I. INTRODUCTION

The ytterbium atom has two fermionic and five bosonic isotopes, a $^1S_0$ ground state, a long-lived metastable $^6S^1P^0_1$ state, and transitions at convenient wavelengths for laser cooling and trapping. All this makes Yb a superb candidate for a variety of applications such as development of optical atomic clocks [1], study of degenerate quantum gases [2], quantum information processing [3], and studies of fundamental symmetries [4]. The best quantum gases [2], quantum information processing [3], and studies of fundamental symmetries [4] have also been proposed for searches for the electron electric-dipole (EDM) which constrains extensions of the standard model of particle physics. The best limit to date on the value of the electron electric-dipole moment (EDM) which constrains extensions of the standard model to date on the value of the electron electric-dipole moment (EDM) which constrains extensions of the standard model [4] is $d_{e} = 1932(35)$ [10]. However, fit of the $C_6$ and $C_8$ coefficients for the $^1S_0$ state was rather uncertain, with strong correlation between the $C_6$ and $C_8$ fit parameters [15].

Knowledge of the $C_6$ and $C_8$ long-range interaction coefficients in Yb-Yb dimers is critical to understanding the physics of dilute gas mixtures. Recently, we evaluated the $C_6$ coefficient for the Yb-Yb $^1S_0 + ^1S_0$ dimer and found it to be $C_6 = 1929(39)$ [19], in excellent agreement with the experimental result $C_6 = 1932(35)$ [10]. However, the same method cannot be directly applied to the calculation of the van der Waals coefficients with Yb-Yb $^1S_0 + ^3P^0_1$ dimer owing to the presence of the $^3P^0_1 \rightarrow ^1S_0$ decay channel.

In this work, we develop the methodology for an accurate evaluation of the van der Waals coefficients of dimers involving excited state atoms with a strong decay channel to the ground state and evaluate $C_6$ and $C_8$ coefficients of particular experimental interest. We carefully study the uncertainties of all quantities calculated in this work so the present values can be reliably used to analyse existing measurements and to facilitate planning of the future experimental studies. The methodology developed in this work can be used for evaluation of van der Waals coefficients in a variety of systems.

II. GENERAL FORMALISM

We investigate the molecular potentials asymptotically connecting to the $|A\rangle + |B\rangle$ atomic states. The wave function of such a system constructed from these states is

$$|M_A, M_B; \Omega\rangle = |A\rangle_1 |B\rangle_1,$$

where

- $|A\rangle_1$ and $|B\rangle_1$ are the atomic states;
- $M_A$ and $M_B$ are the magnetic quantum numbers of the atomic states;
- $\Omega$ is the total angular momentum of the system.

The excited molecular states asymptotically connected to the $^1S_0 + ^3P^0_1$ separated Yb atom limit were investigated by Takasu et. al. in [12]. They reported the successful production of a subradiant $^1S_0$ state of a two-atom Yb system in a three-dimensional optical lattice. The properties of the long-range potential were studied and the van der Waals coefficients $C_3$, $C_6$, and $C_8$ were predicted. However, fit of the $C_6$ and $C_8$ coefficients for the $^1S_0$ state was rather uncertain, with strong correlation between the $C_6$ and $C_8$ fit parameters [15].
where the index I(II) describes the wave function located on the center I(II) and \( \Omega = M_A + M_B \). Here, the \( M_{A(B)} \) is the projection of the appropriate total atomic angular momentum \( J_{A(B)} \) on the internuclear axis. We assume that \( \Omega \) is a good quantum number for all calculations in this work (Hund’s case (c)).

The molecular wave functions can be obtained by diagonalizing the molecular Hamiltonian

\[
\hat{H} = \hat{H}_A + \hat{H}_B + \hat{V}(R)
\]

in the model space. Here, \( \hat{H}_A \) and \( \hat{H}_B \) represent the Hamiltonians of the two noninteracting atoms and \( \hat{V}(R) \) is the residual electrostatic potential defined as the full Coulomb interaction energy in the dimer excluding interactions of the atomic electrons with their parent nuclei.

Unless stated otherwise, throughout this paper we use atomic units (a.u.); the numerical values of the elements of the atomic electrons with their parent nuclei.

The potential \( V(R) \) may be expanded as an expression in the multipole interactions:

\[
V(R) = \sum_{l,L=0}^{\infty} V_{lL}/R^{l+L+1},
\]

where \( V_{lL} \) are given by

\[
V_{lL}(R) = \sum_{\mu=-1}^{l} \frac{(-1)^{l}(l + L)!}{(l - \mu)!(l + \mu)!(l - \mu)!(L + \mu)! \sqrt{l} / \mu} \times \left( T^{(l)}_{\mu} \right)_I \left( T^{(L)}_{-\mu} \right)_{II}.
\]

Here, \( l_s = \min(l, L) \) and the multipole spherical tensors are

\[
T^{(K)}_{\mu} = -\sum_i r_i^K C^{(L)}_{\mu}(\hat{r}_i),
\]

where the summation is over atomic electrons, \( r_i \) is the position vector of electron \( i \), and \( C^{(L)}_{\mu}(\hat{r}_i) \) are the reduced spherical harmonics.

We now restrict our consideration to the dipole-dipole and dipole-quadrupole interactions. Introducing designations \( d_{\mu} \equiv T^{(1)}_\mu \), \( Q_{\mu} \equiv T^{(2)}_\mu \), \( V_{dd} \equiv V_{11}/R^4 \), and \( V_{dq} \equiv V_{12}/R^4 \), we obtain from Eq. (3):

\[
V_{dd}(R) = -\frac{1}{R^3} \sum_{\mu=-1}^{1} w^{(1)}_{\mu} (d_{\mu})_I (d_{-\mu})_{II},
\]

\[
V_{dq}(R) = \frac{1}{R^4} \sum_{\mu=-1}^{1} w^{(2)}_{\mu} [(d_{\mu})_I (Q_{-\mu})_{II} - (Q_{\mu})_I (d_{-\mu})_{II}],
\]

where the dipole and quadrupole weights are

\[
\begin{align*}
    w^{(1)}_{\mu} &\equiv 1 + \delta_{\mu,0}, \\
    w^{(2)}_{\mu} &\equiv \frac{6}{\sqrt{(1 - \mu)! (1 + \mu)! (2 - \mu)! (2 + \mu)!}},
\end{align*}
\]

Numerically, \( w^{(2)}_{-1} = w^{(2)}_{+1} = \sqrt{3} \) and \( w^{(2)}_{0} = 3 \).

