

Relativistic coupled-cluster-theory analysis of energies, hyperfine-structure constants, and dipole polarizabilities of Cd^+

Cheng-Bin Li,^{1,*} Yan-Mei Yu,^{2,†} and B. K. Sahoo^{1,3,‡}

¹State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China

²Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

³Atomic, Molecular and Optical Physics Division, Physical Research Laboratory, Navrangpura, Ahmedabad 380009, India



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Roles of electron correlation effects in the determination of attachment energies, magnetic-dipole hyperfine-structure constants, and electric-dipole ($E1$) matrix elements of the low-lying states in the singly charged cadmium ion (Cd^+) have been analyzed. We employ the singles and doubles approximated relativistic coupled-cluster (RCC) method to calculate these properties. Intermediate results from the Dirac-Hartree-Fock approximation, the second-order many-body perturbation theory, and considering only the linear terms of the RCC method are given to demonstrate propagation of electron correlation effects in this ion. Contributions from important RCC terms are also given to highlight the importance of various correlation effects in the evaluation of these properties. At the end, we also determine $E1$ polarizabilities (α^{E1}) of the ground and $5p\ ^2P_{1/2,3/2}$ states of Cd^+ in the *ab initio* approach. We estimate them again by replacing some of the $E1$ matrix elements and energies from the measurements to reduce their uncertainties so that they can be used in the high-precision experiments of this ion.

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I. INTRODUCTION

The distinct electronic structure of a singly charged cadmium ion (Cd^+) has an interesting history in the discovery of the hollow cathode spectrum of cadmium [1] and in the preparation of the Cd-vapor laser in the early days of laser physics [2]. With the advent of ion-trapping and laser-cooling techniques, today the singly charged ions can be well controlled and adopted for carrying out high-precision measurements [3,4]. In fact, the $^{113}\text{Cd}^+$ ion has been under consideration for a compact microwave atomic clock [5] for space research and has achieved a fractional uncertainty of 6.6×10^{-14} to date [6]. Also, trapping of the Cd^+ ion in a semiconductor chip has been demonstrated [7]. One of the other important applications of the Cd^+ ion is it can be used for quantum-information processing. The entanglement between a single trapped Cd^+ ion with a single photon has already been realized [8]. This ion has also been observed in the interstellar medium and the metal-poor stars by the Hubble Space Telescope [9–11]. Thus, understanding of the spectroscopic properties of the Cd^+ ion is of immense interest.

High-precision measurements of the ground-state hyperfine structures of the $^{111}\text{Cd}^+$ and $^{113}\text{Cd}^+$ ions have been reported [6,12–15]. Among these, measurement in the $^{113}\text{Cd}^+$ ion was carried out more precisely for the atomic clock purpose [6]. Apart from the ground state, there are no precise measurements of hyperfine splitting in other excited states available. Similarly, lifetimes of the first two excited states, $5p\ ^2P_{1/2}$ and

$5p\ ^2P_{3/2}$, have been measured to quite high accuracy (about 0.4% uncertainty) [16]. There are also measurements of some of the other excited states available with reasonable accuracies [17]. Therefore, it is necessary to perform theoretical calculations of these quantities to understand the roles of electron correlation effects and predict some of the results to guide the experimentalists in carrying out their measurements and in testing the capabilities of many-body methods to produce these quantities.

Likewise the experiments, there have not been many theoretical calculations performed to investigate the role of electron correlation effects in Cd^+ . Using the GRASP2K package, Yu *et al.* employed the multiconfiguration Dirac-Fock method to calculate the low-lying resonance excitation energies, the absorption oscillator strengths, and the first ionization potential of Cd^+ [18]. Later, Ding *et al.* extended these calculations to give the excitation energies between some of the high-lying states and transition probabilities due to the forbidden transitions [19]. Also, Glowacki and Migdalek performed calculations on the oscillator strengths of the $5s_{1/2}$ - $5p_{1/2,3/2}$ transitions by employing a relativistic configuration-interaction method [20]. Some of the excitation energies and transition matrix elements have been reported using the third-order many-body perturbation theory [MBPT(3) method] [21] and the relativistic coupled-cluster (RCC) method with the linearized terms of singles and doubles excitations (LCCSD method) [22]. A RCC method considering important nonlinear terms in the singles and doubles excitations (CCSD method) has also been applied before to give magnetic-dipole hyperfine-structure constants (A_{hf}) and the lifetimes of a few states [23]. In a recent work, third-order hyperfine-induced dipole polarizabilities were estimated to determine the black-body radiation shift for the Cd^+ clock transition [24]. However, electric-dipole ($E1$)

*cbli@wipm.ac.cn

†ymyu@aphy.iphy.ac.cn

‡bijaya@prl.res.in

polarizabilities (α^{E1}) of none of the states in this ion are known yet. Also, the roles of electron correlation effects in the evaluation of spectroscopic properties of Cd^+ have not been demonstrated explicitly in any of the above theoretical studies. In this work, we intend to analyze these effects in the evaluation of energies, A_{hf} values, and $E1$ matrix elements. We give results considering lower-order many-body methods for better understanding of how correlation effects propagate from lower to all-order levels in the calculations of the above properties in the considered ion. Furthermore, we present α^{E1} values of the ground, $5p^2P_{1/2}$, and $5p^2P_{3/2}$ states of Cd^+ by combining experimental energies and precise values of $E1$ matrix elements.

The remaining part of the paper is organized as follows. In Sec. II, we give the description of the many-body methods employed in the present work. The results are given and discussed in Sec. III before concluding the work in Sec. IV. Unless stated otherwise, atomic units (a.u.) are used throughout the paper.

