

## ARTICLE

# Theoretical Study on Divergence Problems of Single Reference Perturbation Theories

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Divergences of the single reference perturbation theories due to the addition of diffusion basis functions have been investigated for both closed-shell and open-shell molecular systems. It is found that the oscillatory range of perturbation energies of open-shell systems increases as the spin multiplicity of systems changes from 2 to 4. Feenberg transformation is exploited to treat the divergence problems. It is found numerically that within the interval of Feenberg parameter there exists a minimum perturbation order at which the perturbation series become convergent. It is also found for the open-shell systems that the magnitude of the corresponding Feenberg parameter becomes larger as the spin multiplicity of the system of interest changes from 2 to 4.

**Key words:** Single reference perturbation theory, Divergence, Diffuse function, Spin multiplicity, Feenberg transformation

## I. INTRODUCTION

Since the work of Møll and Plesset (MP) in 1934 [1], MP perturbation theory has been widely used in quantum chemistry for closed-shell atomic and molecular systems. Due to its great success, the single reference Rayleigh-Schrödinger perturbation theory has also been extended to open-shell systems [2–13]. Among them, to list a few, there are unrestricted MP (UMP), the single reference open-shell version of CASPT2 [2], the restricted open-shell Møller-Plesset theory (ROMP) of Amos *et al.* [3], OPT1 and OPT2 of Murray and Davidson [4], the restricted Møller-Plesset theory (RMP) of Knowles *et al.* [5], the Z-averaged perturbation theory (ZAPT) of Lee and Jayatilaka [7], and the open-shell perturbation theory (OSPT) of Chen [10]. Lee *et al.* [11] compared the performances of OPT1, OPT2, RMP, ROMP and ZAPT. Formaldehyde ( $\text{H}_2\text{CO}^+$ ) and hydroxymethylene ( $\text{HCOH}^+$ ) radical cations are two challenging examples for open-shell perturbation theories to predict their relative stabilities. Ma *et al.* [12] found that UMP2 and RMP2 predicted wrongly that hydroxymethylene radical cation was more stable. Chen *et al.* [13] showed that ZAPT2 and the single reference version of CASPT2 also failed in this case and only OSPT2 predicted correctly that  $\text{H}_2\text{CO}^+$  is more stable than  $\text{HCOH}^+$ .

Divergence problems are often unavoidable in perturbation theories [14] as well as coupled cluster theories [15, 16]. For both closed-shell and open-shell systems, if the eigenvalues of zeroth order Hamiltonian become degenerate or quasi-degenerate, the perturbation series will be divergent even at lower orders. It is usually thought these problems may be solved with the so-called multireference perturbation theories [17–31] such as the CASPT2 [2], the block-correlated second-order perturbation theory of Li *et al.* [26], the valence bond perturbation theory of Wu *et al.* [27], and the multireference Rayleigh-Schrödinger perturbation theory of Yi and Chen [31].

In 1996, Olsen *et al.* found a surprising divergent case of MP perturbation theory due to the addition of diffuse functions [32], in which the MP series are divergent at high orders. Olsen *et al.* attempted to explain this divergent problem with a simple two-state model [33]. Larsen *et al.* [34] reported subsequently the divergent behaviors of molecular electric dipole moments of HF calculated with MP perturbation theory at a stretched geometry in the cc-pVDZ basis set. Similar high-order divergence cases without addition of diffuse functions for molecules at stretched geometries were also investigated by Chen *et al.* [13], Murray *et al.* [35], Wheel *et al.* [36], and Leininger *et al.* [37]. Finley proposed the so-called maximum radius of convergence perturbation theory to yield rapid convergence of Rayleigh-Schrödinger perturbation series [38]. Yokoyama *et al.* tested Finley's theory with Be, Ne,  $\text{H}_2$ , and HF molecules [39]. Feenberg *et al.* [40, 41] introdu-

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ced a parameter  $\lambda$  into the system's Hamiltonian to accelerate the convergence speed of Rayleigh-Schrödinger perturbation series. The Feenberg transformation was exploited to improve the convergence of MP series by Schmidt *et al.* [42], Dietz *et al.* [43], and He *et al.* [44].

