Correlation trends in the nuclear anapole moment interaction of the Be atom in BeCl

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The parity-violating nuclear anapole moment effect can be used as a tool to test nuclear models and gain deep understanding of nuclear structure. Diatomic molecules such as BeCl are considered as good candidates in search for the nuclear anapole moment effect, because such molecules have close-lying molecular levels with opposite parity, where degeneracy can very easily occur in external fields, leading to a dramatic amplification of the tiny parity-violating effect. In order to interpret the results of precision measurements effectively, a parity-violating interaction parameter W_A, which depends on molecular structure, needs to be calculated with high-accuracy. In this work, the calculations of the W_A parameter for the Be atom in BeCl are carried out with various electron correlation approaches such as the open-shell single determinant average-of-configuration Dirac-Hartree-Fock (DHF), the relativistic density functional theory (DFT), the second-order Møller-Plesset method (MP2), the relativistic coupled cluster method with single, double, and perturbative triple excitation, namely CCSD and CCSD(T). The influence of electron correlations on the calculated W_A parameter is investigated and discussed.

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1. Introduction

The nuclear anapole moment interaction is first proposed by Zel'dovich [1]. It is one of the three main sources accounting for the nuclear spin dependent parity violating (NSDPV) effects [2], and comes from the interaction between the electromagnetic current and the nuclear weak current [3]. The effective Hamiltonian, which describes the nuclear anapole moment interaction, takes the following form [4, 5, 6],

$$H_A \equiv \frac{\kappa_A G_F}{\sqrt{2}} \left(\boldsymbol{\alpha} \cdot \hat{\boldsymbol{I}} \right) \rho(\mathbf{r}) \tag{1.1}$$

where $\rho(\boldsymbol{r})$ is the nuclear density distribution, G_F is the Fermi weak interaction constant [7], $\hat{\boldsymbol{I}}$ is the unit vector along the nuclear spin, and $\boldsymbol{\alpha}$ are the Dirac matrices. κ_A is a dimensionless effective coupling constant, which describes the magnitude of the nuclear anapole moment interaction.

The nuclear anapole moment effect has been observed in the ^{133}Cs atom [8, 9]. Some measurements have also been proposed on other atoms, such as ^{137}Ba [10], ^{163}Dy [11], ^{171}Yb [12], and ^{212}Fr [13]. In diatomic molecules with a $^2\Sigma_{1/2}$ ground state, the effect is strongly enhanced because of close-lying molecular levels with opposite parity, where degeneracy can be very easily occur in external fields, leading to a dramatic amplification of the tiny parity-violating effect [14]. Recently, measurements with improved sensitivity were demonstrated for the BaF molecule [15, 16], and the corresponding theoretical investigations for BaF as well as its homologues have also been carried out [10, 17, 18, 19, 20, 21].

The BeCl molecule has a $^2\Sigma_{1/2}$ ground state, and is considered as a promising candidate in search for the nuclear anapole moment effect. For $^2\Sigma_{1/2}$ ground state, Eq. (1.1) can be written as follows [5, 10],

$$H_A = \kappa_A W_A \hat{\boldsymbol{I}} \cdot \left(\hat{\boldsymbol{n}} \times \boldsymbol{S}_{eff} \right) \tag{1.2}$$

where $\boldsymbol{S}_{eff}$ stands for the effective spin of the open-shell electron, and $\hat{\boldsymbol{n}}$ is the unit vector along the molecular axis.

The effective coupling constant κ_A can be obtained both experimentally and theoretically. On the one hand, κ_A can be determined by measuring parity-violating transitions in atoms or molecules when the parameter W_A is known. On the other hand, κ_A can also be calculated directly from nuclear theories. For instance, κ_A takes the following form in a nuclear model [4, 5, 6],

$$\kappa_A \simeq 1.15 \times 10^{-3} (-1)^{I-l+\frac{1}{2}} \left(\frac{I+1/2}{I+1} \right) \mu g A^{\frac{2}{3}} \tag{1.3}$$

where l is the orbital angular momentum of the unpaired valence nucleon, g is a weak interaction coupling constant with values of around 4.6 [4] and 1 [22] for proton and neutron respectively, μ is the nuclear magnetic moment, and A is the total number of nucleons in the nucleus.

