Atomic Structure of Nd\(^{9+}\) for Highly Charged Ion Clocks

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1. Introduction

Highly charged ion (HCI) clocks have been suggested to be some of the most interesting candidates for future frequency metrology, with the aim of breaking precision limits lower than \(10^{-18}\) and aiding in the quest for powerful tools to be used research in physics beyond the Standard Model. The experimental advances in fabrication, cooling, and trapping of highly charged ions have enabled the measurement of the optical spectroscopy of several categories of highly charged ions, such as Nd-like ions [1], the Ho\(^{14+}\) ion [2], the Pr\(^{9+}\) ion [3], the Ni\(^{11+}\)–Ni\(^{14+}\) ions [4], etc. Very recently, the sympathetic cooling and the coherent laser spectroscopy of Ar\(^{13+}\) were demonstrated [5]. All of this progress makes HCIs accessible for high-resolution spectroscopy and precision fundamental studies.

HCIs have high sensitivities to variations in fundamental constants as a consequence of their strong relativistic effects and higher ionization energies. Such high sensitivities can be further enhanced by the electronic-orbital-crossing phenomenon that occurs in inter-configurations. As an Sb-like lanthanide ion, the Nd\(^{9+}\) ion has the core \([1s^2,\ldots,4d^{10},5s^2]\) and three valence electrons in the \(5p\) and \(4f\) shells. The reordering of the \(5p\) and \(4f\) electronic orbital binding energies along the Sb-like isoelectronic sequences generates rich optical transitions over inter-configurations. However, the energy levels due to such
$5p - 4f$ crossings may be very complicated. In particular, the $5s$ orbital has a binding energy that is close to those of the $5p$ and $4f$ shells. This indicates that the two $5s$ electrons should be included in the valent field, considering the Nd$^{9+}$ ion as a five-valent system. For many-electron valent systems, the configuration interaction method (CI) is a widely adopted method, and, in principle, it has no limit for the number of valence electrons. However, calculations of many-valence-electron systems have many practical difficulties in terms of their computational techniques, especially when the number of valence electrons is beyond 4. The accurate prediction of the optical transition in HCl’s with valence electrons in the $4f$ shell is especially challenging. Berengut et al. studied the $4f$–$5p$ level crossing in Nd$^{9+}$ [6]. Complete and consistent information about Nd$^{9+}$ ions remains scarce.

In this work, we adopted two different CI methods—the multi-reference configuration interaction (MRCI) method [7–9] and the configuration interaction plus many-body perturbation theory (CI+MBPT) theory [10,11]. The comparative computation based on the MRCI and CI+MBPT methods ensures the consistency and reliability of our predicted results with minimal uncertainty. Our results show that the $5p$–$4f$ crossing generates wealthy laser-accessible states over the $5p^24f$ and $5p4f^2$ configurations. The long-lived states that are suitable for making clocks are identified. Accurate data on the atomic properties, such as energies, lifetimes, the $g_I$ factor, the magnetic-dipole hyperfine structure (hfs) constants, and the electric quadrupole moment, are predicted. The clock-transition-related properties are calculated, thus validating the dominant systematics that are attainable to below $10^{-19}$. High coefficients of the relativistic sensitivity to variations in the fine-structure constant $\alpha$ and the violation of the local Lorentz invariance are found for the clock transitions of Nd$^{9+}$, indicating its application to studies of a possible varying fine-structure constant $\alpha$ and the violation of the local Lorentz invariance.

2. Computational Methods

2.1. MRCI

The calculations start with the Dirac–Hartree–Fock (DHF) calculation under the Dirac–Coulomb–Gaunt Hamiltonian that is given by

$$\hat{H} = \sum_i [c(\vec{\beta}_i \cdot \vec{p})_i + (\beta - 1)c^2 + V_{iA}] + \sum_{i<j} \left[ \frac{1}{r_{ij}} - \frac{1}{2} \frac{\vec{\beta}_i \cdot \vec{\beta}_j}{r_{ij}} \right],$$

Equation (1)

where $\vec{\beta}$ and $\vec{p}$ are Dirac matrices, $\vec{p}$ is the kinetic momentum, $m_0c^2$ is the resting mass energy of an electron with the speed of light $c$, $V_{iA}$ is the nuclear potential with the atomic mass number $A$, and $r_{ij}$ is the distance between the $i$-th and $j$-th electrons. The last term in Equation (1) is the Gaunt term, which is the leading term of the Breit interaction. The DHF calculation is combined with the relativistic all-electron correlation-consistent optimized basis sets developed by Dyall et al., which contain the $\{24s;19p;13d;8f;2g\}$, $\{30s;24p;16d;11f;3g;2h\}$, and $\{35s;30p;19d;13f;5g;3h;2i\}$ functions in the $2\zeta$, $3\zeta$, and $4\zeta$ basis sets, respectively [12].