II. THEORETICAL APPROACHES

A. Computational methods

To carry out the calculations, we consider the Dirac-Coulomb (DC) Hamiltonian which is given by

$$H = \sum_i [c\boldsymbol{\alpha} \cdot \mathbf{p}_i + (\beta - 1)c^2 + V_{\text{nuc}}(r_i)] + \sum_{i < j} \frac{1}{r_{ij}}, \quad (1)$$

where c is the velocity of light; $\boldsymbol{\alpha}$ and β are the Dirac matrices; $V_{\text{nuc}}(r)$ is the nuclear potential, which is evaluated adopting the Fermi charge distribution; and $\frac{1}{r_{ij}} = \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} = \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$ is the two-body interaction potential between the electrons located at \mathbf{r}_i and \mathbf{r}_j . Correction due to the Breit interaction is estimated by adding the following potential energy:

$$V_B(r_{ij}) = -\frac{\{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j + (\boldsymbol{\alpha}_i \cdot \hat{\mathbf{r}}_{ij})(\boldsymbol{\alpha}_j \cdot \hat{\mathbf{r}}_{ij})\}}{2r_{ij}}, \quad (2)$$

where $\hat{\mathbf{r}}_{ij}$ is the unit vector along \mathbf{r}_{ij} . We also estimate contributions from the lower-order quantum electrodynamics (QED) interactions due to the vacuum polarization effects and self-energy (SE) effects using the procedure described in Ref. [25].

The ground-state configuration of Cd^+ is $[4d^{10}]5s$, which can be treated as a system with a closed-core and one valence electron outside. Many of the excited states of this ion also have similar configurations while some of the excited states can be described as the one-hole–one-particle excitation from the $[4d^{10}]5s$ configuration. In this work, we would like to determine the states that are described by the closed core with one valence electron outside. However, we take care of correlations of electrons from these states with those described with one-hole–one-particle excitations. We discuss these frameworks in the perturbative expansion and the RCC theory below.

We adopt Bloch's prescription [26] to build up the perturbative series of the atomic wave function starting with the mean-field wave function $|\Phi_v\rangle$, which is obtained by the

Dirac-Hartree-Fock (DHF) approximation, by expressing

$$|\Psi_v\rangle = \Omega_v |\Phi_v\rangle, \quad (3)$$

where Ω_v is known as the wave operator [26] that is responsible for accounting for the residual interactions neglected in the DHF method. Since all the interested atomic states have the same closed core with one valence electron on different orbitals, we construct $|\Phi_v\rangle = a_v^\dagger |\Phi_0\rangle$, with $|\Phi_0\rangle$ representing the DHF wave function of the closed core (V^{N-1} potential). In the MBPT method, we express

$$\Omega_v = \sum_k \Omega_v^{(k)}, \quad (4)$$

where the superscript k denotes the order of residual Coulomb interactions taken into account in the wave operator. Amplitudes of these wave operators are solved successively for higher orders using Bloch's equation, which is given by [26]

$$[\Omega_v^{(k)}, H_0] |\Phi_v\rangle = \left[V_{\text{res}} \Omega_v^{(k-1)} - \sum_{m=1}^{k-1} \Omega_v^{(k-m)} E_v^{(m-1)} \right] |\Phi_v\rangle.$$

In the above expression, H_0 stands for the DHF Hamiltonian, and $E_v^{(m-1)} = \langle \Phi_v | V_{\text{res}} \Omega_v^{(m-2)} | \Phi_v \rangle$ is the m th-order energy.

In the RCC theory framework, the wave operator follows the exponential ansatz [26]. Therefore, we can express

$$|\Psi_v\rangle \equiv \Omega_v |\Phi_v\rangle = e^{T_v} |\Phi_v\rangle, \quad (5)$$

with the excitation operator T_v . Without loss of generality, we further express $T_v = T + S_v$ for computational simplicity, such that T represents excitations due to correlations among the core electrons maintaining the valence electron as the spectator while S_v takes care of the correlation of the valence electron and the valence electron with the core electrons simultaneously. It, thus, yields

$$|\Psi_v\rangle = e^{T+S_v} |\Phi_v\rangle = e^T \{1 + S_v\} |\Phi_v\rangle. \quad (6)$$

Termination of the exponential for the S_v series is natural here owing to the presence of only one valence electron in the state. We consider only all possible singly and doubly excited configurations through the T and S_v RCC operators in the (L)CCSD method approximation. This is denoted by expressing

$$T = T_1 + T_2 \quad \text{and} \quad S_v = S_{1v} + S_{2v} \quad (7)$$

in our calculations. As we have mentioned before, both the T_1 and S_{2v} operators can generate one-hole–one-particle excitations independently acting upon $|\Phi_v\rangle$ in these formulations. For example, when these operators act on the $[4d^{10}]5s$ and $[4d^{10}]5p_{1/2;3/2}$ configurations they can also generate the $4d^9 5s^2$ and $4d^9 5s 5p$ configurations, respectively, along with other singles and doubles configurations. Therefore, even though we do not calculate the low-lying states with the $4d^9 5s^2$ and $4d^9 5s 5p$ configurations explicitly using our RCC method, their correlation contributions are taken into account implicitly while determining different atomic states.

The amplitudes of both the T and S_v operators are obtained by solving the following equations:

$$\langle \Phi_0^* | \bar{H} | \Phi_0 \rangle = 0 \quad (8)$$

and

$$\langle \Phi_v^* | (\bar{H} - \Delta E_v) S_v | \Phi_v \rangle = -\langle \Phi_v^* | \bar{H} | \Phi_v \rangle, \quad (9)$$

where $|\Phi_0^*\rangle$ and $|\Phi_v^*\rangle$ are the excited state configurations with respect to the DHF wave functions $|\Phi_0\rangle$ and $|\Phi_v\rangle$, respectively, and $\bar{H} = (He^T)_l$, with the subscript l representing the linked terms only. The attachment energy $\Delta E_v = E_v - E_0$, for the energy E_0 of the $[4d^{10}]$ configuration, is evaluated by

$$\Delta E_v = \langle \Phi_v | \bar{H} \{1 + S_v\} | \Phi_v \rangle. \quad (10)$$

For the CCSD method, we consider all possible singles and doubles configurations for the excited determinants $|\Phi_0^*\rangle$ and $|\Phi_v^*\rangle$. Again, we use the approximation $\bar{H} = H + HT + HS_v$ in order to obtain results with the LCCSD method approximation.