From experimental point of view, the parameter W_A needs to be known with high accuracy so that the effective coupling constant κ_A can be obtained precisely from the measured signals. The determined κ_A from experiments can be compared with the predicted values from theories. Any deviation may suggest the incompleteness of the current nuclear models.

The nuclear anapole moment interaction is only present in atoms or molecules with unpaired nucleons and unpaired electrons. Due to the scaling factor in Eq. (1.3), it is the dominating contribution to the NSDPV effects in atoms or molecules containing heavy elements [2]. However, in light molecules, the observed NSDPV signals may come from all three sources, and it is possible to distinguish the nuclear anapole moment signal from the rest NSDPV signals by measuring different nuclei [23].

The W_A parameter, which depends on the electronic structure of the atoms or molecules, is defined by the following expression [24],

$$W_A \equiv \frac{G_F}{\sqrt{2}} \langle +\tfrac{1}{2} | \rho(\mathbf{r}) \alpha_+ | -\tfrac{1}{2} \rangle \tag{1.4}$$

with

$$\alpha_+ = \alpha_x + i\alpha_y = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} + i \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}. \tag{1.5}$$

Here, σ_x and σ_y represent the Pauli matrices, and $|\pm\tfrac{1}{2}\rangle$ are two Ω-states. The W_A parameter cannot be measured and can only be calculated using theoretical molecular method. In Sec. **2**, the calculations of the W_A parameter for the beryllium atom in BeCl will be discussed in more detail.

2. Method and computational details

In order to calculate the W_A parameter with high accuracy, we need to take into account the following three main factors: Hamiltonian, basis sets, and electron correlation treatments. To begin with, we need to include relativistic effect into our calculations so that high accuracy is assured. Furthermore, for a good description of the electronic wave functions, large basis sets should be employed. More importantly, since electron correlations, which describe the instantaneous interaction among electrons, are crucial in determination of molecular properties, it should be treated properly in high-accuracy calculations. In this work, we carry out the calculations using various approaches treating electron correlations on different levels and compare their influence on the calculated W_A parameter.

We carry out the calculations using the developer's version of the DIRAC package [25] throughout this work. With respect to the treatment of relativistic effect, the following (relativistic) Dirac-Coulomb Hamiltonian is employed,

$$H_0 = \sum_i [c\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + \beta_i mc^2 + V(r_i)] + \sum_{i<j} \frac{1}{r_{ij}}. \tag{2.1}$$

Here, the Coulomb potential takes into account the finite size of the nuclei, modeled by a Gaussian type distribution [26].

In order to have a good description of the electronic wave functions, we use Dyall's relativistic standard basis sets [27, 28]. Throughout this work, all the calculations are performed using the dyall.v4z basis set [27, 28] at the experimental equilibrium bond length (1.7971 angstrom) [29].

In order to further investigate the influence of electron correlation on the calculated W_A parameter, various electron correlation approaches are employed. We first carry out the calculation

using the open-shell single determinant average-of-configuration Dirac-Hartree-Fock (DHF) [30] method, which does not include electron correlation effects. The relativistic density functional theory (DFT) [31] does not treat electron correlation in a robust way, and in order to further test the performance of the DFT method, we perform the calculations with various functionals, such as the Slater local exchange (SVWN5) functional [32], Perdew-Burke-Ernzerhof (PBE) functional [33, 34], the Becke-Lee-Yang-Parr hybrid functional (B3LYP) [35, 36, 37] and its adapted version (CAMB3LYP*) [38, 39]. Finally, we perform the calculations using the second-order Møller-Plesset (MP2) method [40] and the relativistic coupled cluster method [41]. The relativistic coupled cluster method is considered as the state-of-the-art method in electron correlation treatment. In this work, we employ the relativistic coupled cluster method with single, double, and perturbative triple excitation, namely CCSD and CCSD(T) [41]. The nuclear anapole moment interaction is perturbatively added to the coupled cluster calculations using a finite field (FF) approach [21, 42, 43]. In the coupled cluster calculations, the virtual energy cut-off is 500 a.u. and all the electrons are included into correlation treatment. The calculated W_A parameters (in units of Hz) for the Be atom in the BeCl molecule using various methods such as DHF, DFT, MP2, CCSD, and CCSD(T) are presented in Tab. 1 and in Fig. 1.

