

# Determination of the nuclear quadrupole moment of $^{87}\text{Sr}$

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A new nuclear quadrupole moment,  $Q=0.305(2)$  b, of  $^{87}\text{Sr}$  is determined by combining precise measurement of the electric quadrupole hyperfine structure constant of the  $4d\ ^2D_{5/2}$  state of its ion with calculation. This is a significant improvement over the previous values 0.335(20), 0.327(24), and 0.323(20) b. Relativistic coupled-cluster theory is employed in the calculations and electron correlation effects are included using the single, double, and an important subset of triple excitations. The magnetic dipole and electric quadrupole hyperfine structure constants of a few low-lying states are calculated to a high accuracy. The role of different electron correlation effects in the  $4d\ ^2D_{5/2}$  state is investigated.

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## I. INTRODUCTION

A significantly advanced level of the ion trapping and cooling technique has been employed to measure precisely the magnetic dipole and electric quadrupole hyperfine structure constants ( $A$  and  $B$ ) of the  $4d\ ^2D_{5/2}$  state in the singly ionized stable strontium ( $^{87}\text{Sr}^+$ ) [1]. Recently, the  $^2S_{1/2} \rightarrow ^2D_{5/2}$  transition frequency of  $\text{Sr}^+$  is proposed to be one of the best candidates for an optical frequency standard [2]. Knowledge of accurate  $A$  and  $B$  results of these states is essential for this purpose [3]. Accurate calculations of these results require precise values of the nuclear magnetic moment ( $\mu_I$ ) and quadrupole moment ( $Q$ ) and correct scale of atomic wave functions. It requires a powerful method to provide a correct scale of atomic wave functions that is capable of considering the relativistic and electron correlation effects rigorously. On the other hand, it is also possible to combine precisely the measured  $A$  and  $B$  results with accurately calculated  $A/\mu_I$  and  $B/Q$  results to determine  $\mu_I$  and  $Q$ , respectively. A precise  $\mu_I$  value is available for  $^{87}\text{Sr}$  [4], but the available  $Q$  values have large errors [5–7]. An accurate determination of  $Q$  has many applications in nuclear physics, e.g., it is used to obtain necessary information about local symmetry, magnetic properties, and to find out asymmetry parameters of the nucleus [8,9]. This can also be used to study the magnetic-field dependence of the dielectric properties inside the nuclei [10,11], in determination of electron quadrupole moment [12], and in studies of Mössbauer spectroscopy for the structural determination of the elements containing solid-state compounds [13].

Relativistic coupled-cluster (RCC) theory is referred to as a universal many-body theory [14]. It is successfully applied in atomic [15], molecular [16], and nuclear [17] physics to calculate both the ground- and excited-state properties. It is capable of considering the relativistic and correlation effects to all orders [14] and can be used for accurate calculations of atomic, molecular, nuclear, and subnuclear properties.

In the present work, we report an accurate value of the nuclear quadrupole moment ( $Q$ ) of  $^{87}\text{Sr}$  that is derived by

combining the calculated  $B/Q$  value using the RCC theory and the measured  $B$  value of the  $4d\ ^2D_{5/2}$  state of its ion [1]. Accuracy of the wave functions is verified by calculating  $A$  for the low-lying states. We use the new  $Q$  value to determine  $B$  for other states. We investigate the role of the electron correlation effects from the  $4d\ ^2D_{5/2}$  state results.

## II. THEORY AND METHOD OF CALCULATIONS

The magnetic dipole ( $A$ ) and electric quadrupole ( $B$ ) hyperfine structure constants are given by [18]

$$A = \mu_N g_I \frac{\langle J || \mathbf{T}^{(1)} || J \rangle}{\sqrt{J(J+1)(2J+1)}} \quad (2.1)$$

and

$$B = 2eQ \left\{ \frac{2J(2J-1)}{(2J+1)(2J+2)(2J+3)} \right\}^{1/2} \langle J || \mathbf{T}^{(2)} || J \rangle, \quad (2.2)$$

where  $g_I = \left[ \frac{\mu_I}{I} \right]$  with  $\mu_I$  and  $I$  are the nuclear dipole moment and spin, and  $\mu_N$  is the Bohr magneton.

