Calculation of the hyperfine structure constants in ^{43}Ca$^+$ and ^{87}Sr$^+$

Kai-zhi Yu,[1,2] Li-jin Wu,[1] Bing-cong Gou,[2] and Ting-yun Shi[1]

[1]*Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics,*
The Chinese Academy of Sciences, Wuhan 430071, People's Republic of China
[2]*Department of Applied Physics, Beijing Institute of Technology, Beijing 100081, People's Republic of China*
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A relativistic many-body calculation is performed for the low-lying states of the alkaline earth ions ^{43}Ca$^+$ and ^{87}Sr$^+$. The zeroth-order hyperfine structure constants are evaluated with Dirac-Fock wave functions, and the finite basis sets of the Dirac-Fock equation are constructed by *B* splines. With the finite basis sets, the core polarization and the correlation effect are calculated. The final results for ^{43}Ca$^+$ are $a(4S_{1/2})=-805.3$ MHz, $a(4P_{1/2})=-143.1$ MHz, $a(4P_{3/2})=-30.5$ MHz, $b(4P_{3/2})/Q=151.8$ MHz b^{-1}, $a(3D_{3/2})=-47.8$ MHz, $b(3D_{3/2})/Q=68.1$ MHz b^{-1}, $a(3D_{5/2})=-3.6$ MHz, and $b(3D_{5/2})/Q=100.2$ MHz b^{-1}. The results for ^{87}Sr$^+$ are $a(5S_{1/2})=-1003.2$ MHz, $a(5P_{1/2})=-178.4$ MHz, $a(5P_{3/2})=-35.1$ MHz, $b(5P_{3/2})/Q=274.3$ MHz b^{-1}, $a(4D_{3/2})=-47.4$ MHz, $b(4D_{3/2})/Q=118.2$ MHz b^{-1}, $a(4D_{5/2})=2.5$ MHz, and $b(4D_{5/2})/Q=169.5$ MHz b^{-1}.

I. INTRODUCTION

With the development of experimental studies of the new optical frequency standards, studies of the hyperfine structure have become more and more significant [1–3]. Now single trapped ions have come to play an important role as possible frequency standards, with several different candidate ions, such as ^{43}Ca$^+$ and ^{87}Sr$^+$ and so on. The property of the quadrupole transition in ^{43}Ca$^+$ is being studied at the Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics (People's Republic of China). In 2003, the hyperfine structure of the $^2S_{1/2}$-$^2D_{1/2}$ quadrupole transition at 674 nm in ^{87}Sr$^+$ was observed at the National Physical Laboratory of the United Kingdom [2], before which Martensson had applied many-body perturbation theory in the coupled-cluster formulation to perform a calculation of the hyperfine structure in the 4*d* states of Rb-like Sr [1]. The effective operator form of many-body perturbation theory was developed and applied to calculate hyperfine interactions by Garpman *et al.* [4,5]. An important task of a perturbative calculation is to carry out summations over all intermediate states. Lindgren and Morrison used a single-particle function and a pair function by solving inhomogeneous one- and two-particle equation [5] instead of the summations. However, in this work finite basis sets of the Dirac-Fock equation are constructed by *B* splines. With the finite basis sets, the core polarization and the correlation diagrams are calculated, and the hyperfine structure constants of the low-lying states of the alkaline earth ions ^{43}Ca$^+$ and ^{87}Sr$^+$ are evaluated.

II. THEORETICAL METHOD

For single-electron systems outside closed shells, the generalized hyperfine structure constants are [6]

$$A_K = \langle \gamma jj | T_0^K | \gamma jj \rangle M_0^K = \begin{pmatrix} j & K & j \\ -j & 0 & j \end{pmatrix} \langle \gamma j \| T^K \| \gamma j \rangle M_0^K. \quad (1)$$

