Correlation effects in Yb^+ and implications for parity violation

S. G. Porsev,[1,2] M. S. Safronova,[1] and M. G. Kozlov[2,3]
[1]*Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, USA*
[2]*Petersburg Nuclear Physics Institute, Gatchina, Leningrad District, 188300 Russia*
[3]*St. Petersburg Electrotechnical University "LETI", Prof. Popov Str. 5, St. Petersburg 197376, Russia*
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Calculation of the energies, magnetic dipole hyperfine structure constants, $E1$ transition amplitudes between the low-lying states, and nuclear spin-dependent parity-nonconserving amplitudes for the $^2S_{1/2}$-$^2D_{3/2,5/2}$ transitions in $^{171}Yb^+$ ion is performed using two different approaches. First, we carried out many-body perturbation theory calculation considering Yb^+ as a monovalent system. Additional all-order calculations are carried out for selected properties. Second, we carried out configuration interaction calculation considering Yb as a 15-electron system and compared the results obtained by two methods. The accuracy of different methods is evaluated. We find that the monovalent description is inadequate for evaluation of some atomic properties due to significant mixing of the one-particle and the hole-two-particle configurations. Performing the calculation by such different approaches allowed us to establish the importance of various correlation effects for Yb^+ atomic properties for future improvement of theoretical precision in this complicated system.

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I. INTRODUCTION

The Yb^+ ions have been a subject of heightened interest in recent years owing to use of this system in a number of different applications including quantum information studies [1,2], searches for variations of fundamental constants [3], and development of the optical frequency standards [4–7].

Manipulation and detection of a trapped Yb^+ hyperfine qubit was described in [1]. An efficient scheme to carry out gate operations on an array of trapped Yb^+ ions was suggested in [2]. Yb^+ is of particular interest to the atomic clock development due to the availability of two different (quadrupole [5] and octupole [7]) metastable transitions that can be used as optical frequency standards. In 2012, the performance of the optical frequency standard based on electric-octupole transition $^2S_{1/2}(F=0) \rightarrow {}^2F^o_{7/2}(F=3)$ in a single trapped Yb^+ ion was investigated [7]. This work has demonstrated that the octupole transition in $^{171}Yb^+$ can be used to realize an optical clock with a systematic uncertainty of 7.1×10^{-17} [7]. Moreover, it has been shown that a clock based on a linear combination of the quadrupole and the octupole transition frequencies of Yb^+ can have a significantly reduced blackbody shift [8]. An availability of two metastable transitions suitable for the development of the precision frequency standard made Yb^+ an attractive candidate for the search of the variation of the fine-structure constant.

The $^2S_{1/2} \rightarrow {}^2D_{3/2}$ transition in Yb^+ was also proposed [9] for study of the nuclear spin-dependent (SD) parity-nonconserving (PNC) effects. Such an experiment will be able to yield the nuclear anapole moment that arises due to parity-violating interaction between nucleons in the nucleus [10]. Study of the weak hadronic interactions is of particular interest due to significant discrepancy between constraints on weak nucleon-nucleon couplings obtained from the cesium anapole moment and those obtained from other nuclear parity-violating measurements [11,12].

Accurate calculation of Yb^+ properties is very difficult owing to the large number of low-lying states of the hole-two-particle configurations such as $4f^{13}5d6s$ and their strong mixing with one-particle (monovalent) configurations, such as $4f^{14}6p$. The properties of ytterbium ions were studied in a number of theory papers (see, e.g., [13] and references therein). Because the main configuration of the ground state of Yb^+ is $4f^{14}6s$, this ion can be considered as a system with one electron above the closed shells. Alternatively, one can treat the $4f$ electrons as the valence electrons, and consider Yb^+ as a system with 15 valence electrons. Both approaches have advantages and drawbacks. In the following, we refer to them as a single-electron approach and a many-electron approach.

The advantages of a monovalent (single-electron) method are high accuracy and relative simplicity. In particular, the core-valence correlations can be treated very accurately. However, the problem is that the states belonging to the configurations with the unfilled $4f$ shell, such as $4f^{13}6s^2$ and $4f^{13}5d6s$, are lying very low in Yb^+. A knowledge of their properties is important for a number of experimental schemes mentioned above. A single-electron method is unable to treat such states since these are not monovalent states. Moreover, the states with filled $4f$ shell (such as $4f^{14}6p\ {}^2P^o_{3/2}$) can strongly interact with a closely located state with the unfilled $4f$ shell. This mixing can significantly affect the properties of both states. Again, the single-electron approach does not take into account this interaction that drastically affects the accuracy of this approach for the states where this mixing is large. This effect is illustrated on the example of calculation of the magnetic dipole hyperfine structure (hfs) constant A of the $4f^{14}6p\ {}^2P^o_{3/2}$ state. It was calculated by several different methods that considered Yb^+ as a monovalent system [13–16].

The resulting values are in reasonable agreement with each other but are factor of 2 smaller than the experimental result. As we show in this work, the reason for this discrepancy of theory and experiment is the strong configuration interaction between the $4f^{14}6p\ {}^2P^o_{3/2}$ and $4f^{13}5d6s\ {}^3[3/2]^o_{3/2}$ states.

The many-electron methods, such as the conventional configuration interaction (CI), allow us to study the properties of the states with both filled and unfilled $4f$ shell on equal footing. It also allows us to take into account the configuration

interaction between nearby levels. However, the accuracy of the 15-electron CI approach is generally lower than that of single-electron methods due to omission of the correlation corrections between the core $[1s^2,\ldots,5p^6]$ electrons and the valence electrons. So far, it has not been possible to incorporate successfully the core-valence correlations into a many-electron CI.

In this work, we carried out calculation of Yb^+ properties using both the single-electron approach, with both many-body perturbation theory (MBPT) and all-order methods, and the 15-electron configuration interaction method. The use of the both approaches allows us to study the properties of *all* low-lying states. Since these methods are to some extent complementary to each other, they give us a clearer picture of the importance of various correlation effects and provide more complete theoretical description of the Yb^+ properties. This work will allow us to outline a pathway for the development of more accurate approaches for the calculation of Yb^+ properties of interest to applications listed above. Because of the importance of the Yb^+ for various applications, experimental values of other properties will become available in the future for further theory tests. Yb^+ is an excellent system for benchmark tests of new theoretical approaches capable of describing strong electron correlations. A development of such new approaches is also needed to improve theoretical description of complex atoms, such as Dy or Ho, which is becoming more important owing to recent experimental developments and new proposals with these systems [17–19].