Except the work on the doublet states of NO and CN, and the triplet state of O<sub>2</sub> with ZAPT plus Feenberg transformation by Wheel *et al.* [36], researches are mainly focused on the convergence behaviors of MP series for closed-shell systems so far. In this work, the convergence behaviors of the single reference closed-shell and open-shell perturbation series are investigated with addition of diffuse functions for both closed-shell and open-shell molecules. The effectiveness of Feenberg transformation is studied in detail for parameter  $\lambda$  within the range of  $0 < \lambda < 1$ .

## II. THEORY

In Rayleigh-Schrödinger perturbation theory [45], the Hamiltonian  $\hat{H}$  of the system of interest is divided into two parts as follows

$$\hat{H} = \hat{H}_0 + \hat{V} \quad (1)$$

where  $\hat{H}_0$  is the zero-th order Hamiltonian and  $\hat{V}$  is the perturbation. It is often assumed that  $\hat{H}_0$  is a good approximate to  $\hat{H}$  and can be solved exactly as

$$\hat{H}_0 \psi_i^{(0)} = E_i^{(0)} \psi_i^{(0)} \quad (2)$$

where  $E_i^{(0)}$  and  $\psi_i^{(0)}$  are the  $i$ -th eigenvalue and eigenvector, respectively. The perturbation energy of the  $i$ -th state can be computed order by order through the following equation [13, 28, 45]

$$E_i^{(n)} = \langle \psi_i^{(0)} | \hat{V} | \psi_i^{(n-1)} \rangle \quad (3)$$

with

$$(\hat{H}_0 - E_i^{(0)}) | \psi_i^{(n)} \rangle = \sum_{k=1}^n E_i^{(k)} | \psi_i^{(n-k)} \rangle - \hat{V} | \psi_i^{(n-k)} \rangle \quad (4)$$

where  $E_i^{(k)}$  and  $| \psi_i^{(n-k)} \rangle$  are the  $k$ -th order perturbation energy and wave function, respectively. Eq.(3) is valid for both the closed-shell and open-shell problems.

In order to calculate the perturbation energy as shown in Eq.(3),  $\hat{H}_0$  should be defined explicitly. For the closed-shell atomic and molecular systems,  $\hat{H}_0$  in Eq.(1) has the following form [13, 28]

$$\hat{H}_0 = \sum_{i=1}^N \hat{F}_i \quad (5)$$

where  $N$  is the number of electrons in the system of interest,  $\hat{F}_i$  is the Fock operator [45]. For open-shell

atomic and molecular systems, no unique single particle operator like  $\hat{F}_i$  is available in literature. For example, the single particle operator in CASPT2 for open-shell problems is defined simply as an average of the Fock operators of  $\alpha$  and  $\beta$  spin orbitals. In our previous work of OSPT [10, 13, 28], the single particle operators in the doubly occupied, singly occupied, and fully unoccupied spaces are defined respectively as

$$-\frac{\hat{F}_\alpha}{2} + \frac{3\hat{F}_\beta}{2}, \frac{\hat{F}_\alpha}{2} + \frac{\hat{F}_\beta}{2}, \frac{3\hat{F}_\alpha}{2} - \frac{\hat{F}_\beta}{2}$$

where  $\hat{F}_\alpha$  and  $\hat{F}_\beta$  are the Fock operators for  $\alpha$  and  $\beta$  spin orbitals, respectively. This description is also the same as in GAMESS [46].