For the magnetic-dipole hyperfine constant $K=1$, and for the electric quadrupole $K=2$. In the relativistic case, we get the traditionally used hyperfine constants

$$a = \frac{A_1}{Ij} = \frac{\mu_I}{Ij} \langle \gamma jj | T_0^1 | \gamma jj \rangle = \frac{\mu_I}{Ij} \begin{pmatrix} j & 1 & j \\ -j & 0 & j \end{pmatrix} \langle j \| T^1 \| j \rangle, \quad (2)$$

$$b = 4A_2 = 2Q \langle \gamma jj | T_0^2 | \gamma jj \rangle = 2Q \begin{pmatrix} j & 2 & j \\ -j & 0 & j \end{pmatrix} \langle j \| T^2 \| j \rangle, \quad (3)$$

where I, μ_I, Q, and j are the nuclear spin, magnetic-dipole moment, electric-quadrupole moment, and total angular momentum of the electrons, respectively. Also,

$$\langle \kappa \| T^1 \| \kappa' \rangle = -\alpha(\kappa + \kappa') \langle \kappa \| C^1 \| - \kappa' \rangle$$
$$\times \int \frac{(P_\kappa Q_{\kappa'} + Q_\kappa P_{\kappa'})}{r^2} dr, \quad (4)$$

$$\langle \kappa \| T^2 \| \kappa' \rangle = -\langle \kappa \| C^2 \| \kappa' \rangle \int \frac{(P_\kappa P_{\kappa'} + Q_\kappa Q_{\kappa'})}{r^3} dr, \quad (5)$$

where α is the fine structure constant, C^1 and C^2 are spherical tensors of ranks 1 and 2, P_κ and Q_κ are the large and small radial components of the Dirac-Fock single-particle wave functions, and κ is defined as

$$\kappa = l(l+1) - j(j+1) - \frac{1}{4}. \quad (6)$$

In order to evaluate second- and third-order perturbation diagrams, we need a complete set of single-particle states. We can construct a complete finite basis set of the Dirac-Fock equation by using *B* splines.

The relativistic Hamiltonian for an atomic system is given by

$$H = H_0 + V \quad (7)$$

with

$$H_0 = \sum_{i=1}^{N} [c\alpha_i p_i + (\beta_i - 1)c^2 + V_{nuc}(r_i)] + \sum_{i=1}^{N} u(r_i) \quad (8)$$

and

$$V = \sum_{i<j} \frac{1}{r_{ij}} - \sum_{i=1}^{N} u(r_i). \quad (9)$$

Then we expand the large and small component radial wave functions $P_\kappa(r)$ and $Q_\kappa(r)$ in terms of B splines of order k as

$$P_\kappa(r) = \sum_{i=1}^{n} p_i^{(\kappa)} B_{i,k}(r), \quad Q_\kappa(r) = \sum_{i=1}^{n} q_i^{(\kappa)} B_{i,k}(r). \quad (10)$$

Using the Galerkin method and the MIT-bag-model boundary condition, we obtain a $2n \times 2n$ symmetric generalized eigenvalue equation [7]

$$Av = \epsilon Bv, \quad (11)$$

where the $2n$ vector v is given by

$$v = (p_1, p_2, \ldots, p_n, q_1, q_2, \ldots, q_n), \quad (12)$$

and A is a symmetric $2n \times 2n$ matrix with the form

$$A = \begin{pmatrix} (V_d) + (V_{ex}^{PP}) & c[(D) - (\kappa/r)] + (V_{ex}^{PQ}) \\ -c[(D) + (\kappa/r)] + (V_{ex}^{PQ}) & (V_d) - 2c^2(C) + (V_{ex}^{QQ}) \end{pmatrix}$$
$$+ A'. \quad (13)$$

The details of other matrices, such as $B, A', (C), (D), (V_d)$, and (κ/r) can be found in Ref. [7], and
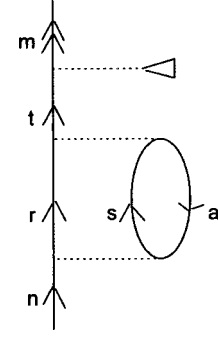

FIG. 1. One of the 65 lowest-order correlation diagrams.

$$(V_{ex})_{ij} = \int B_i(r) V_{ex}(r) B_j(r) dr, \quad (14)$$

where atomic units (a.u.) have been used in the above expression.

Using the above equations, we can construct the matrices A and B. Taking 50 B splines with order $k_B = 9$, we can solve the symmetric generalized eigenvalue equation (11) in a cavity of radius $R_B = 50$ a.u. So we can get the complete finite basis set of the Dirac-Fock equation. Details of B splines can be found in the book of deBoor [8]. Johnson *et al.* have applied the technique of constructing finite basis sets from B splines to calculate the hyperfine constants of the alkali metals ^{7}Li, ^{23}Na, ^{39}K, ^{85}Rb, and ^{133}Cs [9].