Another goal of this paper is to evaluate spin-dependent parity-violating amplitudes for the $4f^{14}6s\ ^2S_{1/2}$-$4f^{14}5d\ ^2D_J$ transitions in Yb^+ and to study the effects of various correlation corrections to this quantity. The calculation of the PNC amplitude is required to analyze the experimental PNC studies and extract the anapole moment (unless the measurements are carried out with several isotopes). Such experimental study with Yb^+ is presently underway in Los Alamos [9]. So far, a nonzero anapole moment was observed only in Cs [10]. The Cs result is in disagreement with the nuclear physics predictions for the Cs anapole moment and constraints on weak nucleon-nucleon couplings [11,12] prompting further investigations. The spin-dependent PNC effects in the $4f^{14}5d\ ^2D_{3/2}$-$4f^{14}6s\ ^2S_{1/2}$ transition of Yb^+ were recently investigated in Ref. [15]. The authors of Ref. [15] treated Yb^+ as a monovalent system. They noted significant cancellation between different terms contributing to the SD PNC amplitudes which merited further investigation carried out here. We note that the total uncertainty in the value of the anapole moment that can be extracted from the experiment with a single isotope includes the theoretical and experimental uncertainties. Other PNC experiments that are presently underway include studies with Yb [20], Fr [21], and Ra^+ [22]. Large atomic parity violation effect was observed in neutral Yb [20].

The paper is organized as follows. Section II is devoted to the single-electron approach. We present the results of calculations of the low-lying energy levels, the magnetic dipole hfs constants, $E1$ transition amplitudes between the low-lying states, and nuclear spin-dependent parity-nonconserving amplitudes for the $^2S_{1/2}$-$^2D_{3/2,5/2}$ transitions. The all-order results are also given for the energy levels and electric dipole matrix elements. In Sec. III, we present the energy levels, magnetic dipole hfs constants, and $E1$ transition amplitudes for the low-lying states calculated in the framework of the 15-electron CI method. We compare the results obtained by either method. If the results differ from each other, the reasons are analyzed. The conclusions are described in Sec. IV. We use atomic units $\hbar = |e| = m_e = 1$ through the paper unless stated otherwise.

II. SINGLE-ELECTRON APPROACH AND RESULTS

In this approach, the $4f$ electrons are considered as the core electrons. We start from the solution of the Dirac-Fock (DF) equations carrying out the self-consistency procedure for the $[1s^2,\ldots,4f^{14}]$ core electrons. Then, the valence orbitals 6–8s, 6–7p, and 5–6d were constructed in the V^{N-1} approximation (N is the total number of the electrons in the system). The basis set used in calculations included virtual orbitals up to $23s,23p,23d,22f$, and $14g$ formed with the help of the recurrent procedure described in Refs. [23,24]. The MBPT corrections can be included by solving the equation

$$H_{\rm eff}\,\psi_n = \varepsilon_n \psi_n \qquad (1)$$

with the effective Hamiltonian defined as $H_{\rm eff} \equiv H_0 + \Sigma$, where H_0 is the Dirac-Fock Hamiltonian and the operator Σ takes into account virtual core excitations.

A. Energy levels

First, we find the energies of the low-lying states in various approximations and compare them with the experimental values [25]. As we already mentioned, we are able to obtain only the energies for the states with filled $4f$ shell in the framework of this approach. In Table I we present the ionization potential (line 1) and the energies of the low-lying states obtained in different approximations. At the DF stage of the calculations, even the order of the levels is incorrect. An inclusion of the second-order MBPT corrections restores the correct order of levels listed in Table I. The second-order MBPT values are listed in the column labeled "MBPT."

As expected, the agreement between the experimental and theoretical energies significantly improves with the inclusion

TABLE I. The comparison of the energy levels calculated in different approximations with experiment [25]. The ionization potential is given in the first line (in a.u.), the energy levels of the excited states are counted from the ground state (in cm^{-1}). The columns labeled "DF" and "MBPT" correspond to the Dirac-Fock and DF + MBPT approximations with the MBPT corrections included in the second order. The higher orders of the MBPT are included in the results listed in the column labeled "MBPT(HO)." The results of the single-double all-order calculation are listed in the column labeled "All-order."

	DF	MBPT	MBPT(HO)	All-order	Experiment
$^2S_{1/2}$	0.41366	0.45211	0.44473	0.45090	0.44775[a]
$^2D_{3/2}$	24272	24450	22711	22820	22961
$^2D_{5/2}$	24752	25952	24178	24261	24333
$^2P^o_{1/2}$	24702	28636	27945	27945	27062
$^2P^o_{3/2}$	27513	32242	31403	31481	30392

[a]This is equal to the ionization potential =98269 cm^{-1} [25].

of the correlation corrections beyond DF approximation. At the same time, the correlations are large and accounting for only the second-order MBPT corrections is not sufficient. To calculate the energy levels (and subsequently other properties) more accurately, we need to take into account the higher orders (HO) of the MBPT. We designate this approximation as MBPT(HO) and label the results of such calculations accordingly in the text and the tables.

In this approach, we include higher-order corrections by introducing screening coefficients C_k for the Coulomb lines in self-energy diagrams (see, e.g., [26]). The latter can be calculated as an average screening of the two-electron Coulomb radial integrals of a given multipolarity k. These coefficients serve as an approximation to the insertion of polarization operator in Coulomb lines. The coefficients C_k were chosen as follows: $C_0 = 1.3$, $C_1 = 0.75$, and $C_k = 1$ for $k \geqslant 2$. The resulting energies are listed in Table I in the column labeled "MBPT(HO)." The ionization potential obtained in the MBPT(HO) approximation agrees with the experiment at the level of 0.07%; the energies of the even-parity states are within 1% from the experimental values, and the energies of the $^2P^o_{1/2}$ and $^2P^o_{3/2}$ states were reproduced with the 3% accuracy.

As a test of the MBPT(HO) approach, we also calculated the energy levels using the linearized single-double coupled-cluster method (also referred to as the all-order method). This method allows us to include the higher-order correlation corrections in an *ab initio* way by effectively summing the dominant correlation contributions to all orders of the perturbation theory. The single-double all-order method was demonstrated to produce very accurate atomic properties for alkali-metal atoms and other monovalent systems. We refer the reader to the review [27] for a description of the all-order approach and its applications. The all-order data are listed in the column labeled "All-order" in Table I. These energy values have been previously listed in [28]. We find that *ab initio* all-order energy levels are close to the MBPT(HO) values, serving as an additional verification of the MBPT(HO) approximation.

B. Magnetic dipole hfs constants and $E1$ transition amplitudes

To calculate magnetic dipole hfs constants and $E1$ transition amplitudes, we construct effective valence operators for the magnetic dipole hyperfine interaction $H_{\rm hfs}$ and the electric dipole operator d. First, we solve the random-phase approximation (RPA) equations, which is equivalent to the summation of the dominant sequence of many-body diagrams to all orders of MBPT [26,29]. Then, we include additional corrections (beyond RPA) to the effective operators: the core-Brueckner, structural radiation (SR), and normalization corrections.