With the knowledge of amplitudes of the wave operators in the MBPT and RCC methods, we evaluate the transition matrix element of a general operator O between the states $|\Psi_i\rangle$ and $|\Psi_f\rangle$ using the expression

$$\frac{\langle \Psi_f | O | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}} = \frac{\langle \Phi_f | \Omega_f^\dagger O \Omega_i | \Phi_i \rangle}{\sqrt{\langle \Phi_f | \Omega_f^\dagger \Omega_f | \Phi_f \rangle \langle \Phi_i | \Omega_i^\dagger \Omega_i | \Phi_i \rangle}}. \quad (11)$$

The expectation values are determined by considering $|\Psi_i\rangle = |\Psi_f\rangle$ in this expression. It can also be noticed that the $\Omega_f^\dagger O \Omega_i$ and $\Omega_f^\dagger \Omega_i$ terms contain the nonterminating series $e^{T^\dagger} O e^T$ and $e^{T^\dagger} e^T$ in the CCSD method. These terms are evaluated self-consistently to infinity as discussed in our recent works [27,28].

To estimate typical contributions from the neglected higher-order excitations, we define a triple excitation RCC operator perturbatively involving the valence orbital as

$$S_{3v}^{\text{pert}} = \frac{1}{4} \sum_{ab,pqr} \frac{(HT_2 + HS_{2v})_{abv}^{pqr}}{\Delta E_v + \epsilon_a + \epsilon_b - \epsilon_p - \epsilon_q - \epsilon_r}, \quad (12)$$

where a and b represent the occupied orbitals and p , q , and r represent the virtual orbitals, and the ϵ 's are their corresponding orbital energies. Since this operator involves the valence orbital, it will give the dominant triples contributions that are neglected in the CCSD method. We include this operator in the property evaluating expression to estimate uncertainties due to the neglected higher-level excitations.

B. Atomic properties of concern in this work

We are interested in analyzing the correlation trends in the hyperfine-structure constants (A_{hf}) and the $E1$ transition matrix elements of the low-lying states of Cd^+ . Using the accurate values of the $E1$ matrix elements, we also determine α^{E1} values. General expressions used for these calculations are given below.

The expression for the magnetic-dipole hyperfine-structure constant is given by [29]

$$A_{\text{hf}} = \mu_N g_I \frac{\langle J | | \mathbf{T}_{\text{hf}}^{(M1)} | | J \rangle}{\sqrt{J(J+1)(2J+1)}}, \quad (13)$$

where μ_N is the nuclear magneton and g_I is the ratio of the nuclear-magnetic-dipole moment μ_I and the nuclear spin I . The single-particle matrix element of the hyperfine interaction operator $T_{\text{hf}}^{(M1)} = \sum_i t_{\text{hf}}^{(1)}(r_i)$ is given by

$$\langle \kappa_f | | t_{\text{hf}}^{(1)} | | \kappa_i \rangle = -(\kappa_f + \kappa_i) \langle -\kappa_f | | \mathbf{C}^{(1)} | | \kappa_i \rangle \times \int_0^\infty dr \frac{(P_f Q_i + Q_f P_i)}{r^2}. \quad (14)$$

We have used $g_I = -1.1897722$ and $g_I = -1.2446018$ [30] for the $^{111}\text{Cd}^+$ and $^{113}\text{Cd}^+$ ions, respectively.

We also extract $E1$ matrix elements (in a.u.) from the experimentally known transition probabilities (in s^{-1}) using the following relation:

$$A_{if}^{E1} = \frac{2.02613 \times 10^{18}}{\lambda_{if}^3 g_i} | \langle J_i | | \mathbf{D} | | J_f \rangle |^2, \quad (15)$$

where $g_i = 2J_i + 1$ is the degeneracy factor of the state $|\Psi_i\rangle$ with the angular momentum J_i and λ_{if} is the transition wavelength in \AA . These values are used to compare with our calculations and also to determine the α^{E1} values more precisely.

The expression for the static dipole polarizability is conveniently given by

$$\alpha_i^{E1} = \alpha_i^S + \frac{3M_i^2 - J_i(J_i + 1)}{J_i(2J_i - 1)} \alpha_i^T, \quad (16)$$

where α_i^S and α_i^T are known as the scalar and tensor components of the electric-dipole polarizability for the state $|\Psi_i\rangle$ with angular momentum J_i and its component M_i .

We employ the CCSD method in the equation-of-motion framework [31] using Dyall's relativistic triple- ζ basis function [32] from the DIRAC package [33] to obtain the *ab initio* values of scalar and tensor polarizabilities. A finite-field approach is adopted to express the energy of the $|\gamma_i, J_i, M_i\rangle$ state, for the additional quantum number γ_i , in the presence of an isotropic electric field with strength in the z direction \mathcal{E}_z as

$$E_{\gamma_i, J_i, M_i}(\mathcal{E}_z) = E_{\gamma_i, J_i, M_i}(0) - \frac{\mathcal{E}_z^2}{2} \alpha_{zz}^{E1}(\gamma_i, J_i, M_i) - \dots, \quad (17)$$

where $E_{\gamma_i, J_i, M_i}(\mathcal{E}_z)$ and $E_{\gamma_i, J_i, M_i}(0)$ are the total energies of the state in the absence and the presence of the field, respectively. Here, $\alpha_{zz}^{E1}(\gamma_i, J_i, M_i)$ is its z component of α_i^{E1} and is evaluated as the second derivative of $E_{\gamma_i, J_i, M_i}(\mathcal{E}_z)$ with respect to \mathcal{E}_z . After obtaining $\alpha_{zz}^{E1}(\gamma_i, J_i, M_i)$ values, we determine scalar polarizability by using the relation $\alpha_i^S = \sum_{M_i} \alpha_{zz}^{E1}(\gamma_i, J_i, M_i) / (2J_i + 1)$ and tensor polarizability by using the relation $\alpha_i^T = \alpha_{zz}^{E1}(\gamma_i, J_i, J_i) - \alpha_i^S$.