Following Lindgren and Morrison [5], the contribution of the core polarization to the hyperfine interaction can be calculated to all orders:

$$\Delta_{nj}^K = 2\sum_{ark} (-1)^{k+j_m+j_r-1}(2j+1)[(2j_r+1)(2j_a+1)]^{1/2} \left[(-1)^{(3j_a+j_r+K)}\frac{\delta(k,K)}{2K+1}\begin{pmatrix} j & k & j \\ -1/2 & 0 & 1/2 \end{pmatrix}\begin{pmatrix} j_r & k & j_a \\ -1/2 & 0 & 1/2 \end{pmatrix}R^k(mr,na) \right.$$

$$\left. - (-1)^{2j+K}\begin{pmatrix} j & k & j_a \\ -1/2 & 0 & 1/2 \end{pmatrix}\begin{pmatrix} j_r & k & j \\ -1/2 & 0 & 1/2 \end{pmatrix}\begin{Bmatrix} j & K & j \\ j_r & k & j_a \end{Bmatrix}R^k(mr,an) \right]\overline{h}_a^r, \quad (15)$$

$$(\varepsilon_a - \varepsilon_r)\overline{h}_a^{r(N)} = \langle r\|T^K\|a\rangle + \sum_{bsk} [G_1 X^k(rb,as) - G_2 X^k(br,as)]\overline{h}_a^{r(N-1)}, \quad (16)$$

and

$$\overline{h}_a^{r(0)} = \frac{\langle r\|T^K\|a\rangle}{\varepsilon_a - \varepsilon_r}, \quad (17)$$

where R^k is the relativistic Slater integral and

$$R^k(ab,cd) = \int\int \frac{r_<^k}{r_>^{k+1}}[P_a(r_1)P_c(r_1) + Q_a(r_1)Q_c(r_1)]$$
$$\times [P_b(r_2)P_d(r_2) + Q_b(r_2)Q_d(r_2)]dr_1 dr_2, \quad (18)$$

$$X^k(ab,cd) = (-1)^k \langle j_a\|C^k\|j_c\rangle\langle j_b\|C^k\|j_d\rangle R^k(ab,cd), \quad (19)$$

and

$$G_1 = (-1)^{3j_b+j_s+K}\frac{\delta(k,K)}{2K+1}, \quad G_2 = (-1)^{j_b+j_s+K}\begin{Bmatrix} j_r & K & j_a \\ j_b & k & j_s \end{Bmatrix}. \quad (20)$$

With Eqs. (15)–(17), we use an iterative procedure to carry out the core polarization to all orders.

Following Lindgren and Morrison, the diagrams involving at least one double excitation are called the lowest-order

TABLE I. Hyperfine structure constants a for different states of $^{43}Ca^+$ and $^{87}Sr^+$ (units of MHz).

Isotope	States	Our work	Other theory	Experiment
$^{43}Ca^+$	$4S_{1/2}$	−805.348	−819,[a] −794.7[b]	−797.5(2.4),[c] −805(2),[d] −817(15)[e]
	$4P_{1/2}$	−143.068	−148,[a] −144.8[b]	−158.0(3.3),[c] −145.5(1.0),[d] −142(8),[f] −145.4(0.1)[g]
	$4P_{3/2}$	−30.498	−30.9,[a] −29.3[b]	−29.7(1.6),[c] −31.9(0.2),[d] −31.0(0.2)[g]
	$3D_{3/2}$	−47.824	−52,[a] −49.4[b]	−48.3(1.6),[f] −47.3(0.2)[g]
	$3D_{5/2}$	−3.552	−5.2,[a] −4.2[b]	−3.8(0.6)[g]
$^{87}Sr^+$	$5S_{1/2}$	−1003.177	−1000[h]	−1000.5(1.0)[i]
	$5P_{1/2}$	−178.398	−177[h]	
	$5P_{3/2}$	−35.114	−35.3[h]	−36.0(0.4)[i]
	$4D_{3/2}$	−47.356	−46.7[h]	
	$4D_{5/2}$	2.507	1.1[h]	2.1743(14)[j]