The results obtained for the hfs constants are listed in Table II. This table illustrates that the MBPT corrections are generally large and contribute significantly to the hfs constants A. The RPA, core-Brueckner, SR, and normalization corrections also have to be taken into account. The ^2D_J states are particularly sensitive to different corrections. For instance, the RPA correction even changes the sign of $A(^2D_{5/2})$. The SR corrections (which are usually relatively small) are found to be significant in this case and change the values of $A(^2D_{3/2})$ and $A(^2D_{5/2})$ by more than 40%.

The final values of all hfs constants obtained in this work are, in general, in reasonable agreement with the experimental data and other theoretical results with the exception of two cases. We find a significant difference between our value of $A(^2D_{3/2})$ and the value found in [15]. The difference is most probably due to inclusion of the corrections beyond RPA in this work. Our result is in a good agreement with the experiment. All of the theoretical values are in disagreement with the experimental value of the $A(^2P^o_{3/2})$, demonstrating that this hfs constant can not be correctly reproduced in the framework of a single-electron approach. As we will discuss in more detail in the section devoted to the 15-electron CI, this problem arises due to a strong mixing of the $4f^{14}6p\ ^2P^o_{3/2}$ state and a nearby $4f^{14}5d6s\ ^3[3/2]^o_{3/2}$ state. A possible sensitivity of $A(^2P^o_{3/2})$ to the configuration mixing was also mentioned in Ref. [15].

We also calculated the $E1$ amplitudes for the transitions between the low-lying states and compared them with other

TABLE II. The breakdown of different contributions to the hfs constants A (in MHz) ($I = 1/2$, $\mu = 0.4919$ [30]). First row gives the DF values and the following rows give MBPT(HO), RPA, core-Brueckner (σ), structural radiation (SR), and normalization (Norm.) corrections. The row labeled "Total" gives the final numbers. The values are compared with the experimental and other theoretical [13–16] results.

	$^2S_{1/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2P^o_{1/2}$	$^2P^o_{3/2}$
DF	9577	290	111	1542	183
MBPT(HO)	2993	109	38	549	58
RPA	1672	−55	−308	323	132
σ	−762	−13	−5	−10	−5
SR	−188	167	67	−9	−35
Norm.	−201	−9	1	−24	−3
Total	13091	489	−96	2371	330
Experiment	12645(2)[a]	430(43)[b]	−63.6(7)[c]	2104.9(1.3)[a]	877(20)[d]
Ref. [13]	13172			2350	311.5
Ref. [14]	12730			2317	391
Ref. [15]	13217	291		2533	388
Ref. [16]	13332	447	−48	2516	322

[a]Reference [14].
[b]Reference [31] and references therein.
[c]Reference [32].
[d]Reference [33].

available data. The lifetime τ of the $^2P^o_{1/2}$ state was measured with a high precision in Ref. [34] to be equal to 8.12(2) ns. The $^2P^o_{1/2}$ state can decay to the $^2D_{3/2}$ and $^2S_{1/2}$ states. The decay channel to the ground state strongly dominates. The branching ratio from the $^2P^o_{1/2}$ state to the metastable $^2D_{3/2}$ state was measured to be 0.00501(15) [1]. Using two these quantities, we find the transition probabilities

$$W\left(^2P^o_{1/2} \to {}^2S_{1/2}\right) = 0.995/\tau\left(^2P^o_{1/2}\right) = 1.23(5) \times 10^8 \text{ s}^{-1} \quad (2)$$

and

$$W\left(^2P^o_{1/2} \to {}^2D_{3/2}\right) = 0.00501/\tau\left(^2P^o_{1/2}\right) = 6.17(18) \times 10^5 \text{ s}^{-1}. \quad (3)$$

Respectively, the "experimental" reduced matrix elements (MEs) of the electric-dipole moment operator are $|\langle^2S_{1/2}||d||^2P^o_{1/2}\rangle| = 2.471(3)$ a.u. and $|\langle^2D_{3/2}||d||^2P^o_{1/2}\rangle| = 2.97(4)$ a.u.

At the present time, the most precise measurement of the $^2P^o_{3/2}$ lifetime, $\tau(^2P^o_{3/2}) = 6.15(9)$ ns, was carried out in [35]. The $^2P^o_{3/2}$ state mainly decays by the $E1$ transitions to the $^2S_{1/2}$, $^2D_{3/2}$, and $^2D_{5/2}$ states. Then,

$$\frac{1}{\tau\left(^2P^o_{3/2}\right)} \approx W\left(^2P^o_{3/2} \to {}^2S_{1/2}\right) + W\left(^2P^o_{3/2} \to {}^2D_{3/2}\right) + W\left(^2P^o_{3/2} \to {}^2D_{5/2}\right). \quad (4)$$

The transition probabilities $W(^2P^o_{3/2} \to {}^2D_{3/2})$ and $W(^2P^o_{3/2} \to {}^2D_{5/2})$ were calculated in Ref. [13] to be 3.6×10^5 s^{-1} and 1.9×10^5 s^{-1}, respectively. Thus, they are more than two orders of magnitude smaller than $1/\tau(^2P^o_{3/2}) \approx 1.626 \times 10^8$ s^{-1}. Even if the accuracy of $W(^2P^o_{3/2} \to {}^2D_J)$ is not so high (for example, ~20%–30%), it practically does not affect the final accuracy of the $W(^2P^o_{3/2} \to {}^2S_{1/2})$ inferred from the experiment. Using the experimental value of $\tau(^2P^o_{3/2})$, we find the probability of the $^2P^o_{3/2} \to {}^2S_{1/2}$ transition from Eq. (4) yielding $|\langle^2S_{1/2}||d||^2P^o_{3/2}\rangle| \approx 3.36(3)$ a.u. The same experimental value for this reduced ME was quoted in [15].

In Table III, we present the results obtained for the reduced MEs of the electric dipole moment operator d in the DF approximation and list the MBPT(HO), RPA, and other corrections. We emphasize that the core-Bruckner, SR, and normalization corrections are small in this case, and we do not present them separately. The sum of these corrections is given in the table in the row labeled "Other." We also calculated the $E1$ matrix elements using the *ab initio* all-order method [27]. These values are listed in the row labeled "All-order." These results include the dominant SR, normalization, and other corrections to all orders. The MBPT(HO) and single-double all-order results are in close agreement.