Feenberg transformation [40, 41] is one of effective techniques to treat the divergence problems for perturbation series. In comparison with Eq.(1), the Hamiltonian  $\hat{H}$  in the Feenberg transformation is defined in a slightly different way

$$\hat{H} = \frac{1}{1-\lambda} \hat{H}_0 + \left( \hat{V} - \frac{\lambda}{1-\lambda} \hat{H}_0 \right) \quad (6)$$

where  $\lambda$  is a parameter within the range of  $|\lambda| < 1$ , which is usually used to accelerate the convergent speed of the perturbation series. If  $\lambda$  is zero, Eq.(6) becomes the same as Eq.(1). For positive  $\lambda$ , the unperturbed part of the Hamiltonian  $\hat{H}$ ,  $\hat{H}_0/(1-\lambda)$  becomes increased and the perturbation part becomes decreased. This may help to avoid the divergence behavior of the perturbation series. For negative  $\lambda$ , the unperturbed part of the Hamiltonian  $\hat{H}$  becomes decreased while the perturbation part becomes increased, which may be helpful to obtain a relatively large part of the electronic correlation energy at lower orders but might lead to a divergent perturbation series especially at higher orders. Based on these reasons, only  $\lambda$  with the range of  $0 < \lambda < 1$  will be considered in this work. The corresponding  $n$ -th order perturbation energy  $E_\lambda^{(n)}$  of the  $i$ -th state in Eq.(6) can be expressed as a polynomial in  $\lambda$  [42–44]

$$E_\lambda^{(n)} = (1-\lambda) \sum_{k=0}^{n-2} \binom{n-2}{k} \lambda^{n-2-k} (1-\lambda)^k E_i^{(k+2)}, \quad (n \geq 2) \quad (7)$$

Eq.(3) and (7) will be exploited to discuss the convergence behaviors of series  $E_i^{(n)}$  and  $E_\lambda^{(n)}$ , respectively. The relationships of the perturbation order  $n$  and  $\lambda$  will be also investigated for the convergent  $E_\lambda^{(n)}$  series. In this work, the perturbation series will be regarded as convergent with the convergence criterion  $E_\lambda^{(n)} \leq 10^{-11}$  hartree.

## III. RESULTS AND DISCUSSION

In this work, two types of basis sets are used, which are 6-31+G [47] and aug-cc-pVDZ [48]. The molecules

under study are the singlet states of  $N^{3-}$  and  $O^{2-}$ , doublet states of OH,  $NH_2$  and F, triplet states of C,  $CH_2$ , NH and O, and the quadruplet state of N. The one electron and two electron integrals of basis functions are calculated with GAMESS [46]. The MP and OSPT perturbation energies of closed-shell and open-shell systems are computed to higher orders with programs in our group. For comparison and check of convergence of perturbation series, full configuration interaction results are also computed with our group's programs.

### A. Closed-shell systems

Olsen *et al.* reported that the MP perturbation series of Ne and HF systems were divergent due to the addition of diffuse functions. The number of electrons in these two systems is 10. We found numerically for small systems that the MP perturbation series is divergent only for systems with 10 electrons if diffuse functions are added. For examples, the MP perturbation series of  $Li_2$ , LiH, BH,  $B^-$ , and  $N^-$  are always converged whether diffuse functions are added or not. Therefore,  $N^{3-}$  and  $O^{2-}$  are chosen for present study although the underlying reason is still unclear. The basis set is 6-31+G [47]. FIG. 1 and FIG. 2 show the convergence behaviors of  $N^{3-}$  and  $O^{2-}$ , respectively. The perturbation energies are computed to more than 100 orders for  $N^{3-}$  and  $O^{2-}$  respectively. As shown in FIG. 1 and FIG. 2, if  $\lambda$  is zero, which means that no Feenberg transformation is carried out, the MP perturbation series are divergent. The MP perturbation energies are oscillatory. The divergent patterns for both  $N^{3-}$  and  $O^{2-}$  are similar, and the sign of perturbation energy is changed almost order by order. As the  $\lambda$  increases to a suitable value, such as 0.13, 0.14 or 0.23 for  $N^{3-}$  and 0.29, 0.33 or 0.40 for  $O^{2-}$  respectively, the perturbation series become convergent. On the other hand, when  $\lambda$  becomes close to 1, the convergence speed of the Feenberg perturbation series becomes slow and even divergent for both anions.