[a]Reference [14].   [f]Reference [18].
[b]Reference [15].   [g]Reference [21].
[c]Reference [16].   [h]Reference [1].
[d]Reference [17].   [i]Reference [19].
[e]Reference [20].   [j]Reference [2].

correlations; these are third-order hyperfine diagrams. There are 65 such correlation diagrams. The algebraic expression for one of these diagrams is shown in Fig. 1; it is

$$
a_m^+ a_n^+ \sum_{rsta} \frac{\langle m|T_Q^K|t\rangle\langle ta|r_{12}^{-1}|rs\rangle\langle rs|r_{12}^{-1}|na\rangle}{(\varepsilon_m - \varepsilon_t)(\varepsilon_n + \varepsilon_a - \varepsilon_r - \varepsilon_s)}
$$

$$
= a_m^+ a_n^+ \sum_{rstak} \delta(j_t,j) \frac{(2j_r + 1)(2j_a + 1)(2j_s + 1)}{2k+1}
$$

$$
\times \begin{pmatrix} j & k & j_r \\ -1/2 & 0 & 1/2 \end{pmatrix}^2 \begin{pmatrix} j_a & k & j_s \\ -1/2 & 0 & 1/2 \end{pmatrix}^2
$$

$$
\times \frac{\langle m|T^K|t\rangle R^k(ta,rs)R^k(rs,na)}{(\varepsilon_m - \varepsilon_t)(\varepsilon_n + \varepsilon_a - \varepsilon_r - \varepsilon_s)}, \tag{21}
$$

where T_Q^K is the hyperfine operator. From this expression, we can see that the sums run over all the virtual states of r, s, and t as the well as core states of a. The two $3j$ symbols $\begin{pmatrix} j & k & j_r \\ -1/2 & 0 & 1/2 \end{pmatrix}$ and $\begin{pmatrix} j_a & k & j_s \\ -1/2 & 0 & 1/2 \end{pmatrix}$ give $|j-j_r| \leq k \leq j+j_r$ and $|j_a-j_s| \leq k \leq j_a+j_s$, $0 \leq j_r,j_s \leq \infty$, $j_t=j$. In the above expres-

sion, $j_m=j_n=j$; the total angular momentum for the valence state is used. For numerical calculation it is impossible to take j_r,j_s up to infinity. We can choose a finite value j_{max} as the maximum and let $j_r,j_s \leq j_{max}$. But how can we choose j_{max}? First we take a small positive floating number eps as the precision, and search using j_{try} to make the absolute value of the difference of the calculated results of the correlation diagram for two neighboring j_{try} less than eps. When we find such a j_{try}, we take this j_{try} as j_{max}.

In our program, we calculated all 65 such diagrams. In addition to the 65 diagrams, there are numerous second- and higher-order correlation diagrams, which are rather time consuming to evaluate and expected to be small [10]. Therefore, in order to estimate the effects of these diagrams, we have considered only a few of them rather than evaluating all of them explicitly. Estimated values based on their sizes and on the results of earlier work on Rb [11], Ba$^+$ [12], and Mg$^+$ [13] have been assumed in obtaining the final results. In order to get higher precision, we treated the atomic nuclei as Fermi nuclei, not point charges, in our calculations. We used the Gauss integral which has higher precision.

TABLE II. Hyperfine structure factors b for different states of $^{43}Ca^+$ and $^{87}Sr^+$.

Isotope	States	b/Q (MHz b^{-1})		b (MHz)	
		Our work	Other theory	Our work	Experiment
$^{43}Ca^+$	$4P_{3/2}$	151.798	155[a]	−6.7(1.4)	−6.7(1.4),[b] −6.9(1.7)[c]
	$3D_{3/2}$	68.067	68[a]	−3.0(0.6)	−3.7(1.9)[c]
	$3D_{5/2}$	100.208	97[a]	−4.4(0.9)	−3.9(6.0)[c]
$^{87}Sr^+$	$5P_{3/2}$	274.279	271[d]	88.5(5.4)	88.5(5.4)[e]
	$4D_{3/2}$	118.238	115[d]	38.2(2.3)	
	$4D_{5/2}$	168.513	160[d]	54.4(3.3)	49.11(6)[f]

[a]Reference [14].   [d]Reference [1].
[b]Reference [17].   [e]Reference [19].
[c]Reference [21].   [f]Reference [2].