Based on the single-electron wavefunctions obtained with the DHF calculation, a string-based Hamiltonian-direct configuration interaction [7–9] calculation was carried out. The electron excitation from the occupied to the virtual orbitals comprised configuration spaces with different sizes by tailoring the numbers of the active electrons and the correlated orbitals to balance the computational cost and accuracy. The maximum of 28 electrons that occupied the $3d$, $4s$, $4p$, and $4d$ orbitals were set in order to allow for a single (S) excitation; five electrons in the $5s$, $5p$, and $4f$ shells were assigned to be valence electrons for single and double (SD) excitations; virtual orbitals with energy less than 10 a.u. were included in the CI space, which contained $9sp9df6g$ (which indicates $s$- and $p$-orbitals with $n \leq 9$, $d$- and $f$-orbitals with $n \leq 8$, and $g$-orbitals with $n \leq 6$) in the $2\zeta$ basis set, $10sp9df6g7h$ in the
2.2. CI+MBPT

The CI+MBPT calculation is based on the Dirac–Coulomb–Breit Hamiltonian, which is similar to Equation (1), with the one-electron Dirac–Fock operator

\[ h_{DF} = c(\mathbf{f}_i \cdot \mathbf{p}_i) + (\beta - 1)mc^2 - \frac{Z}{r} + V_{NDF}(r), \]  

(2)

and the Breit term

\[ B_{ij} = -\frac{1}{2r_{ij}}(\mathbf{f}_i \cdot \mathbf{f}_j + (\mathbf{f}_i \cdot \mathbf{r}_{ij})(\mathbf{f}_j \cdot \mathbf{r}_{ij})/r_{ij}^2), \]  

(3)

where \( V_{DF} \) is the potential of the \( N_{DF} \) electrons included in the self-consistent DHF procedure. Herein, \( N_{DF} \) is either all \( N \) electrons of the atom or some subset of them. The choice of the potential may impact the calculation results. The QED interaction is included by adopting the radiative potential method, which was originally developed by Flambaum and Ginges [14]. The remaining valence and virtual orbitals (pseudostates) are constructed as a linear combination of B-spline basis functions. The configuration space is constructed by allowing SD excitation from the leading configurations, \( 5s^25p^24f \) and \( 5s^25p^4f^2 \), up to \( 8spd f \), alongside the entirety of the SD excitations from the \( 4d \) shells for the large-side CSFs, while the small-side CSFs are restricted to \( 6spd f \) for the SD excitations and \( 8spd f \) for an additional S excitation. Correlations with the frozen core orbitals, i.e., those below \( 4d \) and the virtual orbitals beyond the valence basis set, are treated using the second-order MBPT. The B-spline basis set includes virtual orbitals up to the main quantum number \( n \leq 30 \) and angular momentum \( l \leq 4 \). We use the 'use-valence' flag to include valence–valence MBPT diagrams for orbitals above the valence basis set and below the MBPT basis set. The CI+MBPT calculation was carried out by using the AMBiT code [11].