The energy \( \mathcal{E} \equiv E_A + E_B \), where \( E_A \) and \( E_B \) are the atomic energies of the \( |A\rangle \) and \( |B\rangle \) states, is obtained from

\[
\left( \hat{H}_A + \hat{H}_B \right) (M_A, M_B; \Omega) = \mathcal{E} (M_A, M_B; \Omega).
\]

The molecular wave functions \( \Psi^{\Omega}_{\Omega} \) can be formed as a linear combination of the wave functions given by Eq. (1).

\[
\Psi^{\Omega}_{\Omega} \equiv \{ \frac{1}{\sqrt{2}} (|A\rangle_1 |B\rangle_{II} + (-1)^P |B\rangle_1 |A\rangle_{II}), A \neq B \}
\]

where we set \( P = 0 \) for ungerade symmetry and \( P = 1 \) for gerade symmetry. We have taken into account that the states \( A \) and \( B \) that are of interest to the present work are the opposite parity states of Yb atom (when \( A \neq B \)).

Applying the formalism of Rayleigh-Schrödinger perturbation theory in the second order \([22]\) and keeping the terms up to \( 1/R^6 \) in the expansion of \( V(R) \) we obtain the dispersion potential in two-atom basis:

\[
U(R) \equiv \langle \Psi^{\Omega}_{\Omega} | V(R) | \Psi^{\Omega}_{\Omega} \rangle
\]

\[
\approx \langle \Psi^{\Omega}_{\Omega} | \hat{V}_{dd} | \Psi^{\Omega}_{\Omega} \rangle + \sum_{\Psi_i \neq \Psi^{\Omega}_{\Omega}} \frac{\langle \Psi^{\Omega}_{\Omega} | \hat{V}_{dd} | \Psi_i \rangle \langle \Psi_i | \hat{V}_{dd} | \Psi^{\Omega}_{\Omega} \rangle}{\mathcal{E} - E_i} + \frac{\langle \Psi^{\Omega}_{\Omega} | \hat{V}_{dq} | \Psi_i \rangle \langle \Psi_i | \hat{V}_{dq} | \Psi^{\Omega}_{\Omega} \rangle}{\mathcal{E} - E_i},
\]

The intermediate molecular state \( |\Psi_i\rangle \) with unperturbed energy \( E_i \) runs over a complete set of two-atom states, excluding the model-space states, Eq. (1).

The dispersion potential can be approximated as

\[
U(R) \approx \frac{-C_3}{R^3} - \frac{C_6}{R^6} - \frac{C_8}{R^8}.
\]

**A. First-order corrections**

The first-order correction, which is determined by the first term on the right-hand side of Eq. (9), is associated with the \( C_3 \) coefficient in Eq. (10). For the states considered in this work, this coefficient is nonzero only for the molecular potential asymptotically connecting to the \( ^3S_0 + ^1P_1 \) atomic states. It depends entirely on the reduced matrix element (ME) of the electric-dipole operator \( |^3P_1| |d| ^1S_0 \rangle \) and is given by a simple formula

\[
C_3(\Omega_p) = (-1)^{P+\Omega} (1 + \delta_{\Omega,0}) \frac{|\langle ^3P_1 | |d| ^1S_0 \rangle|^2}{3}.
\]
Specifically,

\[ C_3(0_{g/u}) = \pm \frac{2}{3} \left| \langle 3P_1 | d | S_0 \rangle \right|^2, \]
\[ C_3(1_{g/u}) = \pm \frac{1}{3} \left| \langle 3P_1 | d | S_0 \rangle \right|^2, \]

where the upper/lower sign corresponds to gerade/ungerade symmetry.

**B. Second-order corrections**

The second-order corrections, associated with the \( C_6 \) and \( C_8 \) coefficients, are given by the second and third terms on the r.h.s. of Eq. (9).

\[ -\frac{C_6(\Omega_p)}{R^6} = \sum_{\Psi_i \neq \Psi_{\Omega_p}} \frac{\langle \Psi_{\Omega_p} | \hat{V}_{dd} | \Psi_i \rangle \langle \Psi_i | \hat{V}_{dd} | \Psi_{\Omega_p} \rangle}{\mathcal{E} - E_i}, \]
\[ -\frac{C_8(\Omega_p)}{R^8} = \sum_{\Psi_i \neq \Psi_{\Omega_p}} \frac{\langle \Psi_{\Omega_p} | \hat{V}_{dd} | \Psi_i \rangle \langle \Psi_i | \hat{V}_{dd} | \Psi_{\Omega_p} \rangle}{\mathcal{E} - E_i}, \]

where \( \mathcal{E} = E_A + E_B \) and the complete set of doubled atomic states satisfies the condition

\[ \sum_{\Psi_i} |\Psi_i \rangle \langle \Psi_i| = 1. \]

After angular reduction, the \( C_6 \) coefficient can be expressed as

\[ C_6(\Omega) = \sum_{J_A + 1 \leq J_B} \sum_{J_A - 1 \leq J_B} A_{J_A J_B}(\Omega) X_{J_A J_B}, \]

where

\[ A_{J_A J_B}(\Omega) = \sum_{\mu, M_\mu, M_\beta} \left( \frac{J_A}{-M_\mu} \frac{J_B}{-M_\beta} \right)^2 \]

\[ X_{J_A J_B} = \sum_{\alpha, \beta \neq A, B} \frac{\langle A | d | \alpha \rangle^2 \langle B | d | \beta \rangle^2}{E_{\alpha} - E_A + E_{\beta} - E_B}, \]

with fixed \( J_A \) and \( J_B \).