### B. Open shell systems

In contrast to the closed-shell systems discussed in the subsection above, it seems that there are more divergence cases for open-shell systems. The open systems are the doublet states of F, OH and  $NH_2$ , the triplet states of O, NH and  $CH_2$ , and the quadruplet state of N. The electronic energies of these states are calculated to about 100 orders with OSPT theory [10, 13]. The basis set is 6-31+G. The geometry of  $NH_2$  is the same as that in our previous work [13]. The bond length N–H is 1.013 Å, and the bond angle is 103.2°. The convergence behaviors of OSPT series for  $NH_2$  are shown in FIG. 3. The OSPT series of  $NH_2$  is also divergent like the closed-shell case. The absolute values of the higher

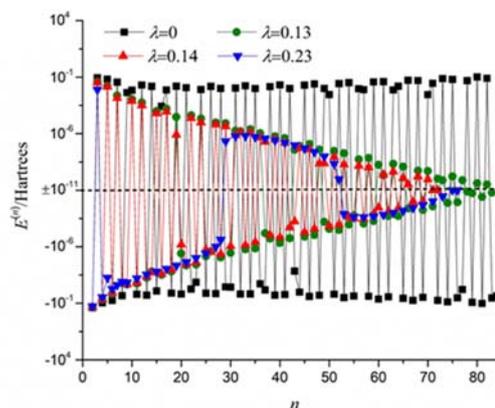


FIG. 1 The convergence behavior of MP series with Feenberg parameter  $\lambda$  for the singlet  $N^{3-}$ . The basis set is 6-31+G.

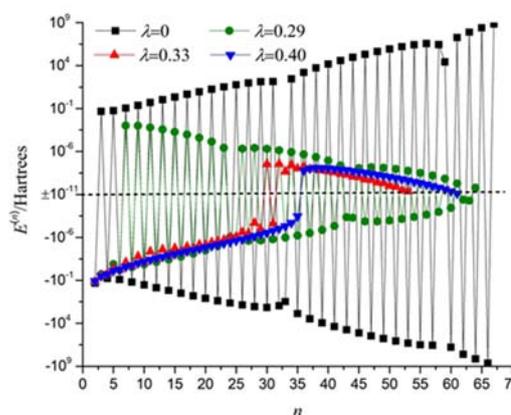


FIG. 2 The convergence behavior of MP series with Feenberg parameter  $\lambda$  for the singlet  $O^{2-}$ . The basis set is 6-31+G.

order perturbation energies are almost constant, but they have alternating signs. As  $\lambda$  becomes bigger than zero, such as  $\lambda=0.15$ , 0.23, 0.40, the Feenberg series become converged. The experimental bond length of O–H is 0.9697 Å [49]. The convergence behaviors of OSPT and Feenberg series of F and OH systems are similar to that of  $NH_2$  as demonstrated in FIG. 3. Therefore, they are not discussed further here. As for  $CH_2$ , the experimental geometry is used to the present study. The bond length and bond angle of  $CH_2$  are 1.077 Å and 134.0°, respectively [50]. The relationships of perturbation energy of  $E_\lambda^{(n)}$  with respect to the perturbation order  $n$  are presented in FIG. 4. An alternation in sign is also observed for OSPT series which corresponds to the curve with  $\lambda=0$  in FIG. 4. In comparison with the behavior of OSPT series of  $NH_2$  in FIG. 3, the magnitudes of OSPT perturbation energies for  $CH_2$  increase order by order. The convergence pattern of  $E_\lambda^{(n)}$  for  $CH_2$  is however different from that of  $NH_2$ , as clearly shown in FIG. 3 and FIG. 4. The experimental bond

