Recoil correction to the ground-state energy of hydrogenlike atoms

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The recoil correction to the ground-state energy of hydrogenlike atoms is calculated to all orders in αZ in the range $Z=1-110$. The nuclear size corrections to the recoil effect are partially taken into account. In the case of hydrogen, the relativistic recoil correction beyond the Salpeter contribution and the nonrelativistic nuclear size correction to the recoil effect amounts to $-7.2(2)$ kHz. The total recoil correction to the ground-state energy in hydrogenlike uranium ($^{238}U^{91+}$) constitutes 0.46 eV. [S1050-2947(98)02506-2]

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I. INTRODUCTION

The complete αZ-dependence formulas for the nuclear recoil corrections to the energy levels of hydrogenlike atoms in the case of a point nucleus were first obtained by a quasipotential method [1] and subsequently rederived by different approaches [2–4]. According to [4], the nuclear size corrections to the recoil effect can be partially included in these formulas by a replacement of the pure Coulomb potential with the potential of an extended nucleus. The total recoil correction for a state a of a hydrogenlike atom is conveniently written as the sum of a low-order term ΔE_L and a higher-order term ΔE_H [1], where ($\hbar=c=1$)

$$\Delta E_L=\frac{1}{2M}\langle a|\{\mathbf{p}^2-[\mathbf{D}(0)\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{D}(0)]\}|a\rangle, \tag{1}$$

$$\Delta E_H=\frac{i}{2\pi M}\int_{-\infty}^{\infty}d\omega\left\langle a\left|\left(\mathbf{D}(\omega)-\frac{[\mathbf{p},V]}{\omega+i0}\right)\right.\right. \times G(\omega+\varepsilon_a)\left.\left.\left(\mathbf{D}(\omega)+\frac{[\mathbf{p},V]}{\omega+i0}\right)\right|a\right\rangle. \tag{2}$$

Here, $|a\rangle$ is the unperturbed state of the Dirac electron in the nuclear potential $V(r)$, $\mathbf{p}$ is the momentum operator, $G(\omega)=[\omega-H(1-i0)]^{-1}$ is the relativistic Coulomb Green function, $H=(\boldsymbol{\alpha}\cdot\mathbf{p})+\beta m+V$, α_l $(l=1,2,3)$, β are the Dirac matrices,

$$D_m(\omega)=-4\pi\alpha Z\alpha_l D_{lm}(\omega),$$

and $D_{ik}(\omega,r)$ is the transverse part of the photon propagator in the Coulomb gauge:

$$D_{ik}(\omega,\mathbf{r})=-\frac{1}{4\pi}\left\{\frac{\exp\,(i|\omega|r)}{r}\delta_{ik}+\nabla_i\nabla_k\frac{(\exp\,(i|\omega|r)-1)}{\omega^2 r}\right\}.$$

In Eq. (2), the scalar product is implicit. For pointlike nuclei, $V(r)=V_C(r)=-\alpha Z/r$. If extended nuclei are considered, $V(r)$ is the potential of the extended nucleus in Eq. (2) and in calculating ε_a, $|a\rangle$, and $G(\omega)$. Therefore the nuclear size corrections are completely included in the Coulomb part of the recoil effect. In the one-transverse-photon part and the two-transverse-photon part (see Ref. [4]), they are only partially included. At least for high Z we expect that this procedure accounts for the dominant part of the nuclear size effect since using the extended nucleus wave function and the extended nucleus Green function strongly reduces the singularities of the integrands in Eqs. (1) and (2) in the nuclear region.

The term ΔE_L contains all the recoil corrections within the $(\alpha Z)^4 m^2/M$ approximation. Its calculation for a point nucleus, based on the virial relations for the Dirac equation [5–7], yields [1]

$$\Delta E_L=\frac{m^2-\varepsilon_{a0}^2}{2M}, \tag{3}$$

where ε_{a0} is the Dirac electron energy for the point-nucleus case.