If \( A \) and \( B \) are the spherically symmetric atomic states and there are no downward transitions from either of them, the \( C_6 \) and \( C_8 \) coefficients for the \( A + B \) dimers are given by well known formulas (see, e.g., [23])

\[ C_6^{AB} = C^{AB}(1,1), \]
\[ C_8^{AB} = C^{AB}(1,2) + C^{AB}(2,1), \]

where the coefficients \( C^{AB}(l, L) \) \( (l, L = 1, 2) \) are quadratures of electric-dipole, \( \alpha_1(\omega) \), and electric-quadrupole, \( \alpha_2(\omega) \), dynamic polarizabilities at an imaginary frequency:

\[ C^{AB}(1,1) = \frac{3}{2\pi} \int_0^\infty \alpha_1^A(\omega) \alpha_1^B(\omega) d\omega, \]
\[ C^{AB}(1,2) = \frac{15}{2\pi} \int_0^\infty \alpha_1^A(\omega) \alpha_2^B(\omega) d\omega, \]
\[ C^{AB}(2,1) = \frac{15}{2\pi} \int_0^\infty \alpha_2^A(\omega) \alpha_1^B(\omega) d\omega. \]

For the Yb-Yb \( ^1S_0 + 3P_0 \) dimer considered in this work, the expressions for \( C_6 \) and \( C_8 \) are more complicated due to the angular dependence, the \( ^3P_0^d \rightarrow ^1S_0 \) decay channel and non-vanishing quadrupole moment of the \( ^3P_0^d \) state. After some transformations, we arrive at the following expression for the \( C_6 \) coefficient in the \(^1S_0 + 3P_0^d \) case:

\[ C_6(\Omega_p) = \sum_{J=0}^2 A_J(\Omega) X_J, \]

where the angular dependence \( A_J(\Omega) \) is represented by

\[ A_J(\Omega) = \frac{1}{3} \sum_{\mu=-1}^1 \left( \frac{w_\mu(1)}{w_\mu(1)} \right) \left( \frac{1}{-\Omega - \mu - \Omega + \mu} \right)^2 \]

with the dipole weights \( w_\mu(1) \) given by Eq. (6) and \( \Omega = 0, 1 \). It is worth noting that \( A_J(\Omega) \) (and, consequently, the \( C_6 \) coefficients) do not depend on gerade/ungerade symmetry.

The quantities \( X_J \) for the \(^1S_0 + 3P_0^d \) dimer are given by

\[ X_J = \frac{27}{2\pi} \int_0^\infty \alpha_1^A(\omega) \alpha_1^B(\omega) d\omega + \delta X_0 \delta_{J,0}, \]

where \( A \equiv ^1S_0 \) and \( B \equiv ^3P_0^d \) and \( \delta X_0 \) is defined below. The possible values of the total angular momentum \( J \) are 0, 1, and 2; \( \alpha_1^A(\omega) \) is the electric-dipole dynamic polarizability of the \( ^1S_0 \) state at the imaginary argument.

The quantity \( \alpha_K(\omega) \) is a part of the scalar electric-dipole (\( K = 1 \)) or electric-quadrupole (\( K = 2 \)) dynamic polarizability of the state \( \Phi \), in which the sum over the intermediate states \( |n \rangle \) is restricted to the states with fixed total angular momentum \( J_n = J \):

\[ \alpha_K^\Phi(\omega) = \frac{2}{(2K+1)(2J+1)} \times \sum_{\gamma_n} \frac{(E_n - E_\Phi)(|\gamma_n, J_n = J ||T^{(K)}||\gamma_n, J_\Phi)|^2}{(E_n - E_\Phi)^2 + \omega^2}. \]

Here, \( \gamma_n \) stands for all quantum numbers of the intermediate states except \( J_n \).

The correction \( \delta X_0 \) to the \( X_0 \) term in Eq. (19) is due to a downward \( ^3P_0^d \rightarrow ^1S_0 \) transition and is given by the following expression:

\[ \delta X_0 = 2 \left| \langle 3P_0^d | | S_0 \rangle \right|^2 \sum_{n\neq 3P_0^d} \frac{(E_n - E_{3S0})(|n\rangle | | S_0 \rangle)^2}{(E_n - E_{3S0})^2 - \omega_0^2} + \left| \langle 3P_0^d | | S_0 \rangle \right|^4 \frac{1}{2\omega_0}, \]
where \( \omega_0 \equiv E_{1s^n} - E_{1s^0} \).

The expression for the \( C_s(1\text{S}_0 + 3\text{P}_0^e) \) coefficient is substantially more complicated, so it is discussed in the Appendix.

### III. Method of Calculation

All calculations were carried out by two methods which allow us to estimate the accuracy of the final values. The first method combines configuration interaction (CI) with many-body perturbation theory (MBPT) \[24\]. In the second method, which is more accurate, CI is combined with the coupled-cluster all-order approach (CI+all-order) that treats both core and valence correlation to all orders \[25-27\].

In both cases, we start from a solution of the Dirac-Fock (DF) equations for the appropriate states of the individual atoms,

\[
H_0 \psi_c = \varepsilon_c \psi_c,
\]

where \( H_0 \) is the relativistic DF Hamiltonian \[24, 26\] and \( \psi_c \) and \( \varepsilon_c \) are single-electron wave functions and energies. The calculation was performed in the \( V^{N-2} \) approximation, i.e., the self-consistent procedure was done for the \([1s^2, \ldots, 4f^{14}]\) closed core. The B-spline basis set, consisting of \( N = 35 \) orbitals for each of partial wave with \( l \leq 5 \), was formed in a spherical cavity with radius 60 a.u. The CI space is effectively complete. It includes the following orbitals: 6–20s, 6–20p, 5–19d, 5–18f, and 5–11g.