C. Parity-nonconserving amplitude

We carried out the calculation of the spin-dependent PNC amplitudes for the $^2S_{1/2} \to {}^2D_{3/2,5/2}$ transitions. The Hamiltonian describing the main part of the nuclear spin-dependent PNC electron-nuclear interaction can be written as follows:

$$H_{\rm SD} = \frac{G_F}{\sqrt{2}} \frac{\varkappa}{I} \boldsymbol{\alpha} \boldsymbol{I} \rho(\boldsymbol{r}), \quad (5)$$

where $G_F \approx 2.2225 \times 10^{-14}$ a.u. is the Fermi constant of the weak interaction, $\varkappa$ is the dimensionless coupling constant, $\boldsymbol{\alpha} = \left(\begin{smallmatrix} 0 & \sigma \\ \sigma & 0 \end{smallmatrix}\right)$, and γ_5 are the Dirac matrices, $\boldsymbol{I}$ is the nuclear spin, and $\rho(\mathbf{r})$ is the nuclear density distribution.

We consider the nucleus to be a uniformly charged sphere. Then,

$$\rho(\boldsymbol{r}) = \frac{3}{4\pi R^3} \theta(R - r).$$

The root-mean-square charge radius is $r_{\rm rms} = 5.2891$ fm [36] and, respectively, the nuclear radius $R = \sqrt{5/3}\, r_{\rm rms} \approx 6.828$ fm.

TABLE III. The breakdown of different contributions to the reduced MEs of the electric dipole moment operator d (in a.u.). First row gives the DF values. The second and third rows give the MBPT(HO) and RPA corrections, respectively. The row labeled "Other" is the sum of the core-Brueckner, structural radiation, and normalization corrections. The row labeled "Total" gives the final numbers. The results of the SD all-order calculation are given in the row labeled "All-order." The values are compared with the experimental and other theoretical [13,15,16] results.

	$\lvert\langle^2S_{1/2}\rvert\rvert d\rvert\rvert^2P^o_{1/2}\rangle\rvert$	$\lvert\langle^2S_{1/2}\rvert\rvert d\rvert\rvert^2P^o_{3/2}\rangle\rvert$	$\lvert\langle^2D_{3/2}\rvert\rvert d\rvert\rvert^2P^o_{1/2}\rangle\rvert$	$\lvert\langle^2D_{3/2}\rvert\rvert d\rvert\rvert^2P^o_{3/2}\rangle\rvert$	$\lvert\langle^2D_{5/2}\rvert\rvert d\rvert\rvert^2P^o_{3/2}\rangle\rvert$
DF	3.24	4.54	3.86	1.70	5.20
MBPT(HO)	−0.16	−0.24	−0.47	−0.23	−0.61
RPA	−0.33	−0.42	−0.32	−0.12	−0.36
Other	0.002	−0.05	−0.006	0.001	−0.002
Total	2.75	3.83	3.06	1.35	4.23
All-order	2.64	3.71	2.98	1.32	
Experiment	2.471(3)[a]	3.36(3)[b]	2.97(4)[a]		
Reference [13]	2.68	3.77	2.97	1.31	4.12
Reference [15]	2.72	3.84	3.09	1.36	
Reference [16]	2.72	3.83	3.06	1.35	4.23

[a]References [1,34].

[b]Reference [35], see also explanation in the text.

If $|i\rangle$ and $|f\rangle$ are the initial and final atomic states of the same nominal parity, then taking into account the nuclear SD part of the PNC interaction in the lowest nonvanishing order, one can write the electric dipole transition matrix element as

$$\langle f|d_{q,\mathrm{SD}}|i\rangle = \sum_n \left[\frac{\langle f|d_q|n\rangle\langle n|H_{\mathrm{SD}}|i\rangle}{E_i - E_n} + \frac{\langle f|H_{\mathrm{SD}}|n\rangle\langle n|d_q|i\rangle}{E_f - E_n}\right], \tag{6}$$

where $|a\rangle \equiv |J_a F_a M_a\rangle$, $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{J}$ is the total angular momentum, M is the projection of $\mathbf{F}$, and H_{SD} is given by Eq. (5).

The expression for the reduced ME of d_{SD} was derived in [37] and is given by

$$\begin{aligned}&\langle J_f F_f||d_{\mathrm{SD}}||J_i F_i\rangle \\ &= \sqrt{I(I+1)(2I+1)(2F_i+1)(2F_f+1)}\sum_n \left[(-1)^{J_f-J_i}\begin{Bmatrix} J_n & J_i & 1\\ I & I & F_i\end{Bmatrix}\begin{Bmatrix} J_n & J_f & 1\\ F_f & F_i & I\end{Bmatrix}\frac{\langle J_f||d||n,J_n\rangle\langle n,J_n||H_{\mathrm{SD}}||J_i\rangle}{E_n - E_i}\right.\\ &\left. + (-1)^{F_f-F_i}\begin{Bmatrix} J_n & J_f & 1\\ I & I & F_f\end{Bmatrix}\begin{Bmatrix} J_n & J_i & 1\\ F_i & F_f & I\end{Bmatrix}\frac{\langle J_f||H_{\mathrm{SD}}||n,J_n\rangle\langle n,J_n||d||J_i\rangle}{E_n - E_f}\right].\end{aligned} \tag{7}$$

For the $^2S_{1/2} \to {}^2D_J$ transitions, where $J = 3/2$ and $5/2$, in ^{171}Yb ($I = 1/2$) we obtain from Eq. (7)

$$\begin{aligned}&\langle {}^2D_J, F_f||d_{\mathrm{SD}}||{}^2S_{1/2}, F_i\rangle \\ &= \sqrt{\frac{3\,(2F_i+1)(2F_f+1)}{2}}\sum_n \left[(-1)^{J-1/2}\begin{Bmatrix} J_n & 1/2 & 1\\ 1/2 & 1/2 & F_i\end{Bmatrix}\begin{Bmatrix} J_n & J & 1\\ F_f & F_i & I\end{Bmatrix}\frac{\langle {}^2D_J||d||n,J_n\rangle\langle n,J_n||H_{\mathrm{SD}}||{}^2S_{1/2}\rangle}{E_n - E_{^2S_{1/2}}}\right.\\ &\left. + (-1)^{F_f-F_i}\begin{Bmatrix} J_n & J & 1\\ 1/2 & 1/2 & F_f\end{Bmatrix}\begin{Bmatrix} J_n & 1/2 & 1\\ F_i & F_f & I\end{Bmatrix}\frac{\langle {}^2D_J||H_{\mathrm{SD}}||n,J_n\rangle\langle n,J_n||d||{}^2S_{1/2}\rangle}{E_n - E_{^2D_J}}\right].\end{aligned} \tag{8}$$

For subsequent calculations, it is convenient to write

$$\langle {}^2D_J,\ F_f\ ||d_{\mathrm{SD}}||{}^2S_{1/2}, F_i\rangle = \langle {}^2D_J, F_f||d\cdot R_1\cdot H_{\mathrm{SD}}||{}^2S_{1/2}, F_i\rangle + \langle {}^2D_J, F_f||H_{\mathrm{SD}}\cdot R_2\cdot d||{}^2S_{1/2}, F_i\rangle, \tag{9}$$

where we denote the terms involving summations over n by R_1 and R_2.