ΔE_H contains the contribution of order $(\alpha Z)^5 m^2/M$ and all contributions of higher order in αZ, which are not included in ΔE_L. To lowest order in αZ, this term represents the Salpeter correction [8]. The calculation of this term to all orders in αZ was performed in [9,10] for the case of a point nucleus. According to these calculations, the recoil correc-

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tion to the Lamb shift of the 1s state in hydrogen constitutes −7.1(9) kHz, in addition to the Salpeter term. This value is close to the $(\alpha Z)^6 m^2/M$ correction (−7.4 kHz) found in [3] and is clearly distinct from a recent result for the $(\alpha Z)^6 m^2/M$ correction (−16.4 kHz) obtained in [11]. [The $(\alpha Z)^6 \ln(\alpha Z) m^2/M$ corrections cancel each other [12,13].] The total recoil correction to the ground-state energy in $^{238}U^{91+}$ was calculated in [9] to be 0.51 eV.

In this work we calculate the recoil correction to the ground-state energy of hydrogenlike atoms in the range $Z = 1$–110 using the formulas (1) and (2) employing the potential of an extended nucleus.

II. LOW-ORDER TERM

Using the virial relations for the Dirac equation in a central field [7], the formula (1) can be transformed to (see Appendix)

$$\Delta E_L = \frac{m^2 - \varepsilon_{a0}^2}{2M} + \frac{1}{2M}\{(\varepsilon_{a0}^2 - \varepsilon_a^2) + \langle a|(\delta V)^2|a\rangle + 2\alpha Z \kappa \langle a|\sigma_z \delta V/r|\rangle - 2\varepsilon_a \langle a|\delta V|a\rangle + 2(m + 2\varepsilon_a \kappa) \times \langle a|\sigma_z \delta V|a\rangle - 2\alpha Z m \langle a|\sigma_x \delta V|a\rangle - 4m\varepsilon_a \langle a|\sigma_x r \delta V|a\rangle\}, \quad (4)$$

where ε_a and ε_{a0} are the Dirac electron energies for an extended nucleus and the point nucleus, respectively, $\kappa = (-1)^{j+l+1/2}(j+1/2)$ is the relativistic angular quantum number, $\delta V = V(r) - V_C(r)$ is the deviation of the nuclear potential from the pure Coulomb potential, and σ_x and σ_z are the Pauli matrices. Here, the notations for the radial matrix elements from [7] are used:

$$\langle a|u|b\rangle = \int_0^\infty [G_a(r)G_b(r) + F_a(r)F_b(r)]u(r)\, dr, \quad (5)$$

$$\langle a|\sigma_z u|b\rangle = \int_0^\infty [G_a(r)G_b(r) - F_a(r)F_b(r)]u(r)\, dr, \quad (6)$$

$$\langle a|\sigma_x u|\rangle = \int_0^\infty [G_a(r)F_b(r) + F_a(r)G_b(r)]u(r)\, dr. \quad (7)$$

$G/r = g$ and $F/r = f$ are the radial components of the Dirac wave function for the extended nucleus, which are defined by

$$\psi_{n\kappa m}(\mathbf{r}) = \begin{pmatrix} g_{n\kappa}(r)\Omega_{\kappa m}(\mathbf{n}) \\ i f_{n\kappa}(r)\Omega_{-\kappa m}(\mathbf{n}) \end{pmatrix}.$$

The first term on the right side of Eq. (4) corresponds to the low-order recoil correction for the point nucleus [see Eq. (3)]. The second term gives the nuclear size correction . We calculate this term for the uniformly charged nucleus. In Table I we display the results of this calculation for the 1s state. The values are expressed in terms of the function $\Delta F_L(\alpha Z)$ which is defined by

TABLE I. Nuclear size correction to the low-order term for the 1s state expressed in terms of the functions $\Delta F_L(\alpha Z)$ and $\Delta P_L(\alpha Z)$, defined by Eqs. (8) and (9), respectively. The values of the nuclear radii employed in the calculation are taken from [16,19–23].