Accurate calculations of  $A/g_I$  and  $B/Q$  require accurate calculations of the  $\langle J || \mathbf{T}^{(1)} || J \rangle$  and  $\langle J || \mathbf{T}^{(2)} || J \rangle$  elements, where  $\mathbf{T}$  operators are given elsewhere [18].

The many-body wave functions for the single valence ( $v$ ) system  $\text{Sr}^+$  using RCC theory can be expressed as [19]

$$|\Psi_v\rangle = e^T \{1 + S_v\} |\Phi_v\rangle, \quad (2.3)$$

where  $|\Phi_v\rangle$  is the open-shell Dirac-Fock (DF) wave function defined as  $|\Phi_v\rangle = a_v^\dagger |\Phi_0\rangle$  and  $|\Phi_0\rangle$  is the closed-shell DF wave function.  $T$  and  $S_v$  are the closed- and open-shell hole-particle excitation operators, respectively. The curly brackets represent the normal ordered form of the operators. In the singles and doubles (CCSD) approximation, the RCC operators are given by

$$T = T_1 + T_2 = \sum_{a,p} a_p^\dagger a_a^\dagger t_a^p + \frac{1}{4} \sum_{ab,pq} a_p^\dagger a_q^\dagger a_b a_a t_{ab}^{pq}, \quad (2.4)$$

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$$S_v = S_{1v} + S_{2v} = \sum_{p \neq v} a_p^\dagger a_v s_v^p + \frac{1}{2} \sum_{b,p,q} a_p^\dagger a_q^\dagger a_b a_v s_{vb}^{pq}, \quad (2.5)$$

where the  $(a, b, c, \dots)$  and  $(p, q, r, \dots)$  subscripts of the second quantized operators ( $a$ ) represent occupied (core) and unoccupied (particle) orbitals, respectively. The amplitudes  $t_a^p$  and  $t_{ab}^{pq}$  correspond to the single ( $T_1$ ) and double ( $T_2$ ) excitation operators in the closed shell and  $s_v^p$  and  $s_{vb}^{pq}$  to the single ( $S_{1v}$ ) and double ( $S_{2v}$ ) excitation operators involving  $v$ . The energy and RCC amplitudes in these closed-shell and single valence open-shell systems are obtained by

$$\langle \Phi^L | \{ \hat{H} e^T \} | \Phi_0 \rangle = E_0 \delta_{L,0}, \quad (2.6)$$

$$\begin{aligned} \langle \Phi_v^L | \{ \hat{H} e^T \} S_v | \Phi_v \rangle &= - \langle \Phi_v^L | \{ \hat{H} e^T \} | \Phi_v \rangle + \langle \Phi_v^L | S_v | \Phi_v \rangle E_v \delta_{L,0} \\ &= - \langle \Phi_v^L | \{ \hat{H} e^T \} | \Phi_v \rangle, \\ &+ \langle \Phi_v^L | S_v | \Phi_v \rangle \langle \Phi_v | \{ \hat{H} e^T \} \{ 1 + S_v \} | \Phi_v \rangle \delta_{L,0}, \end{aligned} \quad (2.7)$$

where the superscript  $L$  ( $=1, 2$ ) represents excited states from the corresponding DF states and the widehat symbol denotes connected terms.  $E_0$  and  $E_v$  are the energies for the closed-shell and open-shell states.  $\delta_{L,0}$  represents the Kronecker delta function, which is zero for  $L=0$ . The difference between  $E_0$  and  $E_v$  can give us the ionization potential energy of the valence electron,  $v$ .