To calculate the nuclear spin-dependent PNC amplitude defined by Eq. (8), one needs to sum over all possible intermediate states or to solve the corresponding inhomogeneous equation. Here, we solve the inhomogeneous equation using the Sternheimer-Dalgarno-Lewis method [38,39] in the valence sector. The results obtained in different approximations are presented in Table IV.

We carried out the calculations in the DF and DF + MBPT(HO) (i.e., including the higher orders of the MBPT) approximations. Note that in these approximations, $\langle {}^2D_J||H_{\mathrm{SD}}||{}^2P^o_{J'}\rangle = 0$ and, respectively, the second term in Eq. (9) is also zero. Then, we solved the RPA equations, which are equivalent to the summation of the corresponding many-body diagrams to all orders for both d and H_{SD} operators in Eq. (8). Smaller contributions that include core-Brueckner, structural radiation, and normalization corrections were also taken into account. When the RPA corrections are included, the intermediate $n P^o_{3/2}$ states also contribute to the spin-dependent PNC amplitude drastically increasing (in absolute value) the second term in Eq. (9).

The initial and final states are the many-electron states. Therefore, we need to account for the core excitations. This contribution (labeled as "core" in Table IV) was calculated in the DF and RPA approximations.

Table IV (see the column labeled "RPA + other") illustrates that the two terms in Eq. (9) are comparable in their magnitude, but have the opposite sign for all $F_i \to F_f$ transitions. Therefore, they partially cancel each other. Unfortunately, the accuracy of the calculation of the second term is expected to be rather poor since the intermediate $^2P^o_{3/2}$ state contributes to the second term at the level of 90%. The quality of the wave function for this state near the nucleus is expected to be low because of the discrepancies of the theoretical and experimental values for the magnetic dipole hfs constant $A(^2P^o_{3/2})$ discussed above. Because of the significant cancellation between terms, the final numbers in Table IV are expected to only give an order-of-magnitude estimate of the spin-dependent PNC amplitudes.

A similar single-electron approach was used by Dzuba and Flambaum in [15] for calculating the PNC amplitude. They have rescaled the *ab initio* value of the ME $\langle n|H_{\mathrm{SD}}|m\rangle$ as

$$\langle n|H_{\mathrm{SD}}|m\rangle_{\mathrm{rescaled}} = \sqrt{\frac{A_{\mathrm{exp}}(n)\,A_{\mathrm{exp}}(m)}{A_{\mathrm{th}}(n)\,A_{\mathrm{th}}(m)}}\langle n|H_{\mathrm{SD}}|m\rangle, \tag{10}$$

where $A_{\mathrm{exp}}(k)$ and $A_{\mathrm{th}}(k)$ are the experimental and theoretical values of the magnetic dipole hfs constant of the state k. The assumption that

$$\left\langle {}^2D_{3/2}|H_{\mathrm{SD}}|{}^2P^o_{3/2}\right\rangle_{\mathrm{rescaled}} \sim \sqrt{A_{\mathrm{exp}}({}^2D_{3/2})\,A_{\mathrm{exp}}\left({}^2P^o_{3/2}\right)} \tag{11}$$

may not hold for the Yb$^+$ ions due to the mixing of the $4f^{14}6p\ {}^2P^o_{3/2}$ and $4f^{13}5d6s\ {}^3[3/2]^o_{3/2}$ states. An admixture of the configuration $4f^{13}5d6s$ to the leading configuration $4f^{14}6p$ of the $^2P^o_{3/2}$ state leads to an additional contribution to the hfs constant $A(^2P^o_{3/2})$ which is proportional to $\langle 4f^{13}5d6s|H_{\mathrm{hfs}}|4f^{13}5d6s\rangle$. This is a large contribution. However, the configuration $4f^{13}5d6s$ does not contribute

TABLE IV. The nuclear spin-dependent PNC amplitude (in units $i\varkappa \cdot 10^{-12}\,|e|a_0$), where a_0 is the Bohr radius. The values obtained in the DF and DF + MBPT(HO) approximations are listed in the columns labeled "DF" and "MBPT(HO)." The RPA and other corrections are included in the results listed in the column labeled "RPA + other." The rows labeled "core" show contributions of the core excitations. The final values (given in the rows labeled "Total") are compared with the results obtained in Ref. [15].

F_f	F_i		DF	MBPT(HO)	RPA + other	Ref. [15]
1	0	$\langle {}^2D_{3/2},F_f\|\|d\cdot R_1\cdot H_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$	6.2	6.6	6.9	
		$\langle {}^2D_{3/2},F_f\|\|H_{\rm SD}\cdot R_2\cdot d\|\|{}^2S_{1/2},F_i\rangle$	0	0	−5.1	
		core	0.7	0.7	0.8	
		Total: $\langle {}^2D_{3/2},F_f\|\|d_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$	6.9	7.3	2.6	3.1(1.9)
1	1	$\langle {}^2D_{3/2},F_f\|\|d\cdot R_1\cdot H_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$	1.5	1.6	1.5	
		$\langle {}^2D_{3/2},F_f\|\|H_{\rm SD}\cdot R_2\cdot d\|\|{}^2S_{1/2},F_i\rangle$	0	0	−3.2	
		core	0.2	0.2	0.2	
		Total: $\langle {}^2D_{3/2},F_f\|\|d_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$	1.7	1.8	−1.5	−1.3(4)
2	1	$\langle {}^2D_{3/2},F_f\|\|d\cdot R_1\cdot H_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$	−3.3	−3.5	−3.6	
		$\langle {}^2D_{3/2},F_f\|\|H_{\rm SD}\cdot R_2\cdot d\|\|{}^2S_{1/2},F_i\rangle$	0	0	1.8	
		core	−0.4	−0.4	−0.4	
		Total: $\langle {}^2D_{3/2},F_f\|\|d_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$	−3.7	−3.9	−2.2	−2.6(1.3)
2	1	$\langle {}^2D_{5/2},F_f\|\|d\cdot R_1\cdot H_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$			0.2	
		$\langle {}^2D_{5/2},F_f\|\|H_{\rm SD}\cdot R_2\cdot d\|\|{}^2S_{1/2},F_i\rangle$			−1.1	
		core			−0.1	
		Total: $\langle {}^2D_{5/2},F_f\|\|d_{\rm SD}\|\|{}^2S_{1/2},F_i\rangle$			−1.0	

explicitly to $\langle 4f^{14}5d|H_{\rm SD}|4f^{13}5d6s\rangle$ because the one-electron ME $\langle 4f|H_{\rm SD}|6s\rangle = 0$. Our values are in agreement with the results of Dzuba and Flambaum [15] within the estimated uncertainties.