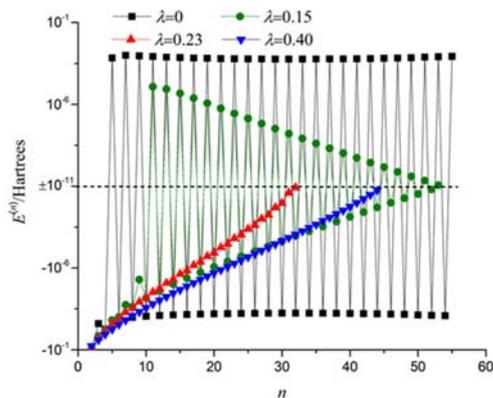


FIG. 3 The convergence behavior of OSPT series with Feenberg parameter  $\lambda$  for the doublet  $\text{NH}_2$ . The basis set is 6-31+G.

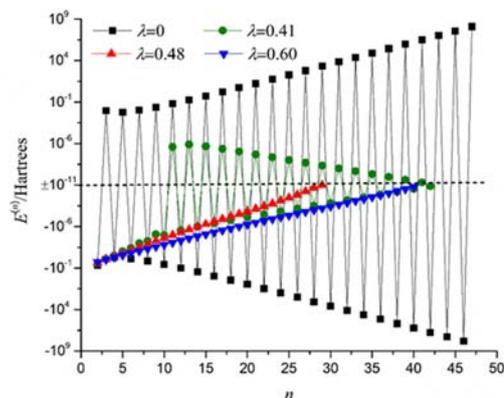


FIG. 5 The convergence behavior of OSPT series with Feenberg parameter  $\lambda$  for the quadruplet N. The basis set is 6-31+G.

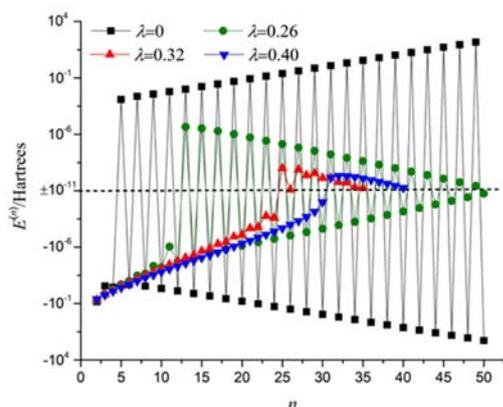


FIG. 4 The convergence behavior of OSPT series with Feenberg parameter  $\lambda$  for the triplet  $\text{CH}_2$ . The basis set is 6-31+G.

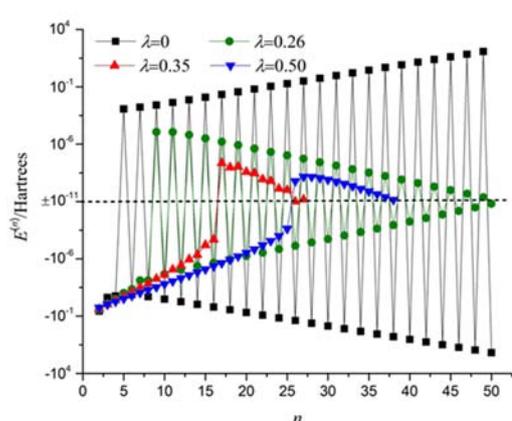


FIG. 6 The convergence behavior of OSPT series with Feenberg parameter  $\lambda$  for the triplet C. The basis set is 6-31+G.

length of N–H is 1.0362 Å [50]. As discussed for the doublet states of F, OH and  $\text{NH}_2$ , the convergence behaviors of O, NH, and  $\text{CH}_2$  are also similar and thus are not discussed further.