The wave functions and the low-lying energy levels are determined by solving the multiparticle relativistic equation for two valence electrons \[28\],

\[
H_{\text{eff}}(E_n) \Phi_n = E_n \Phi_n.
\] (22)

The effective Hamiltonian is defined as

\[
H_{\text{eff}}(E) = H_{\text{FC}} + \Sigma(E),
\] (23)

where \( H_{\text{FC}} \) is the Hamiltonian in the frozen-core approximation. The energy-dependent operator \( \Sigma(E) \) which takes into account virtual core excitations is constructed using the second-order perturbation theory in the CI+MBPT method \[24\] and using linearized coupled-cluster single-double method in the CI+all-order approach \[29\]. \( \Sigma(E) = 0 \) in the pure CI approach. Construction of the effective Hamiltonian in the CI+MBPT and CI+all-order approximations is described in detail in Refs. \[24, 26\]. The contribution of the Breit interaction is negligible at the present level of accuracy and was omitted.

The dynamic polarizability of the \( 2K \)-pole operator \( T^{(K)} \) at imaginary argument is calculated as the sum of three contributions: valence, ionic core, and \( vc \). The \( vc \) term subtracts out the ionic core terms which are forbidden by the Pauli principle. Then

\[
\alpha_K(i\omega) = \alpha_K^v(i\omega) + \alpha_K^{vc}(i\omega),
\] (24)

where both the core and \( vc \) parts are included in \( \alpha_K^v(i\omega) \).

### A. Valence contribution

The valence part of the dynamic polarizability, \( \alpha_K^v(i\omega) \), of an atomic state \( |\Phi\rangle \) is determined by solving the inhomogeneous equation in the valence space. If we introduce the wave function of intermediate states \( |\delta\Phi\rangle \) as

\[
|\delta\Phi\rangle \equiv \text{Re} \left\{ \frac{1}{H_{\text{eff}} - E_{\Phi} + i\omega} \sum_i |\Phi_i\rangle \langle \Phi_i| T^{(K)}_{0} |\Phi\rangle \right\}
\]

\[
= \text{Re} \left\{ \frac{1}{H_{\text{eff}} - E_{\Phi} + i\omega} T^{(K)}_{0} |\Phi\rangle \right\},
\] (25)

where \( \text{Re} \) means the real part, then \( \alpha_v^v(i\omega) \) is given by

\[
\alpha_v^v(i\omega) = 2 \langle \Phi | T^{(K)}_{0} |\delta\Phi\rangle.
\] (26)

Here, \( T^{(K)}_0 \) is the zeroth component of the \( T^{(K)} \) tensor. We include random-phase approximation (RPA) corrections to the \( 2^K \)-pole operator \( T^{(K)}_0 \). The Eqs. \[24, 26\] can also be used to find \( \alpha_v^{vc} \), i.e., the part of the valence polarizability, where summation goes over only the intermediate states with fixed total angular momentum \( J \). We refer the reader to Ref. \[29\] for further details of this approach.

### B. Core contribution

The core and \( vc \) contributions to multipole polarizabilities are evaluated in the single-electron relativistic RPA approximation. The small \( \alpha^{vc} \) term is calculated by adding \( vc \) contributions from the individual electrons, i.e., \( \alpha^{vc}(6s^2) = 2 \alpha^{vc}(6s) \) and \( \alpha^{vc}(6s6p) = \alpha^{vc}(6s) + \alpha^{vc}(6p) \).

A special consideration is required when we need to find the core contribution to \( \alpha_K^{vc}(i\omega) \) of a state \( \Phi \). If we disregard possible excitations of the core electrons to the occupied valence shells, the valence and core subsystems can be considered as independent. Then, the total angular momenta \( J_{\Phi} \) and \( J_n \) of the states \( \Phi \) and \( \Phi_n \), respectively, can be represented as the sum of the valence and core parts \( J = J_v + J_c \). In our consideration, the core of the \( \Phi \) state consists of the closed shells, and \( J_c = 0 \). If we assume that the electrons are excited from the core, while the valence part of the wave function remains the same, we can express the reduced matrix element of the operator \( T^{(K)} \) as

\[
\langle J_{\Phi} || T^{(K)} || J_n \rangle = \langle J_c^0 = 0, J_v, J_{\Phi} || T^{(K)} || J_c^0 = K, J_v, J_n \rangle.
\] (27)

If \( T^{(K)} \) acts only on the core part of the system, we arrive at (see, e.g., \[21\])

\[
\langle J_c^0 = 0, J_v, J_{\Phi} || T^{(K)} || J_c^0 = K, J_v, J_n \rangle = \sqrt{\frac{2J_n + 1}{2K + 1}} \langle J_c^0 = 0 || T^{(K)} || J_c^0 = K \rangle.
\] (28)
Then, using Eq. (20), we can write the core contribution to \( \alpha_{KJ}(i\omega) \) of the \( \Phi \) state as

\[
\alpha_{KJ}^c(i\omega) = \frac{2(2J+1)}{(2K+1)^2(2J_\Phi+1)} \sum_{\gamma_n} \frac{(E_n - E_\Phi)(|J_\Phi = 0||T^{(K)}||J_n = K)|^2}{(E_n - E_\Phi)^2 + \omega^2}, \tag{29}
\]

Taking into account that the core polarizability \( \alpha_{KJ}^c(i\omega) \) of the operator \( T^{(K)} \) in a single-electron approximation can be written as

\[
\alpha_{KJ}^c(i\omega) = \frac{2}{2K+1} \times \sum_{\alpha,n} \frac{\epsilon_n - \epsilon_\alpha}{(\epsilon_n - \epsilon_\alpha)^2 + \omega^2} \left(|n||T^{(K)}||\alpha\right)^2, \tag{30}
\]

where \( |\alpha\rangle \) and \( |n\rangle \) are the single-electron core and virtual states, we arrive at

\[
\alpha_{KJ}^c(i\omega) = \frac{2J+1}{(2K+1)(2J_\Phi+1)} \alpha_{KJ}^c(i\omega). \tag{31}
\]

Finally, \( \alpha_{KJ}(i\omega) \) of the \( \Phi \) state can be approximated as

\[
\alpha_{KJ}(i\omega) = \alpha_{KJ}^c(i\omega) + \frac{2J+1}{(2K+1)(2J_\Phi+1)} \alpha_{KJ}^s(i\omega), \tag{32}
\]

where possible values of \( J \) are from \( \min(0,|J_\Phi - K|) \) to \( J_\Phi + K \).