We consider the Dirac-Coulomb-Breit Hamiltonian in the above equations, which is given by

$$\begin{aligned} H = [H_0] + [V_{es}] &= \sum_i^N \Lambda_i^+ [c \vec{\alpha}_i \cdot \vec{p}_i + (\beta_i - 1)c^2 + V_{\text{nuc}}(r_i) \\ &+ U(r_i)] \Lambda_i^+ + \left[ \sum_{i>j}^N \Lambda_i^+ \Lambda_j^+ V(r_{ij}) \Lambda_j^+ \Lambda_i^+ - \sum_i^N \Lambda_i^+ U(r_i) \Lambda_i^+ \right], \end{aligned} \quad (2.8)$$

where  $H_0$  is the DF Hamiltonian and  $V_{es}$  is the residual terms in atomic unit due to the Coulomb and Breit interactions  $[V(r_{ij})]$  given by

$$V(r_{ij}) = \frac{1}{r_{ij}} - \frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{r_{ij}} + \frac{1}{2} \left\{ \frac{\vec{\alpha}_i \cdot \vec{\alpha}_j}{r_{ij}} - \frac{(\vec{\alpha}_i \cdot \vec{r}_{ij})(\vec{\alpha}_j \cdot \vec{r}_{ij})}{r_{ij}^3} \right\},$$

and  $\Lambda^+$  are the projection operators onto the positive-energy states of the Dirac Hamiltonian in the nuclear  $[V_{\text{nuc}}(r_i)]$  and DF  $[U(r_i)]$  potentials.

We include leading-order triple excitations [CCSD(T)] in the calculation by constructing effective operators as [20]

$$S_{vbc}^{pqr} = \frac{V_{es} \hat{T}_2 + V_{es} \hat{S}_{v2}}{\epsilon_v + \epsilon_b + \epsilon_c - \epsilon_p - \epsilon_q - \epsilon_r}, \quad (2.9)$$

where  $\epsilon_i$  is the DF energy of the electron in the  $i$ th orbital. These operators are correlated with Eq. (2.7). We have given typical Goldstone diagrams representing these triple excitations in Fig. 1.

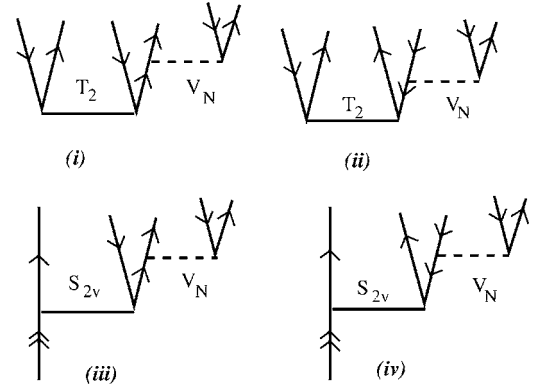


FIG. 1. Typical Goldstone diagrams representing leading-order triple excitations over the CCSD method. Double arrows in the diagrams represent valence electron  $v$ , and  $V_N$  is the normal order form of the residual interaction,  $V_{es}$ .

The expectation value of a Hermitian operator ( $O$ ) in the single valence states can be expressed as

$$\langle O \rangle = \frac{\langle \Psi_v | O | \Psi_v \rangle}{\langle \Psi_v | \Psi_v \rangle} = \frac{\langle \Phi_v | \{ 1 + S_v^\dagger \} e^{T^\dagger} O e^T \{ 1 + S_v \} | \Phi_v \rangle}{1 + N_v}, \quad (2.10)$$

where we define  $N_v = S_v^\dagger e^{T^\dagger} e^T S_v$ . In the CCSD (T) method, both  $e^{T^\dagger} O e^T$  and  $e^T e^T$  truncate naturally at effective five-body terms while expanding this expression using Wick's generalized theorem [21]. Since these operators have to finally connect with  $S_v$  operators, only up to three-body terms contribute to the calculations. We consider all possible effective one-body  $[\bar{O} = (e^{T^\dagger} O e^T)_{\text{one}}]$  terms from the following expressions:

$$\begin{aligned} \bar{O} \simeq O + OT_1 + T_1^\dagger O + OT_2 + T_2^\dagger O + T_1^\dagger OT_1 + T_1^\dagger OT_2 \\ + T_2^\dagger OT_1 + T_2^\dagger OT_2. \end{aligned} \quad (2.11)$$