3. Energy Levels

The excited energies (EEs) of the low-lying states in \( \text{Nd}^{9+} \) obtained with the MRCI calculation are shown in Table 1. We first adopt an intermediate CI model space that correlates 18 core electrons \((4s^24p^64d^{10})\) at the S-excitation level and five valence electrons of the \( 5s, 5p, 4f \) shells at the SD-excitation level; these are referred to as \( '(\text{core}18)_{2\xi}' \), \( '(\text{core}18)_{3\xi}' \), and \( '(\text{core}18)_{4\xi}' \) for the different basis sets. The convergent energy values are obtained at the \( 4\xi \) basis set with a possible error due to the finite-size effect of the basis set, with \( \Delta_{\text{basis}} \) being estimated by the difference between \( '(\text{core}18)_{3\xi}' \) and \( '(\text{core}18)_{4\xi}' \). Two additional calculations are conducted for the \( 2\xi \) basis set: The first calculation includes the triple excitations of the \( 5s, 5p, 4f \) valence electrons, referred to as \( '(\text{core}18)^T' \); this is used to estimate the possible correction due to the triple excitations, \( \Delta_T \), through the difference between \( '(\text{core}18)' \) and \( '(\text{core}18)^T' \); the second calculation extends the inner-core excitations up to the inclusion of 28 core electrons by adding those from the \( 3d \) shell, referred to as \( '(\text{core}28)' \); then, the correction due to more core excitations, \( \Delta_c \), is estimated by the difference between \( '(\text{core}18)' \) and \( '(\text{core}28)' \). The contribution of the QED interaction, \( \Delta_{QED} \), that is absent in the MRCI calculation is taken from the AMBiT calculation. The final results are recommended based on \( '(\text{core}18)_{4\xi}' \) plus \( \Delta_{QED} \), with the corresponding uncertainties assigned according to the rms of \( \Delta_{\text{basis}}, \Delta_T, \) and \( \Delta_c \).
Table 1. The excited energies (EEs) (cm⁻¹) of the energy levels in the Nd⁹⁺ ion obtained with the MRCI calculation.

| Levels | (core18)²⁴ /² | (core28)²⁴ /² | (core18)²⁴ /² | (core18)²⁴ /² | ΔQED | Δn | Δτ | Δε | Final | Unc. |
|--------|----------------|----------------|----------------|----------------|------|----|----|----|-------|-----|
| G0:    | (5p²4f)⁹⁺ /²  | 0              | 0              | 0              | 0    | 0  | −55| −40| 6524  | 69  |
| G1:    | (5p²4f)⁹⁺ /²  | 6568           | 6528           | 6513           | 6569 | 6683| 20 | 15 | −55   | −40 |
| E0:    | (5p²4f)⁹⁺ /²  | 17,352         | 16,606         | 16,649         | 19,142| 20,662| −140| 1521| −703  | −746|
| E1:    | (5p²4f)⁹⁺ /²  | 20,484         | 19,953         | 19,780         | 22,114| 23,243| −81 | 1129| −704  | −531|
| E2:    | (5p²4f)⁹⁺ /²  | 23,687         | 23,081         | 22,903         | 25,859| 27,306| −112| 1446| −784  | −606|
| E3:    | (5p²4f)⁹⁺ /²  | 23,977         | 23,392         | 23,206         | 26,156| 27,533| −95 | 1397| −770  | −585|
| E4:    | (5p²4f)⁹⁺ /²  | 25,615         | 25,032         | 25,463         | 27,728| 29,039| −59 | 1311| −152  | −582|
| E5:    | (5p²4f)⁹⁺ /²  | 26,494         | 26,052         | 26,361         | 28,727| 29,916| −52 | 1190| −132  | −442|
| E6:    | (5p²4f)⁹⁺ /²  | 27,744         | 27,149         | 27,243         | 29,645| 30,968| −44 | 1323| −501  | −605|
| E7:    | (5p²4f)⁹⁺ /²  | 28,061         | 27,466         | 27,403         | 30,327| 31,748| −69 | 1420| −658  | −615|
| E8:    | (5p²4f)⁹⁺ /²  | 29,158         | 28,633         | 28,964         | 31,155| 32,377| −90 | 1222| −194  | −525|
| E9:    | (5p²4f)⁹⁺ /²  | 29,839         | 29,372         | 29,015         | 32,352| 33,713| −101| 1361| −824  | −467|

The EEs obtained by the CI+MBPT calculations are given in Table 2. The changes in the EEs under the V⁹⁺ −5, V⁹⁺ −3, and V⁹⁺ potentials are obvious, more than 2000-3000 cm⁻¹, bringing in certain uncertainty. The Δn considers the changes in the EEs when the valence basis set increases to 10spdf. The final results are given using the results under the V⁹⁺ potential plus ΔQED and Δn.