TABLE III. Energy of the hyperfine interaction W_F at different F in the $3D_{5/2}$ state of ^{43}Ca$^+$ (units of MHz).

F	W_F of ^{43}Ca$^+$ in $3D_{5/2}$
1	38.302
2	32.459
3	23.224
4	10.029
5	−7.878
6	−31.441

TABLE IV. Energy intervals to $F=7$ in the $4D_{5/2}$ state of ^{87}Sr$^+$ (units of MHz).

F	Our work	Experiment[a]
2	−51.166	−44.126
3	−59.986	−52.336
4	−65.399	−57.553
5	−61.965	−54.867
6	−42.885	−38.138
7	0	0

[a]Reference [2].

III. RESULTS AND DISCUSSION

In this paper we evaluated the hyperfine structure constants for the low-lying states of ^{43}Ca$^+$ and ^{87}Sr$^+$. Our results are listed in Tables I and II.

Table I shows the comparison of our evaluated results and other theoretical results and experimental results. From Table I, we can see that the agreement between most of our results and the experimental results for ^{43}Ca$^+$ and ^{87}Sr$^+$ is better than 3%. Our results are also compatible with other theoretical work except for $3D_{5/2}$ of ^{43}Ca$^+$ and $4D_{5/2}$ of ^{87}Sr$^+$.

In Table II, we give out our calculated hyperfine structure b/Q values for ^{43}Ca$^+$ and ^{87}Sr$^+$. Our results are close to those of Ref. [14] and Ref. [1]. The size of the b values, of course, depends on the size of the nuclear quadrupole moment Q. However, there exists no experimental technique for determining nuclear quadrupole moments in a direct way. But with the experimental b values and our calculated b/Q values for the $4P_{3/2}$ state of ^{43}Ca$^+$ and the $5P_{3/2}$ state of ^{87}Sr$^+$, the nuclear quadrupole moments $Q(^{43}$Ca$)=-0.044(9)b$, $Q(^{87}$Sr$)=0.323(20)b$ are derived, and the uncertainties in parentheses are from the experimental uncertainties in $4P_{3/2}$ and $5P_{3/2}$, respectively. These values are compatible with $Q(^{43}$Ca$)=-0.043(9)b$ [17] and $Q(^{87}$Sr$)=0.327(24)b$ [1].

Using our values of $Q(^{43}$Ca$)=-0.044b$ and $Q(^{87}$Sr$)=0.323b$, the b constants of ^{43}Ca$^+$ and ^{87}Sr$^+$ are listed in column 5. And with the calculated values a and b, the energy

of the hyperfine interaction W_F in $D_{5/2}$ states can be derived in the following equation:

$$W_F = \frac{1}{2}a_{D_{5/2}}C + b_{D_{5/2}}\frac{\frac{3}{2}C(C+1) - 2I(I+1)J(J+1)}{2I(2I-1)2J(2J-1)},$$

where $C=F(F+1)-I(I+1)-J(J+1)$, and $a_{D_{5/2}}$ and $b_{D_{5/2}}$ are the two hyperfine structure constants. In the $3D_{5/2}$ state of ^{43}Ca$^+$ $I=\frac{7}{2}$, $J=\frac{5}{2}$ and in the $4D_{5/2}$ state of ^{87}Sr$^+$ $I=\frac{9}{2}$, $J=\frac{5}{2}$. The values of W_F in the $3D_{5/2}$ state of ^{43}Ca$^+$ are listed in Table III. From Table III, we can see that the order of the values W_F of ^{43}Ca$^+$ from maximum to minimum is the normal one, $F=1,2,3,4,5,6$. The energy intervals to $F=7$ in the $4D_{5/2}$ state of ^{87}Sr$^+$ are listed in Table IV, from which we can see that the order of the values W_F of ^{87}Sr$^+$ is $F=7,6,2,3,5,4$, which is compatible with the latest experiment [2]. The order of W_F is mainly determinate by the magnetic-dipole interaction, but if the magnetic-dipole interaction is too small, and the value of b/a is large enough, the order will be abnormal. For example, in the $4D_{5/2}$ state of ^{87}Sr$^+$, the magnetic-dipole constant a is abnormally small, so the order of W_F is abnormal. The different between our data and experiment in ^{87}Sr$^+$ is caused by the difference of a and b. Our data are a little larger than the experimental data, so

TABLE V. Contributions from different parts of the hyperfine operator to the a factors of ^{43}Ca$^+$ and ^{87}Sr$^+$ (units of MHz). H(1) is the Dirac-Fock contribution, H(2) complete polarization, H(3) the first-order correlation, and "total" is H(1) + H(2) + H(3). H(4) is the estimated second- and higher-order correlations, and "final" is total + H(4).