We include effective two-body terms only from

$$e^{T^\dagger} O e^T \simeq OT_1 + T_1^\dagger O + OT_2 + T_2^\dagger O. \quad (2.12)$$

The justification for neglecting other terms from the above expansions is discussed in the next section by calculating contributions from some of the important immediate leading-order diagrams.

Contributions from the normalization factors are given by

$$\text{Normalization Factors} = \langle \Psi_v | O | \Psi_v \rangle \left\{ \frac{1}{1 + N_v} - 1 \right\}. \quad (2.13)$$

### III. RESULTS AND DISCUSSIONS

The orbitals are constructed as linear combinations of Gaussian type orbitals (GTOs) of the form [22]

TABLE I.  $A$  and  $B/Q$  results in  $^{87}\text{Sr}^+$ .

	$A$ (MHz)		$B/Q$ (MHz b $^{-1}$ )
	Calculation	Experiment	
$5s^2S_{1/2}$	-1001.203 <sup>a</sup>	-1000.5(1.0) <sup>e</sup>	
	-1003.177 <sup>b</sup>	-1000.473673(11) <sup>f</sup>	
	-1000 <sup>c</sup>	-990 <sup>g</sup>	
	-987 <sup>d</sup>	-993.5 <sup>h</sup>	
		-1000.5 <sup>i</sup>	
$5p^2P_{1/2}$	-176.561 <sup>a</sup>		
	-178.389 <sup>b</sup>		
	-177 <sup>c</sup>		
$5p^2P_{3/2}$	-35.596 <sup>a</sup>	-36.0(0.4) <sup>i</sup>	272.955 <sup>a</sup>
	-35.114 <sup>b</sup>		274.279 <sup>b</sup>
	-35.3 <sup>c</sup>		271 <sup>c</sup>
$4d^2D_{3/2}$	-45.604 <sup>a</sup>		116.108 <sup>a</sup>
	-47.356 <sup>b</sup>		118.238 <sup>b</sup>
	-46.7 <sup>c</sup>		115 <sup>c</sup>
$4d^2D_{5/2}$	2.145 <sup>a</sup>	2.1743(14) <sup>c</sup>	161.201 <sup>a</sup>
	2.507 <sup>b</sup>		168.513 <sup>b</sup>
	1.1 <sup>c</sup>		160 <sup>c</sup>

<sup>a</sup>This work.<sup>b</sup>[6].<sup>c</sup>[7].<sup>d</sup>[24].<sup>e</sup>[1].<sup>f</sup>[25].<sup>g</sup>[26].<sup>h</sup>[27].<sup>i</sup>[28].

$$F_{i,k}(r) = r^k e^{-\alpha_i r^2}, \quad (3.1)$$

where  $k=0, 1, \dots$  for  $s, p, \dots$  type orbital symmetries, respectively. For the exponents, we use the even tempering condition as

$$\alpha_i = \alpha_0 \beta^{i-1}. \quad (3.2)$$

In our earlier work it was found that GTOs are able to produce accurate hyperfine structure constants in different sizes of systems [20,23]. For the present system we consider  $30s_{1/2}$ ,  $25p_{1/2}$ ,  $25p_{3/2}$ ,  $25d_{3/2}$ ,  $25d_{5/2}$ ,  $20f_{5/2}$ ,  $20f_{7/2}$ ,  $20g_{7/2}$ , and  $20g_{9/2}$  GTOs. The  $\alpha_0$  and  $\beta$  values are considered to be 0.00525 and 2.73, respectively, for all the symmetries. All core electrons are activated in the RCC calculations.

