82+}$ and 0.042–0.045 for $^{207}Pb^{81+}$.

Finally RMF theory reproduces the observed values of μ_I and the HFS within the accuracy of 5% in $^{209}Bi^{82+}$ and 13% in $^{207}Pb^{81+}$. These discrepancies indicate that several problems remain beyond RMF. Especially higher-order correlations of *p-h* excitations may be important; there exist several other calculations of magnetic moments in relativistic models where it is found that core polarization modifies the magnetic moments [31]. Further studies are necessary on this point.

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APPENDIX

To calculate variationally the nucleon system and the electron system, we employ the diagonalization method on the Gaussian bases [32] as follows:

$$\psi(r) = \sum_{k}^{n} c_k r^l e^{-(r/a_k)^2}, \tag{A1}$$

where

$$a_k = (a_1 \beta^{(k-1)/(n-1)}) \tag{A2}$$

and c_k is the expansion coefficient. For the nucleon system, we calculate matrix elements to 20 fm on a mesh of 0.02 fm; and for the electron system, we do to 6000 fm on a mesh of 20 fm. In Table VII, we show parameters used in these calculations.

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