Isotope	States	H(1)	H(2)	H(3)	Total	H(4)	Final
^{43}Ca$^+$	$4S_{1/2}$	−588.933	−117.893	−101.790	−808.616	3.268	−805.348
	$4P_{1/2}$	−101.492	−22.742	−19.335	−143.569	0.501	−143.068
	$4P_{3/2}$	−19.646	−8.495	−2.454	−30.595	0.097	−30.498
	$3D_{3/2}$	−33.206	−0.619	−14.160	−47.985	0.161	−47.824
	$3D_{5/2}$	−14.144	18.204	−7.691	−3.631	0.079	−3.552
^{87}Sr$^+$	$5S_{1/2}$	−736.547	−135.887	−135.886	−1008.320	5.143	−1003.177
	$5P_{1/2}$	−121.576	−24.544	−33.023	−179.143	0.745	−178.398
	$5P_{3/2}$	−21.331	−11.078	−2.835	−35.244	0.130	−35.114
	$4D_{3/2}$	−31.126	−2.413	−13.978	−47.517	0.161	−47.356
	$4D_{5/2}$	−12.977	21.876	−6.459	2.440	0.067	2.507

TABLE VI. Contributions from different parts of the hyperfine operator to the b/Q factors of ^{43}Ca$^+$ and ^{87}Sr$^+$ (units of MHz b^{-1}). Notation is the same as in Table V.

Isotope	States	H(1)	H(2)	H(3)	Total	H(4)	Final
^{43}Ca$^+$	$4P_{3/2}$	96.890	41.020	14.365	152.275	−0.477	151.798
	$3D_{3/2}$	54.445	−2.922	16.808	68.331	−0.264	68.067
	$3D_{5/2}$	77.132	−3.456	26.961	100.637	−0.429	100.208
^{87}Sr$^+$	$5P_{3/2}$	165.747	80.173	29.367	275.287	−1.008	274.279
	$4D_{3/2}$	80.347	17.740	20.567	118.653	−0.415	118.238
	$4D_{5/2}$	110.040	26.267	32.773	169.080	−0.567	168.513

the intervals of energy are a little larger than the experimental ones, but the order is the same.

Tables V and VI show the contributions from different parts of the hyperfine operator to the final results for the hyperfine structure constants a and b/Q factors, respectively. From Table V, we can see that for the $3D_{5/2}$ of ^{43}Ca$^+$ and $4D_{5/2}$ of ^{87}Sr$^+$ the complete polarization is larger than for the other states and has the opposite sign. In particular, for the $4D_{5/2}$ state of ^{87}Sr$^+$, the final result is abnormally small and seems to be inverted because of the complete polarization. From Table VI, we can see that for P states the complete polarization effect is much larger than the correlation effect. But for $3D_{3/2}$ and $3D_{5/2}$ of ^{43}Ca$^+$, the complete polarization effect is much smaller than the correlation effect, and its value has the opposite sign. For $4D_{3/2}$ and $4D_{5/2}$ of ^{87}Sr$^+$, the complete polarization effect is close to the correlation effect. As mentioned above, in addition to the 65 lowest-order correlation diagrams, there are a large number of second- and

higher-order correlation diagrams, which are rather time consuming to evaluate; therefore, we have not evaluated them explicitly. We have considered only a few of them and listed the estimated values in column 7 of Tables V and VI in obtaining the final results for all states. From Tables V and VI, we can see that the estimated values have only a small effect on all the interaction constants except for the magnetic interaction ones in the D states, because the absolute value of the total magnetic interaction in D states is abnormally small, even much smaller than the lowest-order correlation contributions. We hope that our calculated results will be useful in future experiments.

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