III. 15-ELECTRON CONFIGURATION INTERACTION

We demonstrated in the preceding sections that the single-electron method sometimes fails to correctly predict certain properties of the Yb^+ ions due to mixing of configurations outside of the monovalent states space. This mixing can be taken into account within the framework of the 15-electron CI. In this approach, the $4f$ electrons are also considered as the valence electrons.

We again start from the solution of the Dirac-Fock equations, but the construction of the DF orbitals is more complicated than in the monovalent approximation described in the preceding section. The odd-parity low-lying levels belong to three different configurations: $4f^{13}6s^2$, $4f^{14}6p$, and $4f^{13}5d6s$. Therefore, if we construct the basis set in a standard way, i.e., in the V^{N-1} approximation, the $4f^{13}6s^2$ and $4f^{13}5d6s$ states will have much higher energy than the $4f^{14}6p$ states and, respectively, there will be no mixing interaction between these configurations. To avoid this problem, we carry out the initial self-consistency procedure for the $[1s^2,\ldots,4f^{14},6p]$ configuration. Then, all electrons were frozen and two electrons (one from the $4f$ shell and another one from the $6p$ shell) were moved to the $6s$ shell. Thus, the $6s$ orbital was constructed for the $4f^{13}6s^2$ configuration. Next, all electrons were frozen again and one electron from the $6s$ shell was moved to the $5d$ shell. The $5d_{3/2,5/2}$ orbitals were constructed for the $4f^{13}5d6s$ configuration.

The basis set used in the CI calculations included virtual orbitals up to $8s$, $8p$, $7d$, $7f$, and $5g$. The virtual orbitals were constructed as described in [23,24]. As a result, the basis set we used for these calculations is rather short since the size of the configuration space grows very rapidly with the increase of the basis set. The configuration space was formed by allowing single and double excitations for the even-parity states from the configurations $4f^{14}6s$ and $4f^{14}5d$ and for the odd-parity states from the configurations $4f^{14}6p$, $4f^{13}6s^2$, and $4f^{13}5d6s$. To check convergence of the CI, we calculated the low-lying energy levels for three cases: (1) including the single and double excitations to the shells $6s$, $6p$, $5d$, and $5f$ (we designate it $[6sp5df]$), (2) including the single and double excitations to $[7sp6df5g]$, and (3) including the single and double excitations to $[8sp7df5g]$. In the last case, the configuration space consisted of ∼2 300 000 determinants and calculation of the energy levels was rather lengthy.

A. Energy levels

The low-lying energy levels were calculated using the three CI spaces described above. The results are presented in Table V.

We were able to reproduce the low-lying even- and odd-parity states belonging to *five* different configurations $4f^{14}6s, 4f^{14}5d, 4f^{14}6p, 4f^{13}6s^2$, and $4f^{13}5d6s$ (the column $[8sp7df5g]$ in Table V) reasonably well. The theoretical energy levels for the $4f^{14}6p\ {}^2P^o_J$ states are located deeper than the experimental levels. It is not surprising since the initial self-consistency Dirac-Fock procedure was carried out for this configuration. The levels of the $4f^{13}5d6s$ configuration are in reasonable agreement with the experimental data. The $4f^{14}5d\ {}^2D_J$ states are lying 5%–7% higher than the experimental levels. This is also expected because, as we mentioned above, the $5d$ orbital was constructed not for the $4f^{14}5d$ configuration, but for the $4f^{13}5d6s$ configuration. We observe the worst agreement with the experiment for the $4f^{13}6s^2\ {}^2F^o_{7/2}$ state. A reason is a particular sensitivity of this state to the configuration interaction. It was confirmed by calculations carried out with other (smaller) sets of configurations (not

TABLE V. The energy levels of the low-lying excited states counted from the ground state (in cm^{-1}). The columns [$6sp5df$], [$7sp6df5g$], and [$8sp7df5g$] give results obtained using different sets of the configurations described in the text. The results of the single-double all-order calculations are presented in the column labeled "All-order" for comparison. The experimental energy levels [25] are presented in the column labeled "Experiment."

Configuration	Term	[$6sp5df$]	$7sp6df5g$]	[$8sp7df5g$]	All-order	Experiment
$4f^{14}6s$	$^2S_{1/2}$	0	0	0	0	0
$4f^{14}5d$	$^2D_{3/2}$	29978	24237	24615	22820	22961
	$^2D_{5/2}$	30283	25068	25464	24261	24333
$4f^{13}6s^2$	$^2F^o_{7/2}$	24621	26735	26760		21419
$4f^{13}5d6s$	$^3[3/2]^o_{5/2}$	22977	25992	26201		26759
$4f^{14}6p$	$^2P^o_{1/2}$	21266	24057	24289	27945	27062
$4f^{13}5d6s$	$^3[3/2]^o_{3/2}$	26232	28782	28973		28758
	$^3[9/2]^o_{9/2}$	27595	30169	30364		30224
$4f^{14}6p$	$^2P^o_{3/2}$	24288	27093	27324	31481	30392
$4f^{13}5d6s$	$^3[11/2]^o_{11/2}$	27732	30412	30616		30563
	$^3[11/2]^o_{13/2}$	28297	31165	31407		31632
	$^3[5/2]^o_{7/2}$	29928	32329	32531		31979
	$^3[5/2]^o_{5/2}$	30323	32730	32939		32731

included in Table V). We assume that more configurations have to be taken into account to reproduce this energy level with good precision.

It is worth noting that it was essential to include the $5g$ shell into consideration as illustrated by the comparison of the columns [$6sp5df$] and [$7sp6df5g$] in Table V. Most of the observed differences in the energy levels listed in these two columns are due to including configurations involving the $5g$ orbitals into the CI space. A number of levels are very sensitive to these configurations. An addition of the $8s$, $8p$, $7d$, and $7f$ shells (compare the columns [$7sp6df5g$] and [$8sp7df5g$] in the table) led to much smaller changes in the energy levels. Comparison of these three sets appears to indicate that further extension of the CI space (which will be extremely time consuming) will not lead to any qualitative changes for a majority of the states. The results obtained in the framework of the single-double all-order approach are presented in Table V for comparison.