Z	$\langle r^2\rangle^{1/2}$ (fm)	$\Delta F_L(\alpha Z)$	$\Delta P_L(\alpha Z)$
1	0.862	-0.337×10^{-8}	-0.0136
2	1.673	-0.519×10^{-7}	-0.0262
5	2.397	-0.102×10^{-5}	-0.0329
10	3.024	-0.976×10^{-5}	-0.0394
20	3.476	-0.933×10^{-4}	-0.0472
30	3.928	-0.406×10^{-3}	-0.0607
40	4.270	-0.126×10^{-2}	-0.0797
50	4.655	-0.340×10^{-2}	-0.1099
60	4.914	-0.823×10^{-2}	-0.1539
70	5.317	-0.0195	-0.2295
80	5.467	-0.0436	-0.3442
90	5.802	-0.0993	-0.5506
92	5.860	-0.117	-0.6073
100	5.886	-0.224	-0.9038
110	5.961	-0.517	-1.572

$$\Delta E_L = \frac{m^2 - \varepsilon_{a0}^2}{2M}[1 + \Delta F_L(\alpha Z)]. \quad (8)$$

In order to compare the nuclear size correction to the low-order term with the corresponding correction to the higher-order term (see the next section), in the last column of the Table I we display the value $\Delta P_L(\alpha Z)$ which is defined by

$$\Delta E_L = \frac{m^2 - \varepsilon_{a0}^2}{2M} + \frac{(\alpha Z)^5}{\pi n^3}\frac{m^2}{M}\Delta P_L(\alpha Z). \quad (9)$$

Using Eq. (4), one easily finds for an arbitrary ns state and for very low Z ($\alpha Z \ll 1$)

$$\Delta F_L(\alpha Z) = \frac{1}{n}\left(-\frac{12}{5}(\alpha Z)^2(Rm)^2 - \frac{72}{35}(\alpha Z)^3 Rm\right), \quad (10)$$

where $R = \sqrt{5/3}\langle r^2\rangle^{1/2}$ is the radius of the uniformly charged nucleus. The first term in Eq. (10) is a pure nonrelativistic one. It describes the reduced mass correction to the nonrelativistic nuclear size effect. So, if the nuclear size correction to the energy level is calculated using the reduced mass, this term must be omitted in Eq. (10). The second term, which is dominant, arises from the Coulomb part $[\langle a|\mathbf{p}^2|a\rangle/(2M)]$. For the standard parametrization of the proton form factor

$$f(p) = \frac{\Lambda^4}{(\Lambda^2 + p^2)^2}, \quad (11)$$

which corresponds to

$$\rho(r) = \frac{\Lambda^3}{8\pi}\exp(-\Lambda r) \quad (12)$$

and

TABLE II. Higher-order term for the 1s state expressed in terms of the function $P(\alpha Z)$ defined by Eq. (15). The nuclear radii employed in the calculation are the same as in Table I. $P_0(\alpha Z)$ is the related value for the point nucleus and $\Delta P = P - P_0$. $P_S(\alpha Z)$ is the Salpeter contribution obtained by Eq. (16).

Z	$P(\alpha Z)$	$P_0(\alpha Z)$	$\Delta P(\alpha Z)$	$P_S(\alpha Z)$
1	5.4391(3)	5.4299(3)	0.0092(2)	5.4461
2	4.9703(3)	4.9528(3)	0.0175(2)	4.9840
5	4.3281(3)	4.3034(3)	0.0247(2)	4.3731
10	3.828	3.795	0.031	3.9110
20	3.330	3.294	0.036	3.4489
30	3.086	3.044	0.043	3.1786
40	2.977	2.927	0.050	2.9868
50	2.973	2.914	0.060	2.8380
60	3.072	3.006	0.066	2.7165
70	3.295	3.234	0.061	2.6137
80	3.686	3.672	0.013	2.5247
90	4.330	4.521	−0.191	2.4462
92	4.501	4.779	−0.277	2.4315
100	5.40	6.41	−1.01	2.3759
110	7.24	12.43	−5.19	2.3124

$$V(r) = -\frac{\alpha Z}{r}\left(1 - \frac{1}{2}\exp(-\Lambda r)(2+\Lambda r)\right), \qquad (13)$$

the contribution of this term to ΔP_L is

$$\Delta P_L' = -\frac{35}{8}\pi\frac{m}{\Lambda}. \qquad (14)$$

We will see in the next section that this term cancels with the corresponding correction to the Coulomb part of the higher-order term. This implies that the sum of the low-order and higher-order contributions is more regular at $r \to 0$ than each of them separately.