Table 2. The excited energies (EEs) (cm⁻¹) of the energy level in the Nd⁹⁺ ion obtained with the CI+MBPT calculations.

| Level   | V⁹⁺ −5 | V⁹⁺ −3 | V⁹⁺ | ΔQED | Δn | Final |
|---------|--------|--------|------|------|----|-------|
| G0:     | 0      | 0      | 0    | 0    | 0  | 0     |
| G1:     | 6026   | 6115   | 6064 | 20   | −2 | 6062  |
| E0:     | 23,049 | 21,729 | 19,702| −140| 349| 20,072|
| E1:     | 24,519 | 23,266 | 22,472| −81  | 178| 22,510|
| E2:     | 26,895 | 26,359 | 26,607| −95  | −36| 26,490|
| E3:     | 28,831 | 27,597 | 25,471| −112 | 350| 25,710|
| E4:     | 29,131 | 27,622 | 25,880| −95  | 324| 26,110|
| E5:     | 28,892 | 28,110 | 27,464| −52  | 290| 27,702|
| E6:     | 30,553 | 29,770 | 28,378| −44  | 243| 28,937|
| E7:     | 33,434 | 32,054 | 29,917| −69  | 324| 30,172|
| E8:     | 33,159 | 31,793 | 30,539| −90  | 132| 30,582|
| E9:     | 35,055 | 33,999 | 32,785| −101 | 187| 32,871|

The MRCI and CI+MBPT results for the EEs are consistent within a reasonable error range. The EE results prove that the Nd⁹⁺ ion has a 5p²4f ground configuration. The fine-structure splitting via (5p² 4f)⁹⁺ /² and (5p² 4f)⁹⁺ /², labeled as G0 and G1, respectively, is around 6524(69) cm⁻¹ (MRCI result), which is consistent with the earlier calculations [6,15]. Subsequently, the 5p − 4f orbital crossing raises many of the 5p4f² excited states for those below about 30,000 cm⁻¹, which are listed as E0 to E9 in Tables 1 and 2. Another fine-structure splitting state for the ground configuration, G2: 5p⁸4f, is found in the CI+MBPT calculation.

4. The Atomic Properties

Table 3 compares the results obtained with MRCI and AMBiT for the lifetime τ, gᵣ factor, electric quadrupole moment Θ, and magnetic-dipole hyperfine structure constant A for the energy levels in the Nd⁹⁺ ion. The differences in level energies of the MRCI and AMBiT results change the transition wavelengths and then lead to differences in the τ values. The results for τ justify several long-lived excited states that are suitable for making clock transitions. One good example is the G0:(5p²4f)⁹⁺ /² − E0:(5p4f)⁹⁺ /² transition,
which occurs at 485 (80) nm (the MRCI result) and has a natural linewidth that is estimated to be about 2 milli-Hz in terms of the 67.21 s (the MRCI result) upper-state lifetime. In the case of the odd isotope, hyperfine mixing with faster decaying levels may need to be taken into account, as it can change the lifetime of $E_0 \times (5p^4f^2)_{9/2}^s$, or we can choose appropriate hyperfine sublevels $F$ to adjust the hyperfine–mediate transitions. The results for the $g_f$ factor and the electric quadrupole moment $\Theta$ (a.u.), as they show excellent consistency between the MRCI and CI+MBPT calculations, are used for the evaluation of the systematic effect of the clock transition. 

The Nd element has rich, naturally stable isotopes—$^{142,143,144,145,146,148,150}$Nd. The even isotopes have simple energy levels, which is advantageous for setting up the clock transition, whereas the hyperfine structures also have a wide range of usage for atomic clocks. For completeness, we provide the hyperfine structure constant $A$ (MHz) of $^{143}$Nd$^{9+}$ (nuclear spin $I = 3/2$ and nuclear magnetic moment $\mu_I = -1.08\mu_N$, where $\mu_N$ is a nuclear magneton), which has the greatest natural abundance. Table 4 lists some clock-transition-related properties.