We also rewrite the expressions for α_i^S and α_i^T as

$$\alpha_i^{S/T} = 2 \langle \Psi_i^{(0)} | \tilde{D} | \Psi_i^{(1)} \rangle, \quad (18)$$

with the unperturbed wave function $|\Psi_i^{(0)}\rangle$ and its first-order correction due to the dipole operator $|\Psi_i^{(1)}\rangle$, to determine dipole polarizabilities in the spherical coordinate system using the atomic orbitals with definite parities. In this expression, we define the respective effective dipole operator for the scalar and the tensor components as described in Ref. [34] to obtain the corresponding expressions for α_i^S and α_i^T . Using the prescribed formalisms in Refs. [34,35], we solve the wave function $|\Psi_i^{(1)}\rangle$ with the DHF and MBPT(3) methods to

estimate the α_i^S and α_i^T values and then compare them with the results obtained using the CCSD method to understand the propagation of electron correlation effects from lower orders to all orders in these calculations.

Our ultimate intention is to provide very precise values of polarizabilities for experimental use. Thus, we would like to reduce the uncertainties in the *ab initio* results by substituting precisely known energies and $E1$ matrix elements from the experimental observations. For this purpose, we also express formulas for α_i^S and α_i^T in the sum-over-states approach as

$$\alpha_i^S = \frac{2}{3(2J_i + 1)} \sum_{n \neq i} \frac{|\langle J_n || \mathbf{D} || J_i \rangle|^2}{E_n - E_i} \quad (19)$$

and

$$\alpha_i^T = 4 \left(\frac{5J_i(2J_i - 1)}{6(J_i + 1)(2J_i + 1)(2J_i + 3)} \right)^{1/2} \times \sum_n (-1)^{J_i + J_n} \begin{Bmatrix} J_i & 1 & J_n \\ 1 & J_i & 2 \end{Bmatrix} \frac{|\langle J_n || \mathbf{D} || J_i \rangle|^2}{E_n - E_i}. \quad (20)$$

It to be noted that for $J_i \leq 1/2$ the α_i^T component does not contribute to α^{E1} owing to the properties of the above $6j$ symbol.

Since we are dealing with atomic states that are expressed as Slater determinants, the $|\langle J_n || \mathbf{D} || J_i \rangle|^2$ values will have contributions from the core orbitals and the continuum. To account for these contributions, we divide contributions to scalar and tensor components as

$$\alpha_i^{S,T} = \alpha_i^{S,T}(c) + \alpha_i^{S,T}(cv) + \alpha_i^{S,T}(v) \quad (21)$$

following the discussions in Ref. [36], where the notations c , cv , and v in the parentheses represent the contributions from the closed core, core-valence interactions, and valence correlations respectively. It can be shown that due to the presence of the phase factor $(-1)^{J_i + J_n}$ in the tensor component of the polarizability, the closed-core contribution becomes zero. Again, $\alpha_i^{S,T}(v)$ will have contributions from both the bound states and the continuum. The contributions from the

bound states are referred to as ‘‘Main’’ contributions while those from the continuum we denote as ‘‘Tail’’ contributions.

III. RESULTS AND DISCUSSION

We present attachment energies of the $(5-7)S$, $(5-6)P$, $5D$, and $4F$ states of Cd^+ in Table I from different methods using the DC Hamiltonian. As can be seen the results from the CCSD method are about 0.5% accurate compared with the experimental values, which are also quoted in the same table from the National Institute of Science and Technology (NIST) database [37]. We have also given corrections from the Breit and QED interactions estimated using the CCSD method. As can be seen, the DHF values are about 10% smaller than the experimental values for the S and P states. Inclusion of the correlation effects through the second-order MBPT [MBPT(2)] and LCCSD methods overestimate the results compared to the experimental values while the CCSD method gives values close to the experimental results. The higher relativistic corrections to the energies are found to be very small. Agreement between our CCSD results with the experimental values for the energies suggest that we can also obtain the hyperfine-structure constants and $E1$ matrix elements of the above states reliably by employing this method.

In Table II, we give the calculated values of A_{hf}/g_I of the $^{113}\text{Cd}^+$ ion from the employed methods. Likewise the energies, the correlations trends from the DHF and CCSD methods are found to be similar in this property. It has also been observed in the earlier studies that the signs of this quantity in the $D_{5/2}$ states are usually different in the DHF and CCSD methods in the alkali-metal atoms [27,38] and singly charged alkaline-earth-metal ions [39], implying that electron correlation effects are more than 100% in these states. However, we do not find such trend in the considered ion. We also find the Breit interaction contributes insignificantly, but the QED corrections to the A_{hf}/g_I values in the S states are seen to be quite large. Unlike other states, the correlation trends in the F states are found to be different. In this case, the final CCSD values are smaller than the DHF results. After multiplying with the respective g_I values of the $^{111}\text{Cd}^+$ and $^{113}\text{Cd}^+$ ions, we have given the A_{hf} values of all the considered

TABLE I. Trends of attachment energies (in a.u.) from different approximated methods. Results including the relativistic corrections from the Breit and QED interactions are also given. The final results from the CCSD method including higher relativistic corrections are compared with the experimental values that are quoted in the NIST database [37] and differences are given in percentages as Δ .