In Sec. II, we discussed a poor agreement between the experimental value of the magnetic dipole hfs constant $A(4f^{14}6p\ ^2P^o_{3/2})$ and the value obtained in the single-electron approach. A strong interaction of this state with the closely lying $4f^{13}5d6s\ ^3[3/2]^o_{3/2}$ state was suggested as a possible reason of this disagreement. Our calculation with the [$8sp7df5g$] CI space reproduced the difference between the energies of the $^2P^o_{3/2}$ and $^3[3/2]^o_{3/2}$ states almost perfectly (1649 cm^{-1}), although the order of the levels was not correct. The experimental difference is 1634 cm^{-1}. It makes us confident that the configuration mixing of these two states is taken into account sufficiently correctly. We would like to stress that our calculations are purely *ab initio*. No semiempirical parameters were used in the framework of this approach.

In the next section, we present the values of the magnetic dipole hfs constants and $E1$ transition amplitudes between the low-lying states. We compare these results with those obtained in the single-electron approximation and discuss the role of the mixing of monovalent and one-hole–two-particle configurations.

B. hfs constants, $E1$ transition amplitudes, and other observables

The values of the magnetic dipole hfs constants obtained using three sets of configurations are listed in Table VI. We compare these results with the values listed in Table II obtained using the single-electron method. We will discuss the results obtained for the largest [$8sp7df5g$] CI space.

For the even-parity states, the hfs constants found in the 15-electron CI are close to the values obtained at the MBPT(HO) stage (see Table II). Such an agreement looks reasonable. The CI results include the correlation corrections between the $4f$ and other valence electrons. In the single-electron approach, these are core-valence correlations. At the same time, the core excitations from all shells up to $4f$ are completely disregarded in the 15-electron CI approach. The configuration mixing does not play very significant role for the even-parity states considered here because the even states with unfilled $4f$ shell are located rather far from the ground and $^2D_{3/2,5/2}$ states.

The value of $A(^2P^o_{1/2})$ is very close to the result obtained in the single-electron approach in the DF approximation. Our analysis shows that in the many-electron case the contributions of all electrons (except the $6p_{1/2}$) nearly cancels with each other and the final value is determined almost completely by the contribution of the $6p_{1/2}$ electron.

The most significant disagreement between the experimental and theoretical hfs constants in the single-electron approach (by a factor of 2.7) was found for the $^2P^o_{3/2}$ state. This problem is resolved in the many-electron calculation. The 15-electron CI gives the value 765 MHz, which differs from the experiment by only 13% (see Table VI, column [$8sp7df5g$]). The admixture of the $4f^{13}5d6s\ ^3[3/2]^o_{3/2}$ state

TABLE VI. The magnetic dipole hfs constants A (in MHz). The columns [$6sp5df$], [$7sp6df5g$], and [$8sp7df5g$] give results obtained using different sets of the configurations described in the text. The MBPT(HO) results are presented in the column labeled "MBPT(HO)" for comparison. The available experimental values are given in column labeled "Experiment."

Configuration	Term	[$6sp5df$]	[$7sp6df5g$]	[$8sp7df5g$]	MBPT(HO)	Experiment
$4f^{14}6s$	$^2S_{1/2}$	18430	12916	12679	13091	12645(2)[a]
$4f^{14}5d$	$^2D_{3/2}$	690	425	455	489	430(43)[b]
	$^2D_{5/2}$	252	154	164	−96	−63.6(7)[c]
$4f^{13}6s^2$	$^2F^o_{7/2}$	946	973	977		905.0(5)[d]
$4f^{13}5d6s$	$^3[3/2]^o_{5/2}$	4520	3848	3841		
$4f^{14}6p$	$^2P^o_{1/2}$	1264	1437	1532	2371	2104.9(1.3)[a]
$4f^{13}5d6s$	$^3[3/2]^o_{3/2}$	−964	−742	−798		
	$^3[9/2]^o_{9/2}$	−719	−436	−430		
$4f^{14}6p$	$^2P^o_{3/2}$	783	763	765	330	877(20)[e]
$4f^{13}5d6s$	$^3[11/2]^o_{11/2}$	1427	1347	1365		
	$^3[11/2]^o_{13/2}$	2036	1782	1776		
	$^3[5/2]^o_{7/2}$	3208	2776	2770		
	$^3[5/2]^o_{5/2}$	1518	1246	1237		

[a]Reference [14].
[b]Reference [31] and references therein.
[c]Reference [32].
[d]Reference [40].
[e]Reference [33].

to the $4f^{14}6p\ ^2P^o_{3/2}$ state leads to an appearance of the contribution from the one-electron ME $\langle 6s|H_{\rm hfs}|6s\rangle$, which strongly affects the value of this constant. Based on the results obtained in the single-electron approach (see Table II, the row RPA), we estimate that the core-valence correlation corrections will increase this number, making it even closer to the experimental result. Thus, if the interaction between the $^2P^o_{3/2}$ and $^3[3/2]^o_{3/2}$ states is taken into account, the value of $A(^2P^o_{3/2})$ turns out to be in a good agreement with the experimental result.

We found only one experimental result for the states with the unfilled $4f$ shell listed in Table VI (for the $4f^{13}6s^2\ ^2F^o_{7/2}$ state). Our value agrees with the experiment at the level of 7%. An assignment of uncertainties to the hfs constants of these states is not trivial. One source of errors is the insufficiently large CI space. The corresponding uncertainties may be estimated by a comparison of the results obtained for the [$7sp6df5g$] and [$8sp7df5g$] CI spaces. We see that the difference is not so large (at the level of a few percent). Another source of uncertainties is the core-valence correlations omitted in this approach. A magnitude of these corrections can be estimated using the results obtained in DF + MBPT method (see Table II). For the large hfs constants $A(^2S_{1/2})$ and $A(^2P^o_{1/2})$, they contribute ∼30%–35%. In the 15-electron approach, these corrections are expected to be smaller because the CI core $[1s^2,\ldots,5p^6]$ contains less electrons and is more "hard" than the $[1s^2,\ldots,5p^6, 4f^{14}]$ core. Thus, we estimate accuracy of our results to be at the level of 25%–30%. For comparison, we also present in Table VI the results obtained in the framework of the single-electron MBPT(HO) approach.

We also calculated the $E1$ transition amplitudes for the low-lying states. The reduced MEs of the electric dipole operator d are given in Table VII. It is instructive to compare the results obtained by the single-electron and 15-electron CI methods. This comparison is carried out in Table VIII.

The results indicate the following trend. The values of the MEs of the transitions between the ground and $^2P^o_J$ states are closer to the experimental values in the 15-electron CI approach, while DF + MBPT method gives better agreement with the experiment for the $^2P^o_{1/2}$-$^2D_{3/2}$ transition. As we noted above, taking into account the configuration mixing is important for the $^2P^o_{3/2}$ state. This mixing also manifests itself for the reduced ME $|\langle ^2S_{1/2}||d||^2P^o_{3/2}\rangle|$ although its influence is weaker than for the hfs constant $A(^2P^o_{3/2})$.