The convergence behaviors of the quadruplet state of N are shown in FIG. 5. In comparison with the doublet state of  $\text{NH}_2$  in FIG. 3 and the triplet state of  $\text{CH}_2$  in FIG. 4, the OSPT energies of N oscillate much more dramatically. The oscillatory ranges at 45 order change from 0.1 hartree at the doublet state, to 320.0 hartree at the triplet state and more than  $10^6$  hartree at the quadruplet state. This effect of electron spin multiplicity on the oscillatory range is first observed. On the other hand, it seems that the multiplicity effect on the Feenberg series is almost negligible.

### C. Basis set effect

The triplet state of C is chosen for the present study on the basis set effect. In this case 6-31+G and aug-cc-pVDZ are employed for investigation. The conver-

gence behaviors of perturbation series of OSPT and Feenberg for the two basis sets are presented in FIG. 6 and FIG. 7, respectively. As can be seen from these two figures, it seems that the basis set effect on the OSPT series can be ignored. However, the basis set effect on the Feenberg series is more significant. For the same value of parameter  $\lambda$ , more perturbation orders are required to reach the convergent threshold as the basis set is increased from 6-31+G to aug-cc-pVDZ. For example, if  $\lambda$  is 0.50 and the convergence threshold is  $10^{-11}$  hartree as shown in FIG. 6 and FIG. 7, the perturbation orders for 6-31+G and aug-cc-pVDZ are 37 and 44, respectively.

### D. Minimum perturbation order

As discussed in the subsections above, the Feenberg transformation plays an important role in improving the convergence of MP and OSPT series. For various values of the parameter  $\lambda$ , the convergent speeds of MP and OSPT series are different. The relationship between the

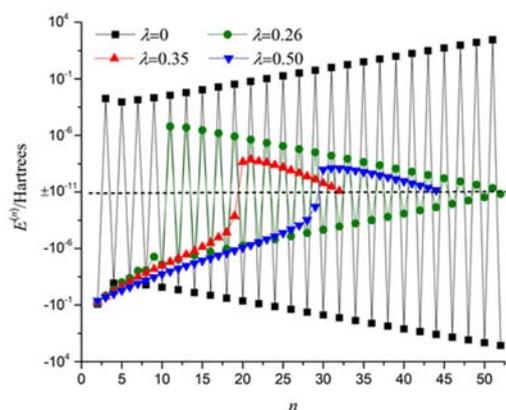


FIG. 7 The convergence behavior of OSPT series with Feenberg parameter  $\lambda$  for the triplet C. The basis set is aug-cc-pVDZ.

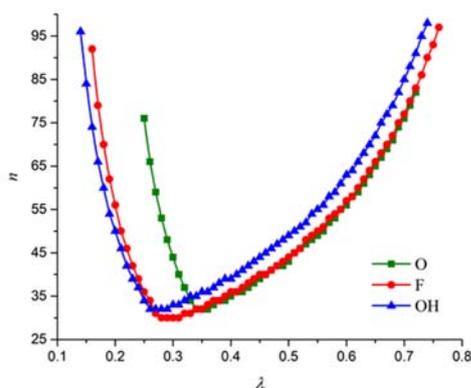


FIG. 8 The perturbation order  $n$  with the Feenberg parameter  $\lambda$  for the doublet states of F and OH, and the triplet state of O. The basis set is 6-31+G.

perturbation order  $n$  and  $\lambda$  are presented in FIG. 8 only for O, F and OH systems because of the limited space. For any pair  $(\lambda, n)$  in the figure, if the perturbation energy  $E_{\lambda}^{(k)}$  is smaller than the convergence criterion for all  $k \geq n$ , the corresponding perturbation series are regarded to be convergent. The convergence threshold in FIG. 8 is  $10^{-10}$  hartree. It can be seen from FIG. 8, there always exists for each of three systems a minimum perturbation order  $n_{\min}$  for  $\lambda$  within the range  $0 < \lambda < 1$ . It can also be found from FIG. 8 that there exists an interval of  $\lambda$  for a specific  $n_{\min}$ . These conclusions are also true for other closed-shell and open-shell systems studied in the present work. They are all listed in Table I. The systems and basis set are listed in the first and second columns, respectively. The interval of  $\lambda$  and the corresponding minimum order  $n_{\min}$  are presented in the third and fourth columns, respectively. For the singlet state of  $O^{2-}$  and the triplet state of NH, because the range of  $\lambda$  is very narrow, only one value of  $\lambda$  is given in the table. Of course, it is possible that the interval of  $\lambda$  may change to one or a few points when the convergence criterion becomes smaller and smaller than the conver-