Transition	DHF	MBPT(2)	LCCSD	CCSD	+Breit	+Breit + QED	NIST	Δ
$5s \ ^2S_{1/2}$	-0.5675749	-0.6259303	-0.6275084	-0.6197197	-0.6193345	-0.6190594	-0.6213690	0.4%
$6s \ ^2S_{1/2}$	-0.2326545	-0.2444164	-0.2445125	-0.2429233	-0.2428409	-0.2427841	-0.2432358	0.2%
$7s \ ^2S_{1/2}$	-0.1284520	-0.1329612	-0.1329438	-0.1323406	-0.1323081	-0.1322858	-0.1324703	0.1%
$5p \ ^2P_{1/2}$	-0.3868446	-0.4203548	-0.4237701	-0.4184912	-0.4181088	-0.4180743	-0.4202703	0.5%
$6p \ ^2P_{1/2}$	-0.1816390	-0.1900302	-0.1905469	-0.1892563	-0.1891522	-0.1891432	-0.1898367	0.4%
$5p \ ^2P_{3/2}$	-0.3775864	-0.4087151	-0.4121132	-0.4070980	-0.4068669	-0.4068698	-0.4089593	0.5%
$6p \ ^2P_{3/2}$	-0.1787987	-0.1867903	-0.1873862	-0.1861016	-0.1860382	-0.1860394	-0.1867692	0.4%
$5d \ ^2D_{3/2}$	-0.2057042	-0.2123090	-0.2130057	-0.2123385	-0.2123199	-0.2123194	-0.2127147	0.2%
$5d \ ^2D_{5/2}$	-0.2050792	-0.2115584	-0.2122487	-0.2116222	-0.2116250	-0.2116246	-0.2120107	0.2%
$4f \ ^2F_{5/2}$	-0.1254789	-0.1270271	-0.1273479	-0.1270349	-0.1270362	-0.1270350	-0.1273736	0.3%
$4f \ ^2F_{7/2}$	-0.1254936	-0.1270419	-0.1273539	-0.1270498	-0.1270502	-0.1270495	-0.1273145	0.2%

TABLE II. Calculated A_{hf}/g_I values (in MHz) from different methods. Multiplying $g_I = -1.1897722$ and $g_I = -1.2446018$ in the total values from the CCSD method and higher relativistic corrections, the A_{hf} values for the respective $^{111}\text{Cd}^+$ and $^{113}\text{Cd}^+$ ions are evaluated. These values are compared with the available experimental results and other calculations.

States	DHF	MBPT(2)	LCCSD	CCSD	ΔBreit	ΔQED	$A_{\text{hf}}^{111\text{Cd}^+}$		$A_{\text{hf}}^{113\text{Cd}^+}$		
							This work	Experiment	This work	Others	Experiment
$5s\ ^2S_{1/2}$	9585.78	12318.07	12821.53	12262.32	-1.80	-91.42	14478(175)	14530.507 [12]	15146(183)	15280 [23]	15199.863 [6]
$6s\ ^2S_{1/2}$	2179.67	2570.42	2668.03	2568.77	0.55	-17.76	3036(41)		3176(43)	3230 [23]	
$7s\ ^2S_{1/2}$	877.01	1011.14	1046.84	1010.28	0.72	-6.88	1195(15)		1250(15)		
$5p\ ^2P_{1/2}$	1477.19	1956.30	2084.25	1969.81	-6.04	-2.51	2333(31)		2441(33)	2430 [23]	
$6p\ ^2P_{1/2}$	440.12	531.94	552.47	534.74	-1.02	-0.61	634(10)		664(10)	667.81 [23]	
$5p\ ^2P_{3/2}$	229.08	337.02	364.65	333.89	0.16	-0.20	397(6)		416(6)	406.02 [23]	400 [14]
$6p\ ^2P_{3/2}$	69.97	96.84	109.17	94.47	0.08	-0.07	112(1)		118(1)	118.12 [23]	
$5d\ ^2D_{3/2}$	28.78	44.18	49.75	52.30	0.13	-0.02	62.4(1.1)		65.2(1.2)		
$5d\ ^2D_{5/2}$	12.22	17.89	20.79	20.39	0.07	0.01	24.4(5)		25.5(5)		
$4f\ ^2F_{5/2}$	0.44	0.25	-0.08	0.40	-0.001	-0.002	0.473(12)		0.494(12)		
$4f\ ^2F_{7/2}$	0.24	0.06	0.05	0.05	-0.0014	0.002	0.060(4)		0.063(5)		

states in the same table. Since the mass differences between ^{111}Cd and ^{113}Cd are very small, we have neglected the small changes in the wave functions to evaluate the A_{hf}/g_I values for the $^{111}\text{Cd}^+$ ion here. We also compare our estimated A_{hf} values of these ions with the available experimental values and other calculations. Very precise values of these quantities for the ground state of both the isotopes are available [6,12–15]. Among them the most precise values are reported for the $^{111}\text{Cd}^+$ and $^{113}\text{Cd}^+$ ions as 14 530.507 349 9(11) MHz [12] and 15 199.862 855 019 2(10) MHz [6], respectively. We have only quoted these values up to three decimal places in Table II. Though measurements of A_{hf} values have not been reported precisely in the other states, a preliminary measurement of hyperfine splitting in the $5p\ ^2P_{3/2}$ state of the $^{113}\text{Cd}^+$ ion suggests that its A_{hf} value is about 400 MHz [14]. It can be seen that our calculations agree with the available experimental values quite well. Therefore, we also anticipate that the values estimated for the other states will have similar accuracies. We had also studied these properties

before using the CCSD method [23] without accounting for the Breit and QED interactions. Moreover, we only included a few nonlinear terms from the nonterminating series of $e^{T^\dagger} O e^T$ and $e^{T^\dagger} e^T$ in Eq. (11). Later, we developed procedures to include contributions from these series self-consistently to infinity (see, e.g., Refs. [27,28]). These are the reasons why we obtain improved values of A_{hf} in this work. Also, details of correlation trends are analyzed by us here.

To gain better understanding of the roles of electron correlation effects in the evaluation of the A_{hf}/g_I values in Cd^+ , we present individual contributions from various CCSD terms in Table III. We give contributions as \bar{O} , corresponding to the effective one-body part of $e^{T^\dagger} O e^T$ and other terms linear in T , S_v , and their Hermitian conjugate (H.c.) operators. Corrections due to normalization of the wave functions are also given explicitly. Contributions from the remaining nonlinear terms are given together. The difference between the DHF value and the \bar{O} contribution for a given state implies the role of core correlations. It can be seen that in the states with the angular momentum $J = 1/2$, the core correlations decrease the values

TABLE III. Contributions from different RCC terms to the A_{hf}/g_I calculations (in MHz) without accounting for the normalization of wave functions are given in the CCSD method approximation. Corrections due to the normalization of wave functions are listed under Norm. Contributions from the nonlinear terms that are not given explicitly here are added together and quoted as Others. Contributions from Hermitian conjugate (H.c.) terms are added up.