### Table 4. Comparison of the lifetime $\tau$ (s), $g_f$ factor, electric quadrupole moment $\Theta$ (a.u.), and magnetic-dipole hyperfine structure constant $A$ (MHz) of the energy levels in the Nd$^{9+}$ ion obtained with the MRCI and AMBiT calculations.

| Level       | $\tau$ (s) | $g_f$   | $\Theta$ (a.u.) | $A$ (MHz) |
|-------------|------------|--------|-----------------|----------|
|             | MRCI      | AMBiT | MRCI            | AMBiT    | MRCI            | AMBiT    |
| G0: (5p^4f)^5/2          | 0.830 | 0.837 | 0.019 | 0.006 | 1.127 | 1.169 |
| G1: (5p^4f)^5/2          | 0.17  | 0.47  | 1.157 | 1.155 | 0.044 | 0.009 | 1.086 | 1.104 |
| E0: (5p^4f)^5/2          | 67.21 | 49.55 | 0.808 | 0.815 | 0.103 | 0.101 | 0.085 | 0.084 |
| E1: (5p^4f)^5/2          | 0.05  | 0.04  | 0.829 | 0.863 | 0.082 | 0.082 | 2    | 86    |
| E2: (5p^4f)^5/2          | 0.11  | 0.46  | 1.011 | 1.014 | 0.076 | 0.064 | 0.085 | 0.084 |
| E3: (5p^4f)^5/2          | 0.40  | 0.16  | 1.040 | 1.048 | 0.098 | 0.091 | 192   | 228   |
| E4: (5p^4f)^5/2          | 0.04  | 0.04  | 0.676 | 0.689 | 0.032 | 0.023 | 1352  | 1326  |
| E5: (5p^4f)^5/2          | 0.15  | 0.05  | 0.726 | 0.897 | 0.034 | 0.032 | 1215  | 1051  |
| E6: (5p^4f)^5/2          | 0.02  | 0.01  | 1.018 | 1.007 | 0.101 | 0.118 | 437   | 579   |
| E7: (5p^4f)^5/2          | 0.46  | 0.52  | 1.187 | 1.184 | 0.091 | 0.079 | 307   | 274   |
| E8: (5p^4f)^5/2          | 0.02  | 0.08  | 1.152 | 1.188 | 0.079 | 0.085 | 502   | 581   |
| E9: (5p^4f)^5/2          | 0.13  | 0.12  | 1.144 | 1.149 | 0.040 | 0.009 | 748   | 703   |

Table 4. The static scalar and tensor electric dipole polarizabilities, $a_5^{(1)}$ and $a_5^{(2)}$ (a.u.), the magnetic dipole polarizabilities, $a^{M1}$ (a.u.), the values of the reduced matrix elements of $\langle J||T^2||J \rangle$ (a.u.), and the coefficient of the relativistic sensitivity $K$ to variations in $\alpha$.

| Items | G0: $\langle 5p^4f \rangle_{5/2}^p$ | G1: $\langle 5p^4f \rangle_{7/2}^p$ | E0: $\langle 5p^4f^2 \rangle_{7/2}^p$ |
|-------|----------------------------------|----------------------------------|----------------------------------|
| $a_5^{(1)}(J)$ | 2.218 | 2.220 | 2.235 |
| $a_5^{(2)}(J)$ | -0.04 | -0.06 | 0.01 |
| $a^{M1}(J)$ | -4.62 | 3.45 | -2.12 |
| $a^{M1}(F,M_J)=(3,2)$ | $-1.53 \times 10^5$ | $-1.28 \times 10^6$ | $-1.12 \times 10^5$ |
| $\langle J||T^2||J \rangle$ | -73.67 | -85.23 | -85.20 |
| $K$ | 0.72 | 6.52 |

### 5. Conclusions

In conclusion, we investigated the atomic structure of the Nd$^{9+}$ ion as a possible clock frequency standard. Many spectroscopic properties, such as energy levels, lifetimes, $g_f$ factors, electric quadrupole moments, electric dipole polarizabilities, and magnetic-dipole hyperfine structure constants of the low-lying atomic states, were provided by using comparative computations based on the MRCI and CI+MBPT methods. The dominant systematics in Nd$^{9+}$ are attainable below the level of $10^{-19}$. Moreover, a strong sensitivity to violation of the Lorentz invariance and variations in the fine-structure constant $\alpha$ was
found in Nd$^{9+}$. All of these findings strongly suggest the aptness of the Nd$^{9+}$ ion as a promising optical clock and cast its great potential for application for the probing of new physics beyond the Standard Model.

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