### IV. RESULTS AND DISCUSSION

#### A. Energy levels

We start from the calculation of the low-lying energy levels of atomic Yb. The calculations were carried out using CI, CI+MBPT, and CI+all-order methods. The results are listed in Table I (see also the Supplemental Material to Ref. [19]) in columns labeled “CI”, “CI+MBPT”, and “CI+All”. Two-electron binding energies are given in the first row, energies in other rows are counted from the ground state. Corresponding relative differences of these three calculations with the experiment are given in cm\(^{-1}\) and in percentages.

#### B. Polarizabilities

In Table II we give a breakdown of the main contributions from the intermediate states to the static electric-dipole and electric-quadrupole polarizabilities of the \( 6s^2 \) \( ^1S_0 \), \( 6s6p \) \( ^3P_0 \), and \( 6s6p \) \( ^3P_1 \) states in the CI+all-order approximation. For the \( ^3P_1 \) state the contributions to the scalar parts of the polarizabilities are presented. While we do not explicitly use the sum-over-states to
TABLE II: A breakdown of the contributions to the 6s² ¹S₀, 6s6p ¹P₀, and 6s6p ¹P₁ electric-dipole, α₁, and electric-quadrupole, α₂, static polarizabilities in the CI+all-order approximation. For the ¹P₁ state, the scalar polarizabilities are given. The row labeled “Other” gives the contribution of all other valence states not explicitly listed in the table. The row labeled “Total” lists the final values obtained as the sum of all contributions. \(|\langle n|T^{(K)}|m\rangle\) are the reduced matrix elements; \(T^{(1)} = d\) and \(T^{(2)} = Q\) stand for the electric-dipole and electric-quadrupole operators, respectively. The theoretical and experimental transition energies are presented in columns \(\Delta E_{\text{th}}\) and \(\Delta E_{\text{exp}}\) (in cm\(^{-1}\)). The contributions to the polarizabilities are given in the column labeled “\(\alpha\)”. We also give the breakdown of the 6s² contribution to the polarizability was analyzed in Ref. [19] (see the Supplemental Material). We compare the ¹P₀ case with the contributions to the scalar part of the ¹P₁ polarizability given in Table II. We find that the main contributions to the 6s6p ¹P₀ and 6s6p ¹P₁ polarizabilities are similar in every respect. In particular, the 5d⁷s ³D₃ states contribute \(\sim 57\%\) to both polarizabilities. The contributions of the 6s6d ³D₂ states are at the level of 7-10%. The higher-excited states not explicitly listed in the table, labeled as “Other”, contribute \(\sim 21\%\) in both cases.

![FIG. 1: (Color online) Low-lying energy levels of Yb. Other states of the 4f¹³5d⁶s² configuration are not shown.](image-url)
TABLE III: The values of the $D \equiv |(6s6p^3P_1^u)[d]|6s^2 1S_0)$ matrix element (in a.u.) and $C_3$ coefficients in the CI+MBPT and CI+all-order approximations.

|          | CI+MBPT | CI+all-order | Experiment     |
|----------|---------|--------------|----------------|
| $C_3(0_u)$ | 0.225   | 0.218        | 0.1940(11)     |
| $C_3(0_g)$ | -0.225  | -0.218       |                |
| $C_3(1_u)$ | -0.113  | -0.109       |                |
| $C_3(1_g)$ | 0.113   | 0.109        | 0.09685        |

*Reference [31]. The experimental number was obtained from the weighted $^3P_1^u$ lifetime $\tau(^3P_1^u) = 845(12)$ ns;
*Reference [7] (this error is pure statistical); 'Reference [2].

contribution (listed in rows “Other”) is significant for all polarizabilities considered here. These contributions are at the level of 15–18%. The uncertainties of the polarizability values are discussed later in Section V

C. $C_3$ coefficients

The values of the $C_3$ coefficients obtained in the CI+MBPT and CI+all-order approximations for the $1S_0 + ^3P_0^g$ dimer are given in Table III (also see the Supplemental Material [32]). We calculated the $|(6s6p^3P_1^u)[d]|6s^2 1S_0)$ matrix element (ME) and then found $C_3$ coefficients using Eq. [12]. The $C_3(0_g)$ and $C_3(1_u)$ have the same numerical values as $C_3(0_u)$ and $C_3(1_g)$, but the opposite sign. Our CI+all-order value for this ME differs from the experimental results by 4-5%. It is not unexpected, because the $1S_0 - ^3P_1$ transition is an intercombination transition and due to cancelation of different contributions its amplitude is relatively small. It may be also affected by the mixing with the core-excited states that are outside of our CI space as is discussed in detail in [19]. As a result, the accuracy of calculation of such MEs is lower. Using Eq. [12] we can estimate the accuracy of $C_3$ coefficients at the level of 8-10%.

D. $C_6$ and $C_8$ coefficients

To find the van der Waals coefficients for the $1S_0 + ^3P_0^g$ and $^3P_0^g + ^3P_0^g$ dimers we computed the dynamic electric-dipole and electric-quadrupole polarizabilities of the $1S_0$ and $^3P_0^g$ states at imaginary frequency and then used Eqs. [15] and [10]. In practice, we computed the $C_6^{AB}$ coefficients by approximating the integral [17] by Gaussian quadrature of the integrand computed on the finite grid of discrete imaginary frequencies [33]. The $C_6$ coefficient for the $1S_0 + 1S_0$ dimer was obtained in Ref. [19].