We present our calculated  $A$  and  $B/Q$  values of  $^{87}\text{Sr}^+$  in Table I. We use  $g_I = -0.24283$  [4] to calculate  $A$ . Our results are compared with the available experimental results and other calculations. In the paper by Yu *et al.*, they have considered only the lowest-order relativistic many-body pertur-

TABLE II. Breit contributions to the  $A$  and  $B/Q$  in MHz and MHz b $^{-1}$ , respectively.

	$5s^2S_{1/2}$	$5p^2P_{1/2}$	$5p^2P_{3/2}$	$4d^2D_{3/2}$	$4d^2D_{5/2}$
$A$	-1.799	-0.665	0.017	-0.138	-0.009
$B/Q$			-0.305	-0.017	-0.090

TABLE III. Break down of the RCC contributions to the  $4d^2D_{5/2}$  state hyperfine structure constants calculation.

RCC terms	$4d^2D_{5/2}$	
	$A$ (MHz)	$B/Q$ (MHz b $^{-1}$ )
$O$ (DF)	-13.006	110.231
$O-\bar{O}$	-0.491	7.781
$\bar{O}S_{1v} + \text{c.c.}$	-2.292	19.259
$\bar{O}S_{2v} + \text{c.c.}$	18.885	27.016
$S_{1v}^\dagger \bar{O}S_{1v}$	-0.101	0.817
$S_{1v}^\dagger \bar{O}S_{2v} + \text{c.c.}$	0.848	0.319
$S_{2v}^\dagger \bar{O}S_{2v} + \text{c.c.}$	-1.696	-1.585
Important effective two-body terms		
$S_{2v}^\dagger OT_1 + \text{c.c.}$	0.023	-0.188
$S_{2v}^\dagger OT_2 + \text{c.c.}$	0.016	-0.134
Norm.	-0.037	-2.649

bation theory (RMBPT) in their calculations [6], in contrast to our RCC theory. Mårtensson's calculations are based on DF ( $O$ ) and a variant of many-body theories [7] to our *ab initio* method. The DF results of Mårtensson's work are almost the same as ours. The difference between these two results could be due to the fact that Mårtensson's calculations omit Breit interaction and use a different method. In Table II, we give Breit interaction contributions to the  $A$  and  $B/Q$  results of various states. Yaun *et al.* have also calculated  $A$  for the the ground state using RMBPT [24].

From Table I, it is clear that our results are very close to the experimental results. This demonstrates the power of the RCC method to produce accurate results. In our earlier work, we found that the  $d$  states are strongly affected by the core electrons [20]. Therefore, it is difficult to calculate the  $4d^2D_{5/2}$  state accurately. This would require us to include core-polarization effects to all orders. It is known that the RCC theory can incorporate core-polarization effects to all orders [20,23]. We give a breakdown of the contributions in Table III from different RCC terms representing various correlation effects to the total calculated  $A$  and  $B/Q$  results of the  $4d^2D_{5/2}$  state and investigate the role of different correlation effects in this state. We find from this table that contributions from  $\bar{O}S_{2v}$ , which at the lowest order corresponds to a core-polarization effect [20,23], play a crucial role in determining the final results. The DF and  $\bar{O}S_{2v}$  contributions have opposite sign and the latter is larger than the former. Contributions from all other RCC terms are comparatively small. This justifies our argument of how strongly the  $d$  states interact with the core electrons in this system. We show all order Goldstone diagrams representing core-polarization effects in Fig. 2.

A couple of experiments have been carried out to measure the  $A$  and  $B$  values in this system [1,25–28]. Among them, Sunaoshi *et al.* have measured the  $A$  of the ground state ( $5s^2S_{1/2}$ ) very precisely using the ion-trap technique with laser-microwave double resonance spectroscopy [25]. Barwood *et al.* have also measured  $A$  for the  $5s^2S_{1/2}$  state and  $A$

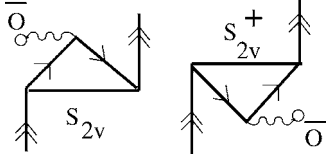


FIG. 2. Goldstone diagrams representing all order core-polarization effects from  $\bar{O}S_{2v}$ .

and  $B$  for the  $4d^2D_{5/2}$  state very accurately using a Paul trap and cooled technique [1].