3. Results and conclusions

Tab. 1 summarizes the calculated W_A parameters for the Be atom in BeCl using various methods such as DHF, DFT, MP2, CCSD, and CCSD(T). As can be seen from Tab. 1 and Fig. 1, the calculated W_A parameters (Hz) tend to be higher from top to bottom, where the electron correlation treatment is steadily improving. The parameter Δ, which describes the relative contributions from the electron correlations, is defined as follows,

$$\Delta = \frac{100\left(Corr - DHF\right)}{DHF}. \tag{3.1}$$

Here, *Corr* represents the calculated results from various electron correlation methods, and *DHF* represents the calculated result from the DHF method. The DHF method does not incorporate

Methods	W_A (Hz)	Δ%
DHF	0.3961	0.0%
DFT(CAMB3LYP*)	0.3973	0.3%
DFT(B3LYP)	0.4138	4.5%
DFT(PBE)	0.4245	7.2%
DFT(SVWN5)	0.4282	8.1%
MP2	0.4626	16.8%
CCSD	0.4847	22.4%
CCSD(T)	0.4822	21.7%

Table 1: Calculated W_A parameters (Hz) for the Be atom in BeCl at the equilibrium bond length using various electron correlation methods.
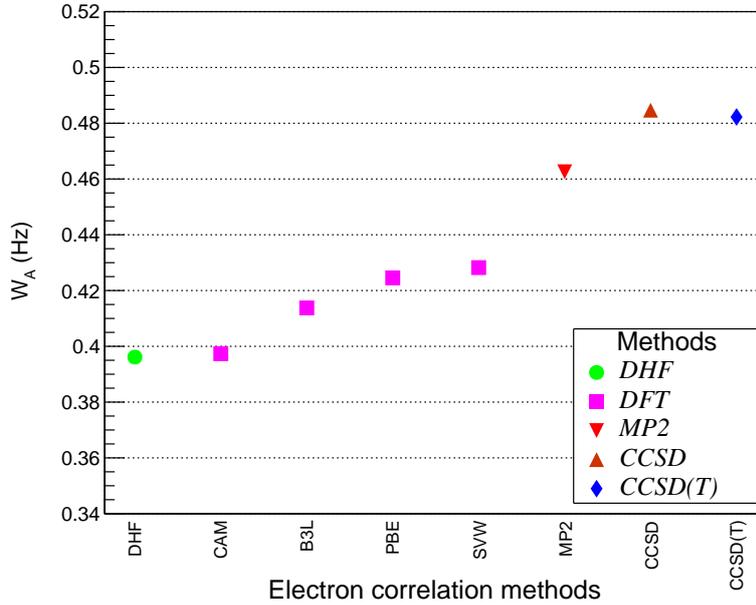
Figure 1: Calculated W_A parameters (Hz) for the Be atom in BeCl at the equilibrium bond length using various electron correlation methods.

the electron correlation effect while the CCSD(T) is considered as the state-of-the-art method in dealing with electron correlations. A direct comparison between the DHF and the CCSD(T) results suggests that electron correlation effect contributes to the nuclear anapole moment effect by approximately 20%, and thus it plays an important role in determination of the W_A parameter and should be taken into account in high-accuracy calculations. Interestingly, the value calculated from the CCSD method is higher than the calculated value from the CCSD(T) method but the difference is very small. This illustrates that, in our case, the perturbative triple excitation tends to lower down the W_A parameter but its contribution is not significant.

In summary, we have calculated the W_A parameter, which can be used for interpreting the measurement of the nuclear anapole moment effect, for the Be atom in BeCl using various methods such as DHF, DFT, MP2, CCSD, and CCSD(T) and using a large basis set. This is the first result of this effect for the BeCl molecule using the relativistic coupled cluster method. Our results show that electron correlations contribute to the the W_A parameter significantly and should be treated properly in high-accuracy calculations.

Acknowledgement

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