The calculation of the $C_6$ and $C_8$ coefficients for the $1S_0 + ^3P_1$ dimer was carried out according to the expressions given by Eqs. [18]-[19] and in the Appendix A.

TABLE IV: A breakdown of the contributions to the $C_6(\Omega)$ for Yb-Yb (1S0 + ^3P1) dimer. The expressions for X, $\delta X$, and $\delta A$ are given by Eqs. [15]-[19]. The $\delta X_0$ term is given separately in the second row; it is included in $J = 0$ contribution. The CI+MBPT and CI+all-order values for $X_J$ are given in columns labeled “MBPT” and “All”.

| $J$ | $X_J$ | $A_J$ | $C_6(\Omega)$ |
|-----|-------|-------|---------------|
|     | MBPT  | All HO | $\Omega = 0$ | $\Omega = 1$ | $\Omega = 0$ | $\Omega = 1$ |
| 0   | 1107  | 1135  | 2.5%         | 4/9           | 1/9           | 504           | 126          |
| $\delta_0$ | 248  | 253   | 2.0%         | 4/9           | 1/9           | 112           | 28           |
| 1   | 4564  | 4480  | -1.9%        | 5/18          | 1/9           | 498           | 1244         |
| 2   | 6752  | 6702  | -0.7%        | 11/45         | 19/90         | 1638          | 1415         |
| Sum | 2753  | 2814  |              |               |               | 73593         |              |

TABLE V: A breakdown of the contributions to the $C_6(\Omega)$ for Yb-Yb (1S0 + ^3P1) dimer. The expressions for $X_J$, $\delta X$, and $\delta A$ are given in Appendix A. The $\delta X_0$ term is designated as $\delta x_0^J$ and is given separately in the fifth row; it is included in the $X_J$ contribution. The CI+all-order values are given for $X_J$, $\delta X$, and $C_6$; the relative differences of the CI+all-order and CI+MBPT values are given in columns labeled “HO” in %.

| $J$, $\delta X$, $\delta A$, $C_6(\Omega)$ |
|------------------------------------------|
| $\delta_x^J$ | 66588 | 0.5% |
| 11.1 | 107772 | 0.0% | 3/5 | 1/5 | 46463 | 21554 |
| 12.1 | 392687 | -0.6% | 1/15 | 7/15 | 26179 | 183254 |
| 13.1 | 249267 | -1.1% | 43/105 | 31/105 | 102081 | 73593 |
| $\delta_x^\alpha$ | 6510 | 1.4% |
| 20.2 | 35061 | 3.5% | 3/5 | 1/5 | 21037 | 7012 |
| 21.2 | 142845 | -0.4% | 1/5 | 2/5 | 28569 | 75138 |
| 22.2 | 213240 | 0.7% | 9/25 | 8/25 | 76766 | 68237 |
| 11.3 | 1061 | -5.6% | $\pm 3/5$ | $\pm 1/5$ | $\pm 637$ | $\pm 212$ |
| 22.4 | 550 | -15% | $\pm 9/25$ | $\pm 3/25$ | $\pm 198$ | $\pm 66$ |
| $C_6(\Omega)$ | 320130 | 411067 |
| $C_8(\Omega)$ | 318461 | 410511 |
TABLE VI: The \(6s^2\) \(S_0\), \(6s6p^3P_0^o\), and \(6s6p^3P_1^o\) electric-dipole, \(\alpha_1\), and electric-quadrupole, \(\alpha_2\), static polarizabilities in the CI+MBPT and CI+all-order approximations (in a.u.). For the \(3P_1^o\) state the scalar parts of the polarizabilities are presented. The values of \(C_6(\Omega_{u/g})\) and \(C_8(\Omega_{u/g})\) coefficients for the \(A + B\) dimers in the CI+MBPT and CI+all-order approximations are listed in the second part of the table. The (rounded) CI+all-order values are taken as final.

| Level | Property | CI+MBPT | CI+all | HO | Final | Other |
|-------|----------|---------|--------|-----|-------|-------|
| \(6s^2\) \(S_0\) | \(\alpha_1\)^a | 138.3 | 140.9 | 1.8% | 141(2) | 141(6)b |
| \(6s6p^3P_0^o\) | \(\alpha_1\)^a | 305.9 | 293.2 | -4.3% | 293(10) | 302(14)b |
| \(6s6p^3P_1^o\) | \(\alpha_1\) | 323.3 | 315.3 | -2.5% | 315(11) | |
| \(6s^2\) \(1S_0\) | \(\alpha_2\) | 2484 | 2550 | 2.9% | 2560(80) | |
| \(6s6p^3P_0^o\) | \(\alpha_2\) | 21294 | 20601 | -3.4% | 20600(700) | |
| \(6s6p^3P_1^o\) | \(\alpha_2\) | 22923 | 22017 | -4.1% | 22000(900) | |
| \(1S_0 + 1S_0\) | \(C_6\)^a | 1901 | 1929 | 1.5% | 1929(39) | 1932(35)e |
| \(C_8\) | 182360 | 187860 | 2.9% | 1.88(6) | 1.9(5)×10^3 |
| \(1S_0 + 3P_0^o\) | \(C_6\) | 2609 | 2561 | -1.9% | 2561(95) | 2709(338)b |
| \(2P_0^o + 3P_0^o\) | \(C_6\) | 3916 | 3746 | -4.5% | 3746(180) | 3886(360)b |
| \(1S_0 + 3P_1^o\) | \(C_6(0\omega_{u})\) | 2649 | 2640 | -0.3% | 2640(103) | 2410(220)f |
| \(C_6(1\omega_{u})\) | 2824 | 2785 | -1.4% | 2785(109) | 2283.6g |
| \(C_6(0\omega_{g})\) | 321097 | 320130 | -0.3% | 3.20(14)×10^5 | |
| \(C_6(1\omega_{g})\) | 412779 | 411067 | -0.4% | 4.11(18)×10^5 | |
| \(C_6(0\omega_{g})\) | 319300 | 318461 | -0.3% | 3.18(14)×10^5 | |
| \(C_6(1\omega_{g})\) | 412180 | 410511 | -0.4% | 4.11(18)×10^5 | |

a Safronova et al. [19], theory.
b Dzuba and Derevianko [34], theory.
c Zhang and Dalgarno [35], based on experiment.
d Sahoo and Das [36], theory.
e Kitagawa et al. [10], experiment.
f Borkowski et al. [2], experiment; the error includes only uncertainty of the fit.
g Takasu et al. [12], experiment.