States	\bar{O}	$OS_{1v} + \text{H.c.}$	$OS_{2v} + \text{H.c.}$	$S_{1v}^\dagger OS_{1v}$	$S_{1v}^\dagger OS_{2v} + \text{H.c.}$	$S_{2v}^\dagger OS_{2v}$	Norm	Others
$5s\ ^2S_{1/2}$	9539.29	1868.98	793.48	91.10	63.00	258.91	-295.38	-57.06
$6s\ ^2S_{1/2}$	2168.24	207.64	164.66	4.95	3.02	63.20	-33.15	-9.79
$7s\ ^2S_{1/2}$	872.61	60.04	64.38	1.03	0.20	27.06	-11.49	-3.55
$5p\ ^2P_{1/2}$	1466.06	397.86	94.04	26.88	13.34	30.77	-42.15	-16.99
$6p\ ^2P_{1/2}$	437.19	64.16	31.46	2.38	2.30	7.31	-7.97	-2.09
$5p\ ^2P_{3/2}$	229.57	61.58	26.54	4.16	3.54	16.83	-6.91	-1.42
$6p\ ^2P_{3/2}$	70.12	10.48	8.62	0.40	0.54	7.48	-1.39	-1.78
$5d\ ^2D_{3/2}$	30.20	7.82	8.84	0.55	0.80	4.05	-0.41	0.45
$5d\ ^2D_{5/2}$	12.77	3.32	3.04	0.23	0.22	0.65	-0.17	0.33
$4f\ ^2F_{5/2}$	0.44	0.04	-0.26	~ 0.00	-0.04	0.30	~ 0.00	-0.08
$4f\ ^2F_{7/2}$	0.25	0.02	-0.24	~ 0.00	-0.04	0.03	~ 0.00	0.03

TABLE IV. Reduced $E1$ matrix elements (in a.u.) of some of the important transitions in Cd^+ from different many-body methods. Our results are also compared with the other reported calculations employing the DHF, MBPT(2), and LCCSD methods in Ref. [22] and values that are extracted from the lifetime measurements [16,17].

$ \Psi_i\rangle \rightarrow \Psi_f\rangle$	DHF	MBPT(2)	LCCSD	CCSD	Ref. [22]			Experiment
					DHF	MBPT(2)	LCCSD ^a	
$5s\ ^2S_{1/2}-5p\ ^2P_{1/2}$	2.427	2.032	1.888	1.970(8)	2.4271	2.0342	1.9392	1.910(4) [16], 1.89(3) [17]
$5s\ ^2S_{1/2}-6p\ ^2P_{1/2}$	-0.063	0.084	0.118	0.079(4)				
$5s\ ^2S_{1/2}-5p\ ^2P_{3/2}$	3.428	2.881	2.678	2.795(11)	3.4280	2.8889	2.7513	2.713(5) [16], 2.79(4) [17]
$5s\ ^2S_{1/2}-6p\ ^2P_{3/2}$	-0.176	0.030	0.087	0.029(3)				
$5p\ ^2P_{1/2}-6s\ ^2S_{1/2}$	1.771	1.689	1.625	1.647(6)				1.72(12) [17]
$5p\ ^2P_{1/2}-5d\ ^2D_{3/2}$	4.011	3.521	3.332	3.475(12)	4.0144	3.7414	3.4401	3.08(13) [17]
$5p\ ^2P_{3/2}-6s\ ^2S_{1/2}$	2.701	2.580	2.482	2.517(10)				2.31(9) [17]
$5d\ ^2P_{3/2}-5d\ ^2D_{3/2}$	1.867	1.649	1.565	1.628(6)	1.8684	1.7444	1.6122	1.57(6) [17]
$5d\ ^2P_{3/2}-5d\ ^2D_{5/2}$	5.581	4.928	4.680	4.868(22)	5.5857	5.2181	4.8195	4.62(5) [17]

^aDenoted as SD method in the original paper.

from the DHF method while for other angular momentum states the values are increasing. As we had discussed in our earlier work [40], the terms OS_{1v} and OS_{2v} (along with their H.c. terms) represent the all-order pair-correlation and core-polarization effects, respectively. Other terms can be interpreted as the higher-order correlations representing one of these kinds. It can be observed from the above table that the pair-correlation and core-polarization effects are equally important in the determination of A_{hf}/g_I values in the S states; the former types are more significant in the $5S$ and $6S$ states while the later effects are slightly larger than the former in the $7S$ state. In the P states also, the pair-correlation effects play the dominant roles. However, the core-polarization effects are found to play significant roles in the states with higher angular momentum. Contributions from the normalization of the wave functions and the nonlinear terms appearing through property evaluation expressions are also found to be non-negligible.

In Table IV, we present the magnitudes of the reduced $E1$ matrix elements for some of the important transitions of Cd^+ . As can be seen, in most of the cases the DHF values are very large and the correlation effects reduce the magnitudes. This trend is different from the studies of the magnetic-dipole hyperfine-structure constants. We also find that the values are reduced slightly from the DHF values in the MBPT(2) method, but then they are reduced drastically in the LCCSD method. The CCSD method gives values intermediate between the

MBPT(2) and LCCSD methods, suggesting that the nonlinear terms of the RCC method cancel with some of the correlation effects arising with the LCCSD method. It is also noticed that the DHF values in the $5s\ ^2S_{1/2}-6p\ ^2P_{1/2}$ and $5s\ ^2S_{1/2}-6p\ ^2P_{3/2}$ transitions have signs opposite those of the results after including the correlation effects. This means that the electron correlation effects are larger than 100% in these transitions. We also quote uncertainties in the CCSD results by analyzing contributions due to the partial triples contributions. We have compared our calculations with the values that are inferred from the lifetime measurements of many excited states reported in the literature [16,17]. Unlike the hyperfine-structure constants, we find large discrepancies between our results with the experimental values in this property. We also give $E1$ matrix elements from other calculations that are reported using the DHF method, the MBPT(2) method, and the RCC theory similar to our LCCSD approximation [defined as the all-order singles and doubles (SD) method] [22]. In our work, we use a Gaussian type of orbital to define the single-particle matrix elements; however B-spline polynomials were used in Ref. [22]. Nevertheless, we find good agreement between these two works in the DHF and MBPT(2) methods. Large differences are observed among the values from the LCCSD and the SD methods. Since the nonlinear terms in the CCSD method increase values obtained with the LCCSD method, we also anticipate that values obtained with the SD method will

TABLE V. Individual contributions from different CCSD terms to the reduced $E1$ matrix elements (in a.u.) of the transitions given in Table IV.