III. HIGHER-ORDER TERM

To calculate the higher-order term (2) we transform it in the same way as it was done in [9]. The final expressions are given by Eqs. (41)–(54) of Ref. [9] where the pure Coulomb potential $[V_C(r) = -\alpha Z/r]$ in Eqs. (42) and (48) has to be replaced by the potential of the extended nucleus $V(r)$. We calculate these expressions for the uniformly charged nucleus by using the finite basis set method with the basis functions constructed from B splines [14]. The algorithm of the numerical procedure is the same as it is described in [9]. The results of the calculation for the 1s state are presented in the second column of Table II. They are expressed in terms of the function $P(\alpha Z)$ defined by

$$\Delta E_H = \frac{(\alpha Z)^5}{\pi n^3}\frac{m^2}{M}P(\alpha Z). \qquad (15)$$

For comparison, in the third column of this table we list the point-nucleus results $[P_0(\alpha Z)]$ that are obtained by the corresponding calculation for $R \to 0$. These point-nucleus results are in good agreement with our previous results from [9]. In the fourth column of the table, the difference $\Delta P = P - P_0$ is listed. Finally, in the last column the Salpeter contribution [8,15]

$$P_S^{(1s)} = -\frac{2}{3}\ln(\alpha Z) - \frac{8}{3}2.984\,129 + \frac{14}{3}\ln 2 + \frac{62}{9} \qquad (16)$$

is displayed.

For low Z the nuclear size correction to the higher-order term is mainly due to the Coulomb contribution

$$\Delta E_H^{(C)} = \frac{1}{2\pi i M}\int_{-\infty}^{\infty} d\omega \frac{1}{(\omega + i0)^2}\langle a|[\mathbf{p},V]G(\omega+\varepsilon_a) \times [\mathbf{p},V]|a\rangle. \qquad (17)$$

It is comparable with the deviation of the complete αZ-dependence value from the Salpeter contribution [in the case of hydrogen $\Delta P = -0.0092(2)$ while $P_0 - P_S = -0.0162(3)$]. To check this result let us calculate the finite nuclear size correction to the Coulomb part of the $(\alpha Z)^5 m^2/M$ contribution. Taken to the lowest order in αZ, formula (17) yields

$$\Delta E_H^{(C)} = -\frac{(2\pi)^3}{2M}|\phi_a(0)|^2\int d\mathbf{p}\frac{\sqrt{p^2+m^2}-m}{(\sqrt{p^2+m^2}+m)^2}\frac{p^2\tilde{V}^2(p)}{\sqrt{p^2+m^2}}, \qquad (18)$$

where $\phi_a(0)$ is the nonrelativistic wave function at $r=0$ and $\tilde{V}(p)$ is the nuclear potential in the momentum representation. Using the standard parametrization of the proton form factor

$$\tilde{V}(p) = -\frac{\alpha Z}{2\pi^2 p^2}\frac{\Lambda^4}{(\Lambda^2+p^2)^2} \qquad (19)$$

and separating the point-nucleus result from Eq. (18), we can write for an ns state

$$\Delta E_H^{(C)} = \frac{(\alpha Z)^5}{\pi n^3}\frac{m^2}{M}(-4/3 + \Delta P^{(C)}), \qquad (20)$$

where

$$\Delta P^{(C)} = -4\int_0^{\infty} dp \frac{p^2}{(\sqrt{p^2+m^2}+m)^3}\frac{m}{\sqrt{p^2+m^2}} \times \left(\frac{\Lambda^8}{(\Lambda^2+p^2)^4} - 1\right). \qquad (21)$$

Evaluation of this integral to the lowest order in m/Λ yields

$$\Delta P^{(C)} = \frac{35}{8}\pi\frac{m}{\Lambda}. \qquad (22)$$

As we noted above, the correction (22) cancels with the corresponding correction to the low-order term [see Eq. (14)]. For $\langle r^2\rangle^{1/2} = 0.862(12)$ fm [16], which corresponds to $\Lambda = \sqrt{12}/\langle r^2\rangle^{1/2} = 0.845 m_p = 793$ MeV, the formula (22) yields $\Delta P^{(C)} = 0.008\,86$ while the exact calculation of the integral