A breakdown of the contributions to the \(C_6(\Omega)\) coefficients for Yb–Yb \(S_0 + 3P_0^o\) dimer is given in Table V. We list the quantities \(X_{k,Î,Îs}^A\) and coefficients \(A_{k,Î,Îs}^B\) (the analytical expressions for them are given in the Appendix A). The \(\delta X_{11}^{(1)}\) and \(\delta X_{20}^{(2)}\) terms are given separately in the first and fifth rows; they are included in the \(X_{11}^{(1)}\) and \(X_{20}^{(2)}\) contributions, respectively. For calculation of \(\delta X_{11}^{(1)}\) we used the values \([|3P_1^o^0Q|3P_1^0]| = 17.73\) a.u. and the static \(1S_0\) polarizability \(\alpha_1^2(0) = 140.9\) a.u. obtained in the CI+all-order approximation. The coefficients \(A_{11}^{(1)}\) and \(A_{22}^{(2)}\) contain \((-1)^p\), therefore their sign is different for gerade and ungerade symmetry resulting in slightly different values for \(C_6(\Omega_{u})\) and \(C_8(\Omega_{g})\). In Table V the \(+/−\) sign corresponds to the ungerade/gerade symmetry, respectively.

The CI+all-order values are given for \(X_{k,Î,Îs}^A\) and \(C_6\); the relative differences of the CI+all-order and CI+MBPT values are given in column labeled “HO” in %.

Our final results for polarizabilities and the van der Waals \(C_6\) and \(C_8\) coefficients are summarized in Table VI.

The \(6s^2\) \(S_0\), \(6s6p^3P_0^o\), and \(6s6p^3P_1^o\) electric-dipole, \(\alpha_1\), and electric-quadrupole, \(\alpha_2\), static polarizabilities in the CI+MBPT and CI+all-order approximations are listed in a.u. For the \(3P_1^o\) state the scalar parts of the polarizabilities are presented. The values of \(C_6(\Omega_{u/g})\) and \(C_8(\Omega_{u/g})\) coefficients for the \(A + B\) dimers in the CI+MBPT and CI+all-order approximations are listed in the second part of the table. The (rounded) CI+all-order values are taken as final. The relative contribution of the higher-order corrections is estimated as the difference of the CI+all-order and CI+MBPT results, it is listed in column labeled “HO” in percent.

V. DETERMINATION OF UNCERTAINTIES

We compare frequency-dependent polarizabilities calculated in the CI+MBPT and CI+all-order approximations for all \(\omega\) used in our finite grid to estimate the uncertainties of the \(C_6\) and \(C_8\) coefficients. We find that the difference between the CI+all-order and CI+MBPT frequency-dependent polarizability values is largest for \(\omega = 0\) and decreases significantly with increasing \(\omega\). This is reasonable because for large \(\omega\) the main contribution to the polarizability comes from its core part. But the core parts are the same for both CI+all-order and CI+MBPT approaches.
Therefore, the fractional uncertainty $\delta C^{AB}(l, L)$ ($l, L = 1, 2$) may be expressed via fractional uncertainties in the static multipole polarizabilities of the atoms $A$ and $B$ [37],

$$\delta C^{AB}(l, L) = \sqrt{(\delta \alpha^{A}_l(0))^2 + (\delta \alpha^{B}_l(0))^2}. \quad (33)$$

The absolute uncertainties induced in $C^{AB}_6$ and $C^{AB}_8$ ($A \neq B$) are given by

$$\Delta C^{AB}_6 = \Delta C^{AB}(1, 1),$$
$$\Delta C^{AB}_8 = \sqrt{(\Delta C^{AB}(1, 2))^2 + (\Delta C^{AB}(2, 1))^2}. \quad (34)$$

The polarizabilities and their absolute uncertainties are presented in Table VI. The uncertainties of the electric-quadrupole static and dynamic polarizabilities were discussed in detail in Ref. [19]; the uncertainty of the $3^P_0$ polarizability was determined to be 3.4%. Table II illustrates that the accuracy of calculation of the $3^P_0$ and $3^P_1$ energy levels is practically the same ($\sim 2.5\%$ at the CI+all-order stage). We use the same method of solving the homogeneous equation to determine both the $3^P_0$ and $3^P_1$ polarizabilities. The main contributions to these polarizabilities are also very similar. Based on these arguments, we assume that the uncertainty of the scalar part of the $3^P_0$ polarizability can be estimated at the level of 3.5%.

Our estimates of the uncertainties of the electric-quadrupole polarizabilities are based on the differences between the CI+MBPT and CI+all-order values. Besides that we take into account that in all cases the dominant contribution comes from the low-lying state which energies we reproduce well (see Table II). Based on the size of the higher-order correction, we assign the uncertainties 3–4% to these polarizabilities. These results, as well as the final (recommended) values of the polarizabilities, are presented in Table VII (see also Ref. [22]).

Using Eqs. (33) and (34) we estimated the fractional uncertainties of the $C_6$ coefficient for the $1^S_0 + 3^P_{0,1}$ dimers at the level of 4–4.5%. The uncertainty of the $C_8(1^S_0 + 3^S_1)$ coefficient is 3.2% and the uncertainties of the $C_8(1^S_0 + 3^P_0)$ coefficients are $\sim 4.5\%$. The difference of the CI+all-order and CI+MBPT values (4.5%) is taken as an uncertainty for the $C_8(3^P_0 + 3^P_1)$ coefficient.