The nuclear  $Q$  value can be obtained by measuring the coupling constant due to the electric-field gradient at the nucleus and accounting Sternheimer corrections [29]. As mentioned before, it can also be determined by combining a precise measured  $B$  and accurately calculated  $B/Q$  results. In Table IV, we present experimental  $B$  results of the  $5p^2P_{3/2}$  and  $4d^2D_{5/2}$  states. Among them, the  $B$  result of the  $4d^2D_{5/2}$  state is measured to an accuracy of 0.1%. Combining this result with our  $B/Q$  result of the same state, we obtain  $Q = 0.305b$ . We calculate  $B$  in other states by substituting this new value of  $Q$ , and these are given in the same table. It shows that our calculated  $B$  value of the  $5p^2P_{3/2}$  state is within the uncertainty of the available experimental result.

The error in this method arises from the exclusion of higher-order excitations by the CCSD(T) method and suppressed terms from Eq. (2.10). We attempt to verify systematically contributions from the lowest-order triple and quadruple excitations and we would like to estimate possible errors in the determination of  $Q$ . In a recent work, Porsev and Derevianko [30] have shown that for some systems the effect of triple excitations of fourth order in the residual interaction,  $V_{es}$ , plays a significant role in the linearized CCSD (lin-CCSD) method. Indeed, most of these triple excitations have been taken into account in the evaluation of the CCSD amplitudes through the nonlinear terms of Eq. (2.7). A certain class of triple excitations to the CCSD method have been considered using the CCSD(T) approach through Eq. (2.9). The difference of the CCSD and CCSD(T) results at linearized and nonlinearized methods may give a signature of the importance of the contributions of these triple excitations. We present these results for  $A$  and  $B/Q$  of the  $4d^2D_{5/2}$  state of  $^{87}\text{Sr}^+$  in Table V. Again, we try to construct more triple excitations in the following way for better understanding of these effects in the present system. As discussed by Sur *et al.* [31], it is possible to obtain more accurate leading-order triple and quadruple excitations than the CCSD(T) method by constructing a singles and doubles unitary coupled-cluster [UCCSD(T)] method. We consider all these extra diagrams in the lowest order for the calculations of the hyperfine structure constants of the  $4d^2D_{5/2}$  state of  $^{87}\text{Sr}^+$ ,

TABLE IV. Comparison of experimental and our calculated  $B$  results in MHz. New  $Q$  value is used to calculate  $B$ .

	$5p^2P_{3/2}$	$4d^2D_{3/2}$	$4d^2D_{5/2}$
Experiment	88.5(5.4)[28]		49.11(6)[1]
This work	83.251	35.413	49.166

TABLE V. Estimation of contributions from the leading-order triple excitations to the CCSD(T) method in the  $4d^2D_{5/2}$  state of  $^{87}\text{Sr}^+$  hyperfine interactions. Here we use the notation lin-CCSD(T) for the linearized CCSD(T) method.

	lin-CCSD	lin-CCSD(T)	CCSD	CCSD(T)
$A$ (MHz)	0.889	0.892	2.141	2.145
$B/Q$ (MHz $b^{-1}$ )	169.568	169.597	161.174	161.201