Transition	\bar{O}	OS_{1i}	$S_{1f}^\dagger O$	OS_{2i}	$S_{2f}^\dagger O$	$S_{1f}^\dagger OS_{1i}$	$S_{1f}^\dagger OS_{2i}$	$S_{2f}^\dagger OS_{1i}$	$S_{2f}^\dagger OS_{2i}$	Norm	Others
$5s\ ^2S_{1/2}-5p\ ^2P_{1/2}$	2.424	-0.118	-0.002	-0.155	-0.208	0.014	-0.007	-0.001	0.029	-0.045	0.039
$5s\ ^2S_{1/2}-6p\ ^2P_{1/2}$	-0.062	-0.123	0.168	0.054	0.086	-0.018	-0.005	0.004	-0.009	-0.002	-0.014
$5s\ ^2S_{1/2}-5p\ ^2P_{3/2}$	3.424	-0.176	0.008	-0.211	-0.289	0.019	-0.011	-0.001	0.046	-0.062	0.048
$5s\ ^2S_{1/2}-6p\ ^2P_{3/2}$	-0.175	-0.163	0.226	-0.011	0.125	-0.025	-0.006	0.005	-0.014	-0.0005	0.068
$5p\ ^2P_{1/2}-6s\ ^2S_{1/2}$	1.773	0.194	-0.306	0.007	0.018	-0.0004	0.007	-0.011	-0.0006	-0.028	0.006
$5p\ ^2P_{1/2}-5d\ ^2D_{3/2}$	4.011	-0.360	0.085	-0.118	-0.045	0.010	-0.008	-0.002	0.027	-0.051	-0.074
$5p\ ^2P_{3/2}-6s\ ^2S_{1/2}$	2.704	0.276	-0.433	0.003	0.020	0.002	0.009	-0.016	-0.0005	-0.043	-0.004
$5p\ ^2P_{3/2}-5d\ ^2D_{3/2}$	1.867	-0.157	0.036	-0.053	-0.065	0.005	-0.004	0.0005	0.013	-0.023	0.009
$5p\ ^2P_{3/2}-5d\ ^2D_{5/2}$	5.581	-0.475	0.109	-0.159	-0.192	0.015	-0.010	0.002	0.041	-0.072	0.028

TABLE VI. Correlation trends in the determination of α^{E1} values (in a.u.) using various approximations in Cd^+ .

Method	$5s\ ^2S_{1/2}$	$5p\ ^2P_{1/2}$	$5p\ ^2P_{3/2}$	
	Scalar	Scalar	Scalar	Tensor
DHF	36.792	33.913	39.927	-6.433
MBPT(3)	22.273	27.964	31.982	-4.327
CCSD	24.637	25.817	30.594	-3.681
CCSD + Experiment	25.2(6)	25.2(1.5)	28.1(6)	-2.3(4)

be larger after taking into account the nonlinear contributions. Therefore, large discrepancies between the CCSD values and the experimental results may be able to be addressed by including full triples and quadruple excitations in the RCC theory.

We also give contributions from the individual terms of the CCSD method to the $E1$ amplitudes in Table V. It can be found from the differences between the DHF values and the \bar{O} contributions that the core correlations are negligible in this property. The pair-correlation effects arising through the S states in the S - P transitions and the P states in the P - D transitions are found to be quite large. However, this trend seems to be the reverse for the core-polarization correlation contributions. Correlation contributions from the other terms are found to be very small. This indicates that it would be necessary to include correlation effects that can influence the pair-correlation and core-polarization correlations strongly in order to achieve more precise values of the $E1$ matrix elements.

We intend to present now the dipole polarizabilities of the atomic states of Cd^+ . These quantities are very useful for the high-precision measurements. Thus, we would like to estimate them more precisely for the general interest. It is worth noting that the allowed transitions among low-lying states are very useful for the cooling mechanism of singly charged ions. Knowledge of accurate values of α^{E1} for the states associated with these transitions will be required for such studies. In this view, we determine the α^{E1} values of the ground, $5p\ ^2P_{1/2}$, and $5p\ ^2P_{3/2}$ states of Cd^+ here.

First, we present *ab initio* results of α^{E1} in Table VI obtained with the DHF, MBPT(3), and CCSD methods in the perturbative and finite-field approaches as described in Sec. III. As can be seen, the DHF method predicts relatively larger values and the MBPT(3) method, which uses energies and $E1$ matrix elements at the level of the MBPT(2) method approximation, brings down the results. Then, the CCSD method gives an intermediate value between those two lower-order methods for the ground state while it decreases further the α^{E1} values in all other states. Since the correlation effects with respect to the DHF values are found to be strong in these quantities, we would like to reduce their uncertainties by substituting the precise data of $E1$ matrix elements from the lifetime measurements of the low-lying states of Cd^+ and experimental energies with the CCSD results. For this purpose, we have used the sum-over-states approach to estimate the most accurate data and we quote the values in the Table VI as CCSD + Experiment. As seen, these semiempirical values differ significantly from the corresponding CCSD results. The reason for this is obvious from the comparison of the $E1$ matrix elements from the CCSD method with the experimental

TABLE VII. Breakdown of contributions to α^{E1} values (in a.u.) of the ground, $5p\ ^2P_{1/2}$, and $5p\ ^2P_{3/2}$ states in Cd^+ by combining experimental data and calculations from the CCSD method. Intermediate contributions to Main are quoted, in which precisely available experimental $E1$ matrix elements are used. We also use the $E1$ matrix elements from our previous work, Ref. [24], which are not discussed in this paper, to estimate their contributions. Both the Tail and Core-valence contributions are given from the DHF method, while the Core correlations are determined using the random-phase approximation (RPA).