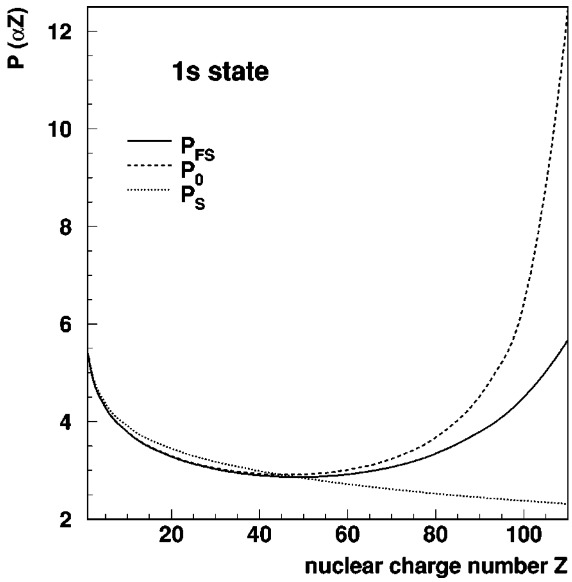

FIG. 1. The function $P_{FS}(\alpha Z)$, compared to $P_0(\alpha Z)$ and $P_S(\alpha Z)$.

(21) amounts to $\Delta P^{(C)}=0.008\,74$. These results are in good agreement with the corresponding result $[\Delta P=0.0092(2)]$ from Table II.

IV. DISCUSSION

In this work we have calculated the recoil correction to the ground-state energy of hydrogenlike atoms for extended nuclei in the range $Z=1$–110. This correction is conveniently written in the form

$$\Delta E=\frac{(\alpha Z)^2}{2M}+\frac{(\alpha Z)^5}{\pi}\frac{m^2}{M}P_{FS}(\alpha Z). \tag{23}$$

The function $P_{FS}(\alpha Z)=P(\alpha Z)+\Delta P_L(\alpha Z)$ is shown in Fig. 1. For comparison, the point-nucleus function $P_0(\alpha Z)$ and the Salpeter function $P_S(\alpha Z)$ are also presented in this figure. Table III displays the values of the recoil corrections (in eV) in the range $Z=10$–110.

In the case of hydrogen we find that the recoil correction amounts to $\Delta E=-7.2(2)$ kHz beyond the Salpeter contribution and the nonrelativistic nuclear size correction to the recoil effect [the first term in Eq. (10)]. It almost coincides with the point-nucleus result. This is caused by the fact that the nuclear size correction to the higher-order term [Eq. (22)] and the relativistic nuclear size correction to the low-order term [Eq. (14)] cancel each other.

For high Z, where the αZ expansion as well as the reduced mass approximation are not valid any more, we should not separate any contributions from the total recoil effect. In the case of hydrogenlike uranium ($^{238}U^{91+}$), the total recoil correction constitutes $\Delta E=\Delta E_L+\Delta E_H=0.46$ eV and is by 10% smaller than the corresponding point-nucleus value ($\Delta E_{\rm PN}=0.51$ eV) found in [9]. This improvement affects the current numbers of the Lamb shift prediction [17].

TABLE III. Recoil corrections in eV. For comparison, the nonrelativistic recoil correction is given separately. The last column displays the deviation from the point-nucleus results for the total recoil effect. The mass values are given in nuclear mass units. They were taken from [24], except for $Z=110$ where we adopted the value of [21].

Z	M/A	Nonrel. recoil	Total recoil	Finite size effect
10	20.2	0.037	0.037	
20	40.1	0.075	0.075	
30	65.4	0.104	0.105	
40	91.2	0.134	0.137	
50	118.7	0.163	0.171	
60	144.2	0.196	0.215	–0.001
70	173.0	0.227	0.269	–0.003
79	197.0	0.26	0.33	–0.01
80	200.6	0.26	0.34	–0.01
82	207.2	0.27	0.36	–0.01
90	232.0	0.30	0.44	–0.03
92	238.0	0.30	0.46	–0.05
100	257.1	0.34	0.61	–0.14
110	268.0	0.42	0.97	–0.75

Finally, we note a very significant amount of the nuclear size effect for $Z=110$. According to Table III, the finite nuclear size modifies the point-nucleus result by more than 40%.