and some of the corresponding Goldstone diagrams are shown in Fig. 3 (i)–(iv). These contributions to the  $A$  and  $B/Q$  results are 0.045 MHz and 0.342 MHz  $b^{-1}$ , respectively. We consider total contributions from these methods to the hyperfine structure constant calculations of the  $4d^2D_{5/2}$  state as the maximum possible source of error in the CCSD(T) method. We also find separately contributions from some of the neglected leading higher-order diagrams from Eq. (2.10), which are shown in Fig. 3 (v)–(vi) with their exchange diagrams, and we consider this as a second possible source of error. Contributions from these diagrams to the  $A$  and  $B/Q$  of the  $4d^2D_{5/2}$  state in  $^{87}\text{Sr}^+$  are 0.002 MHz and 0.007 MHz  $b^{-1}$ , respectively. These results also justify the truncation of the exponential form given in Eqs. (2.11) and (2.12) for the present calculations and save a lot of computational time. By considering the quadrature formula of the maximum possible errors from the calculation and systematic error present in the experimental result of  $B$ , we obtain the  $Q$  value of  $^{87}\text{Sr}$  precisely as 0.305(2).

We also give other estimated results of the  $Q$  value in Table VI. Heider and Brink have determined  $Q$  by using an

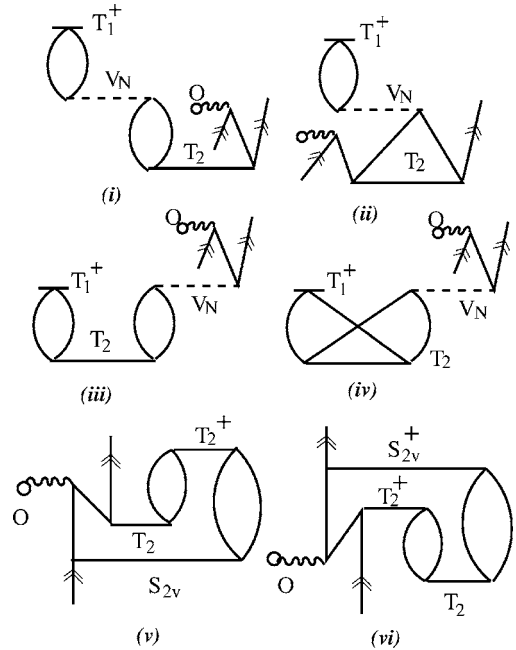


FIG. 3. Some of the important Goldstone diagrams considered to account for errors: (a) diagrams (i)–(iv) and their complex conjugate (c.c.) diagrams are the typical higher-order contributions to the CCSD (T) method and (b) diagrams (v)–(vi) are the leading-order diagrams of those that are neglected in the property calculations.

TABLE VI.  $Q$  value from various works in barn (b).

Heider and Brink [5]	Yu <i>et al.</i> [6]	Mårtensson [7]	This work
0.335(20)	0.323(20)	0.327(24)	0.305(2)

antishielding correction estimated by Sternheimer [5]. Both Mårtensson and Yu *et al.* have calculated this quantity using their  $B/Q$  results with an old experimental  $B$  result of the  $5p\ ^2P_{3/2}$  state, which has a large systematic error. They also do not give the uncertainty in their calculations.

#### IV. CONCLUSION

We employ the RCC theory to study both the magnetic dipole and electric quadrupole hyperfine structure constants

very accurately in the singly ionized stable isotope of strontium. It shows the power of the method to incorporate correlation effects and the potential to produce accurate results. We obtain an accurate value of the nuclear quadrupole moment,  $Q=0.305(2)$ , of  $^{87}\text{Sr}$  by combining a precise experimental result of its ion with our sub-1% calculation.