TABLE I The minimum order  $n$  of convergent perturbation series and the corresponding range of the parameter  $\lambda$ . The convergence criterion is  $10^{-10}$  hartree.

| Systems <sup>a</sup> | Basis set   | Range of $\lambda$ | $n_{\min}$ |
|----------------------|-------------|--------------------|------------|
| $N^{3-}$ (1)         | 6-31+G      | 0.15–0.16          | 66         |
| $O^{2-}$ (1)         | 6-31+G      | 0.33               | 51         |
| OH (2)               | 6-31+G      | 0.26–0.29          | 32         |
| F (2)                | 6-31+G      | 0.28–0.31          | 30         |
| NH <sub>2</sub> (2)  | 6-31+G      | 0.23–0.24          | 32         |
| C (3)                | 6-31+G      | 0.35–0.36          | 27         |
| C (3)                | aug-cc-pVDZ | 0.33–0.34          | 29         |
| O (3)                | 6-31+G      | 0.34–0.36          | 32         |
| NH (3)               | 6-31+G      | 0.34               | 35         |
| CH <sub>2</sub> (3)  | 6-31+G      | 0.32–0.33          | 33         |
| N (4)                | 6-31+G      | 0.46–0.47          | 26         |
| N (4)                | aug-cc-pVDZ | 0.47–0.49          | 26         |

<sup>a</sup> The number in the brackets is the spin multiplicities.

gence threshold  $10^{-10}$  hartree in FIG. 8. Further, it can also be easily found for all open-shell systems in Table I that the corresponding  $\lambda$  with respect to the minimum order  $n_{\min}$  increases as the spin multiplicities of systems change from 2 to 4, although  $\lambda$  is still not constant for systems with the same spin multiplicity. This effect of spin multiplicity on  $\lambda$  is more or less similar to the effect of the multiplicity on the oscillatory range of perturbation energies for open-shell systems as discussed in the second subsection above.

#### IV. CONCLUSION

In this work, two closed-shell systems ( $N^{3-}$  and  $O^{2-}$ ) and eight open-shell systems (OH, F, NH<sub>2</sub>, C, O, NH, CH<sub>2</sub>, and N) are employed to investigate the divergence problems of MP and OSPT series due to the addition of diffusion basis functions. It is found numerically for small systems that the MP perturbation series is divergent only for systems with 10 electrons. In comparison with the divergence behaviors of MP series of closed-shell systems, the OSPT perturbation energies have exactly alternating signs for open-shell systems studied in this work. It is also found that the oscillatory ranges of OSPT perturbation energies are dependent on the spin multiplicities of systems and increase as the spin multiplicity changes from 2 to 4.

Feenberg transformation is one of effective techniques to accelerate the convergence speed of MP and OSPT series. It is found for both closed-shell and open-shell systems that there always exists a minimum perturbation order  $n_{\min}$  for some  $\lambda$  within the range of  $0 < \lambda < 1$ , at which the Feenberg perturbation series become convergent. It is also found that such a value of  $\lambda$  increases as the spin multiplicities of systems change from 2 to

4. These new features of the Feenberg perturbation series will deepen our understanding of Feenberg transformation. Feenberg transformation can also improve the performances of low order perturbation theories as studied by Schaefer *et al.* with ZAPT [36]. The similar work to our low order open-shell perturbation theories will be carried out in near future.

## V. ACKNOWLEDGMENTS

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