Contributions	$E1$ amplitude	Source	α^{E1}
Scalar polarizability of the ground state			
From Main			
$5p\ ^2P_{1/2}$	1.910(4)	Experiment [16]	6.047(25)
$(6-12)p\ ^2P_{1/2}$		This work [24]	0.016
$5p\ ^2P_{3/2}$	2.713(5)	Experiment [16]	11.551(43)
$(6-12)p\ ^2P_{3/2}$		This work [24]	0.011
From $4d^9\ 5s5p$ configurations		This work [24]	2.6(5)
Tail		This work	0.012
Core-valence		This work	-0.018
Core		This work	4.986
Scalar polarizability of the $5p\ ^2P_{1/2}$ state			
From Main			
$5s\ ^2S_{1/2}$	1.910(4)	Experiment [16]	-6.047(25)
$6s\ ^2S_{1/2}$	1.72(12)	Experiment [17]	5.57(80)
$(7-12)s\ ^2S_{1/2}$		This work [24]	0.393
$5d\ ^2D_{3/2}$	3.08(13)	Experiment [17]	15.2(1.3)
$6d\ ^2D_{3/2}$		This work [24]	3.546
$(7-12)d\ ^2D_{3/2}$		This work [24]	0.809
$4d\ ^9S\ ^2D_{3/2}$	0.49(2)	Experiment [17]	0.57(2)
Tail		This work	0.375
Core-valence		This work	-0.193
Core		This work	4.986
Scalar polarizability of the $5p\ ^2P_{3/2}$ state			
From Main			
$5s\ ^2S_{1/2}$	2.713(5)	Experiment [16]	-5.775(21)
$6s\ ^2S_{1/2}$	2.31(9)	Experiment [17]	5.37(42)
$(7-12)s\ ^2S_{1/2}$		This work [24]	0.426
$5d\ ^2D_{3/2}$	1.57(6)	Experiment [17]	2.09(16)
$(6-12)d\ ^2D_{3/2}$		This work [24]	0.209
$5d\ ^2D_{5/2}$	4.62(5)	Experiment [17]	18.06(39)
$(6-12)d\ ^2D_{3/2}$		This work [24]	1.961
$4d^9\ 5s^2\ ^2D_{3/2}$	0.29(4)	Experiment [17]	0.11(3)
$4d^9\ 5s^2\ ^2D_{5/2}$	0.58(4)	Experiment [17]	0.54(8)
Tail		This work	0.341
Core-valence		This work	-0.189
Core		This work	4.986
Tensor polarizability of the $5p\ ^2P_{3/2}$ state			
From Main			
$5s\ ^2S_{1/2}$	2.713(5)	Experiment [16]	5.775(21)
$6s\ ^2S_{1/2}$	2.31(9)	Experiment [17]	-5.37(42)
$(7-12)s\ ^2S_{1/2}$		This work [24]	-0.426
$5d\ ^2D_{3/2}$	1.57(6)	Experiment [17]	1.67(13)
$(6-12)d\ ^2D_{3/2}$		This work [24]	0.167
$5d\ ^2D_{5/2}$	4.62(5)	Experiment [17]	-3.61(8)
$(6-12)d\ ^2D_{3/2}$		This work [24]	-0.392
$4d^9\ 5s^2\ ^2D_{3/2}$	0.29(4)	Experiment [17]	0.09(3)
$4d^9\ 5s^2\ ^2D_{5/2}$	0.58(4)	Experiment [17]	-0.11(2)
Tail		This work	-0.084
Core-valence		This work	0.010

values in Table IV. We have also quoted the uncertainties to the results obtained from the combined experimental and CCSD results. The breakdown of various contributions to these quantities for the CCSD + Experiment approach is given in Table VII. It can be noticed that we have also used many matrix elements in this approach from our CCSD method that are not quoted in Table IV but that are given in another of our recent works [24]. We also give contributions from Tail, core-valence, and core-correlation contributions to the sum-over-states approach in Table VII. Since the Tail and core-valence correlation contributions are extremely small, they are estimated using the DHF method. Comparatively, the core-correlation contributions to the scalar polarizabilities are larger. We have estimated these contributions using the RPA as described by us earlier [41]. Our final values for the ground and $5p\ ^2P_{3/2}$ states are found to be quite precise, but we still get a quite sizable amount of uncertainty to the α^{E1} value of the $5p\ ^2P_{1/2}$ state owing to the large uncertainty associated with the $5p\ ^2P_{1/2}$ - $6s\ ^2S_{1/2}$ transition.

IV. SUMMARY

We have investigated electron correlation trends in the energies, hyperfine-structure constants, and electric-dipole matrix elements of the singly charged ion. We have employed mean-field, finite-order perturbation, and all-order coupled-cluster theories in the relativistic framework to carry out these analyses. Our results employing singles and doubles approximated relativistic coupled-cluster methods are found to agree very well with the experimental results, but the electric-dipole matrix elements do not agree well with those extracted

from the lifetime measurements. Further theoretical studies are required to explain the reasons for such large discrepancies. We have also given the hyperfine-structure constants of many states. These results will be useful to guide the experimentalists to measure them precisely and test the validity of our calculations. Correlation trends to the *ab initio* values of the dipole polarizabilities in the first three low-lying states of Cd^+ are also given using the Dirac-Hartree-Fock approximation, the third-order many-body theory, and the singles and doubles approximated coupled-cluster methods. We also deduce them more accurately by replacing the calculated $E1$ matrix elements by the precisely known electric-dipole matrix elements wherever available and combining with the experimental energies in a sum-over-state approach. These quantities will be helpful to carry out high-precision measurements in the Cd^+ ion.

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