We conclude that *all* $|\langle ^2D_J||d||^2P^o_{J'}\rangle|$ matrix elements are obtained to better accuracy in the single-electron method. In the single-electron approach, the $5d$ orbital was constructed for the $f^{14}5d$ configuration which is "native" for the ^2D_J states. In the 15-electron CI approach, it was constructed for the $f^{13}5d6s$ configuration. Most likely, the set of configurations used to form the wave function of the ^2D_J states is not sufficiently large (even for the biggest CI space that we have considered) to correctly reproduce their properties.

TABLE VII. The absolute values of the reduced MEs $|\langle\gamma'||d||\gamma\rangle|$ (in a.u.), where γ are the even-parity states and γ' are the odd-parity states.

	$f^{14}6s\ ^2S_{1/2}$	$f^{14}5d\ ^2D_{3/2}$	$f^{14}5d\ ^2D_{5/2}$
$f^{14}6p\ ^2P^o_{1/2}$	2.51	2.53	
$f^{14}6p\ ^2P^o_{3/2}$	3.32	1.05	3.27
$f^{13}6s^2\ ^2F^o_{7/2}$			0.063
$f^{13}5d6s\ ^3[3/2]^o_{5/2}$		0.00075	0.0037
$f^{13}5d6s\ ^3[3/2]^o_{3/2}$	1.10	0.27	0.86

TABLE VIII. Comparison of the reduced MEs of the electric dipole moment found in the single-electron approach (the row DF + MBPT) and in the 15-electron CI approach (the row 15-el. CI). The values in the row DF + MBPT include the MBPT(HO), RPA, and smaller corrections. The experimental values are presented in the third row.

	$\lvert\langle^2S_{1/2}\lvert\lvert d\rvert\rvert^2P^o_{1/2}\rangle\rvert$	$\lvert\langle^2S_{1/2}\lvert\lvert d\rvert\rvert^2P^o_{3/2}\rangle\rvert$	$\lvert\langle^2D_{3/2}\lvert\lvert d\rvert\rvert^2P^o_{1/2}\rangle\rvert$	$\lvert\langle^2D_{3/2}\lvert\lvert d\rvert\rvert^2P^o_{3/2}\rangle\rvert$	$\lvert\langle^2D_{5/2}\lvert\lvert d\rvert\rvert^2P^o_{3/2}\rangle\rvert$
DF + MBPT	2.75	3.83	3.06	1.35	4.23
15-el. CI	2.51	3.32	2.53	1.05	3.27
Experiment	2.471(3)[a]	3.36(3)[b]	2.97(4)[a]		

[a]References [1,34].
[b]Reference [35], see also explanation in the text.

In the recent work of Huntemann *et al*. [7], the quadrupole moment Θ of the $4f^{13}6s^2\ ^2F^o_{7/2}$ state was measured to be $\Theta = -0.041(5)\,ea_0^2$. The quadrupole moment Θ of a state $|\gamma J\rangle$ (where γ designates all quantum numbers except J) is determined as

$$\Theta = 2\sqrt{\frac{J(2J-1)}{(2J+3)(2J+1)(J+1)}}\langle\gamma J||Q_2||\gamma J\rangle, \qquad (12)$$

where Q_2 is the electric quadrupole operator.

We carried out the calculation of $\Theta(4f^{13}6s^2\ ^2F^o_{7/2})$ for three increasing CI spaces $[6sp5df]$, $[7sp6df5g]$, and $[8sp7df5g]$. The results are presented in Table IX. As illustrated by the table, our result obtained for the largest CI space coincides with the theoretical value of Ref. [41] and is five times greater (in absolute value) than the experimental result. At the same time, we see that Θ is very sensitive to the configuration interaction. The quadrupole moment is rather small due to large cancelations of one-electron contributions, which is expected to make its accurate calculation more difficult. All this makes the result obtained even for the biggest CI space $[8sp7df5g]$ rather inconclusive. Based on our calculations, we can only roughly estimate this quantity as $\Theta(4f^{13}6s^2\ ^2F^o_{7/2}) \sim -0.1\,ea_0^2$.

Finally, we note that an attempt to take into account core-valence correlations by combining the 15-electron CI with the MBPT was unsuccessful. The main problem, which was repeatedly discussed earlier (see, e.g., [42]), is instability of the MBPT for the mean-field potential V^N, which includes a large number of valence electrons. An accounting for the MBPT corrections leads to an appearance of huge contribution from the subtraction diagrams [43]. These diagrams are calculated only in the second order of the MBPT. This is insufficient for accurate treatment of the core-valence correlations.

This problem does not allow us to calculate the SD PNC amplitude more accurately by the 15-electron CI method than it was done in the single-electron approach because the matrix element of the SD PNC Hamiltonian $\langle^2D_J||H_{\rm SD}||^2P^o_{3/2}\rangle$ is greatly increased when we include the RPA and other corrections. To perform similar calculation in the framework of the 15-electron CI, we need to include the subtraction diagrams into consideration, which makes this approach very unstable.

Formulating CI + all-order approach that can treat two-particle–one-hole states on the same footing as the monovalent states appears to be a promising way for a development of methodologies capable to further improve the calculation accuracy of the Yb^+ properties.

TABLE IX. The quadrupole moment Θ of the $4f^{13}6s^2\ ^2F^o_{7/2}$ state (in ea_0^2). The results are presented for three CI spaces $[6sp5df]$, $[7sp6df5g]$, and $[8sp7df5g]$ and compared with the experimental and another theoretical value.

	Θ
$[6sp5df]$	−0.40
$[7sp6df5g]$	−0.06
$[8sp7df5g]$	−0.20
Other theory [41]	−0.22
Experiment [7]	−0.041(5)

IV. CONCLUSION

To conclude, we calculated the energies, magnetic dipole hfs constants, $E1$ transition amplitudes between the low-lying states, and the nuclear spin-dependent parity-nonconserving amplitudes for the $^2S_{1/2}$-$^2D_{3/2,5/2}$ transitions. Our calculations were carried out in the framework of the single-electron DF + MBPT method and by the 15-electron CI method. All-order calculations were also carried out for selected properties using the linearized single-double coupled-cluster method.

The specific character of Yb^+ ion manifests itself due to the presence of the low-lying states with unfilled $4f$ shell. A configuration interaction between them and the states with filled $4f$ shell significantly affects the properties of both types of states. We demonstrated this configuration mixing by analyzing the properties of the $4f^{14}6p\ ^2P^o_{3/2}$ state. In particular, we found that an admixture of the nearby $4f^{13}5d6s\ ^3[3/2]^o_{3/2}$ state should be taken into account. Various contributions to the spin-dependent parity-violating amplitude are discussed and a method to improve accuracy further is proposed.

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