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APPENDIX

Using the identity $\mathbf{p}^2=(\boldsymbol{\alpha}\cdot\mathbf{p})^2$, the Coulomb part of the low-order term can be written as

$$\Delta E_L^{(C)}=\left\langle a\left|\frac{p^2}{2M}\right|a\right\rangle=\frac{1}{2M}\langle a|(\varepsilon_a-\beta m-V)^2|a\rangle$$
$$=\frac{1}{2M}[\varepsilon_a^2+m^2+\langle a|(V^2-2\varepsilon_a V)|a\rangle$$
$$+2m\langle a|\beta(V-\varepsilon_a)|a\rangle]. \tag{A1}$$

As described in detail in [18], the Breit part of the low-order term can be transformed to

$$\Delta E_L^{(B)} = -\frac{1}{2M}\langle a|[\mathbf{D}(0)\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{D}(0)]|a\rangle$$
$$= -\frac{1}{2M}\left\langle a\left|\frac{\alpha Z}{r}\left(\boldsymbol{\alpha}+\frac{(\boldsymbol{\alpha}\cdot\mathbf{r})}{r^2}\right)\cdot\mathbf{p}\right|a\right\rangle$$
$$= -\frac{\alpha Z}{2M}\left\langle a\left|\frac{1}{r}\left(2\varepsilon_a-2\beta m-2V+\frac{i\kappa}{r}\alpha_r\beta\right)\right|a\right\rangle$$
$$= \frac{1}{2M}[2\alpha Z\langle a|V/r|a\rangle-2\alpha Z\varepsilon_a\langle a|1/r|a\rangle$$
$$+2\alpha Z\langle a|m\beta/r|a\rangle+2\kappa\alpha Z\int_0^\infty g_a f_a dr, \qquad (A2)$$

where $\alpha_r=(\boldsymbol{\alpha}\cdot\mathbf{r})/r$ and $\kappa=(-1)^{j+l+1/2}(j+1/2)$ is the relativistic angular quantum number of the state a. In the following we will use the notations of Ref. [7],

$$A^s=\int_0^\infty(G^2+F^2)r^s dr, \qquad (A3)$$

$$B^s=\int_0^\infty(G^2-F^2)r^s dr, \qquad (A4)$$

$$C^s=2\int_0^\infty GFr^s dr, \qquad (A5)$$

where $G/r=g$ and $F/r=f$ are the radial components of the Dirac wave function for the extended nucleus, and the radial scalar product defined by Eqs. (5)–(7). Using Eq. (2.9) of Ref. [7], we find

$$\Delta E_L=\frac{1}{2M}\{\varepsilon_a^2-m^2+\langle a|\delta V(\delta V-2\varepsilon_a)|a\rangle$$
$$-\alpha Z(\alpha ZA^{-2}-\kappa C^{-2}-2mB^{-1})\}, \qquad (A6)$$

where $\delta V=V-V_C=V+\alpha Z/r$. From Eqs. (2.8)–(2.10) of Ref. [7], one obtains

$$\alpha ZA^{-2}-\kappa C^{-2}=-2\kappa\langle a|\sigma_z\delta V/r|a\rangle+2m\langle a|\sigma_x\delta V|a\rangle, \qquad (A7)$$

$$2\alpha ZmB^{-1}=2(m^2-\varepsilon_a^2)+2(m+2\varepsilon_a\kappa)\langle a|\sigma_z\delta V|a\rangle$$
$$-4m\varepsilon_a\langle a|\sigma_x r\,\delta V|a\rangle. \qquad (A8)$$

Substituting Eqs. (A7) and (A8) into Eq. (A6), we find

$$\Delta E_L=\frac{m^2-\varepsilon_a^2}{2M}+\frac{1}{2M}\{\langle a|(\delta V)^2|a\rangle+2\alpha Z\kappa\langle a|\sigma_z\delta V/r|a\rangle$$
$$-2\varepsilon_a\langle a|\delta V|a\rangle+2(m+2\varepsilon_a\kappa)\langle a|\sigma_z\delta V|a\rangle$$
$$-2\alpha Zm\langle a|\sigma_x\delta V|a\rangle-4m\varepsilon_a\langle a|\sigma_x r\,\delta V|\rangle\}. \qquad (A9)$$

Separating the point-nucleus result from the right side of Eq. (A9), we get Eq. (4).

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