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- [1] G. P. Barwood, K. Gao, P. Gill, G. Huang, and H. A. Klein, *Phys. Rev. A* **67**, 013402 (2003).
- [2] G. P. Barwood, G. Huang, H. A. Klein, P. Gill, and R. B. M. Clarke, *Phys. Rev. A* **59**, R3178 (1999).
- [3] W. Itano, *J. Res. Natl. Inst. Stand. Technol.* **105**, 829 (2000).
- [4] L. Olschewski, *Z. Phys.* **249**, 205 (1972).
- [5] S. M. Heider and G. O. Brink, *Phys. Rev. A* **16**, 1371 (1977).
- [6] K. Z. Yu, L. J. Wu, B. C. Gou, and T. Y. Shi, *Phys. Rev. A* **70**, 012506 (2004).
- [7] A Mårtensson-Pendrill, *J. Phys. B* **35**, 917 (2002).
- [8] For instance, see *Proceedings of the 12th International Conference on Hyperfine Interactions*, edited by W. E. Evenson, H. Jaeger, and M. O. Zacate [Hyperfine Interact. 136/137 (2001)].
- [9] G. Scatz and A. Weidinger, *Nuclear Condensed Matter Physics—Nuclear Methods and Applications*, (Wiley, Chichester, England, 1996), p. 63.
- [10] P. Nagel, A. Fleischmann, S. Hunklinger, and C. Enss, *Phys. Rev. Lett.* **92**, 245511 (2004).
- [11] A. Würger, A. Fleischmann, and C. Enss, *Phys. Rev. Lett.* **89**, 237601 (2002).
- [12] T. Kiyama and M. Itoh, *Phys. Rev. Lett.* **91**, 167202 (2003).
- [13] G. Martinez-Pinedo, P. Schwerdtfeger, E. Caurier, K. Langanke, W. Nazarewicz, and T. Sohnel, *Phys. Rev. Lett.* **87**, 062701 (2001).
- [14] R. F. Bishop and H. G. Kuemmel, *Phys. Today* **40**(3), 52 (1987).
- [15] B. P. Das, K. V. P. Latha, B. K. Sahoo, C. Sur, R. K. Chaudhuri, and D. Mukherjee, *J. Theor. Comput. Chem.* **4**, 1 (2005).
- [16] U. Kaldor, *J. Chem. Phys.* **87**, 467 (1987); **87**, 4693 (1987).
- [17] K. Kowalski, D. J. Dean, M. Hjorth-Jensen, T. Papenbrock, and P. Piecuch, *Phys. Rev. Lett.* **92**, 132501 (2004).
- [18] K. T. Cheng and W. J. Childs, *Phys. Rev. A* **31**, 2775 (1985).
- [19] D. Mukherjee and S. Pal, *Adv. Quantum Chem.* **20**, 281 (1989).
- [20] B. K. Sahoo, T. Beier, B. P. Das, R. K. Chaudhuri, and D. Mukherjee, *J. Phys. B* **39**, 355 (2006) and references therein.
- [21] I. Lindgren and J. Morrison, *Atomic Many-Body Theory*, edited by G. Ecker, P. Lambropoulos, and H. Walther (Springer-Verlag, Berlin, 1985).
- [22] R. K. Chaudhuri, P. K. Panda, and B. P. Das, *Phys. Rev. A* **59**, 1187 (1999).
- [23] B. K. Sahoo, R. K. Chaudhuri, B. P. Das, H. Merlitz, and D. Mukherjee, *Phys. Rev. A* **72**, 032507 (2005).
- [24] X. Yuan, S. N. Panigrahy, R. W. Dougherty, T. P. Das, and J. Andriessen, *Phys. Rev. A* **52**, 197 (1995).
- [25] H. Sunaoshi *et al.*, *Hyperfine Interact.* **78**, 241 (1993).
- [26] R. Beigang, W. Makat, A. Timmermann, and P. J. West, *Phys. Rev. Lett.* **51**, 771 (1983).
- [27] K. T. Lu, J. Q. Sun, and R. Beigang, *Phys. Rev. A* **37**, 2220 (1988).
- [28] F. Buchinger *et al.*, *Phys. Rev. C* **41**, 2883 (1990); **42**, 2754 (1990).
- [29] D. Sundholm and J. Olsen, *Phys. Rev. Lett.* **68**, 927 (1992).
- [30] S. G. Porsev and A. Derevianko, *Phys. Rev. A* **73**, 012501 (2006).
- [31] C. Sur, R. K. Chaudhuri, B. K. Sahoo, B. P. Das, and D. Mukherjee, e-print physics/0502033.