VI. CONCLUSION

To conclude, we evaluated the electric-dipole and electric-quadrupole static and dynamic polarizabilities for the $6s^2 1^S_0$, $6s6p^3^P_0$, and $6s6p^3^P_1$ states and estimated their uncertainties. The $C_6$ and $C_8$ coefficients are evaluated for the Yb-Yb dimers. The uncertainties of our calculations of the van der Waals coefficients do not exceed 5%. Our result $C_8 = 1.88(6) \times 10^5$ for the $1^S_0 + 1^S_0$ dimer is in excellent agreement with the experimental value $C_8 = 1.9(5) \times 10^5$ [10]. The quantities calculated in this work allow future benchmark tests of molecular theory and experiment. Most of these quantities are determined for the first time. Methodology developed in this work can be used to evaluate properties of other dimers with excited atoms that have a strong decay channel.

Acknowledgement

We thank P. Julienne for helpful discussions. This research was performed under the sponsorship of the U.S. Department of Commerce, National Institute of Standards and Technology, and was supported by the National Science Foundation under Physics Frontiers Center Grant No. PHY-0822671 and by the Office of Naval Research. The work of S.G.P. was supported in part by US NSF Grant No. PHY-1212442 and RFBR Grant No. 11-02-00943. The work of A.D. was supported in part by the US NSF Grant No. PHY-1212482.

Appendix A: $C_8$ coefficients for the $1^S_0 + 3^P_0$ dimer

Following formalism of Section III the $C_8$ coefficient may be expressed as:

$$C_8(\Omega_p) = \sum_{A, B \neq \alpha, \beta} \frac{\langle AB | \tilde{V}_{dq} | \alpha \beta \rangle \langle \alpha \beta | \tilde{V}_{dq} | AB \rangle + (-1)^p \langle AB | \tilde{V}_{dq} | \alpha \beta \rangle \langle \alpha \beta | \tilde{V}_{dq} | BA \rangle}{E_{\alpha} + E_{\beta} - \varepsilon},$$

which can be further reduced to:

$$C_8(\Omega_p) = \sum_{k=1}^{4} \sum_{J_a, J_b} A_{k}^{J_a J_b}(\Omega_p) X_{k}^{J_a J_b},$$
where

\[ A_{1}^{J_{\alpha}J_{\beta}}(\Omega) = \sum_{\mu M_{\alpha}M_{\beta}} \left\{ w^{(2)}_{\mu} \left( \begin{array}{ccc} J_{A} & 1 & J_{\alpha} \\ -M_{A} & \mu & M_{\alpha} \end{array} \right) \left( \begin{array}{ccc} J_{B} & 2 & J_{\beta} \\ -M_{B} & -\mu & M_{\beta} \end{array} \right) \right\}^{2}, \]

\[ X_{1}^{J_{\alpha}J_{\beta}} = \sum_{\alpha \beta} \frac{|\langle A|d|\alpha\rangle(\Omega)|^{2}|\langle B|Q|\beta\rangle(\Omega)|^{2}}{E_{\alpha} - E_{A} + E_{\beta} - E_{B}}, \]

\[ A_{2}^{J_{\alpha}J_{\beta}}(\Omega) = \sum_{\mu M_{\alpha}M_{\beta}} \left\{ w^{(2)}_{\mu} \left( \begin{array}{ccc} J_{A} & 1 & J_{\alpha} \\ -M_{A} & \mu & M_{\alpha} \end{array} \right) \left( \begin{array}{ccc} J_{B} & 2 & J_{\beta} \\ -M_{B} & -\mu & M_{\beta} \end{array} \right) \right\}^{2}, \]

\[ X_{2}^{J_{\alpha}J_{\beta}} = \sum_{\alpha \beta} \frac{|\langle A|Q|\alpha\rangle(\Omega)|^{2}|\langle B|d|\beta\rangle(\Omega)|^{2}}{E_{\alpha} - E_{A} + E_{\beta} - E_{B}}. \]

\[ A_{3}^{J_{\alpha}J_{\beta}}(\Omega_{p}) = (-1)^{p} \sum_{\mu M_{\alpha}M_{\beta}} (-1)^{J_{\alpha}+J_{\beta}+J_{\alpha}+J_{\beta}+1} w^{(2)}_{\mu} w^{(2)}_{\alpha}, \]

\[ X_{3}^{J_{\alpha}J_{\beta}} = \sum_{\alpha \beta} \frac{\langle A|d|\alpha\rangle(\Omega)\langle \alpha|Q|B\rangle(\Omega)\langle B|Q|\beta\rangle(\Omega)\langle \beta|d|A\rangle(\Omega)}{E_{\alpha} - E_{A} + E_{\beta} - E_{B}}, \]

\[ A_{4}^{J_{\alpha}J_{\beta}}(\Omega_{p}) = (-1)^{p} \sum_{\mu M_{\alpha}M_{\beta}} (-1)^{J_{\alpha}+J_{\beta}+J_{\alpha}+J_{\beta}+1} w^{(2)}_{\mu} w^{(2)}_{\alpha}, \]

\[ X_{4}^{J_{\alpha}J_{\beta}} = \sum_{\alpha \beta} \frac{\langle A|Q|\alpha\rangle(\Omega)\langle \alpha|d|B\rangle(\Omega)\langle B|d|\beta\rangle(\Omega)\langle \beta|Q|A\rangle(\Omega)}{E_{\alpha} - E_{A} + E_{\beta} - E_{B}}. \]

The total angular momenta \( J_{\alpha} \) and \( J_{\beta} \) of the intermediate states \( \alpha \) and \( \beta \) are fixed in all of the equations above.

We are interested in the case when \( A = 1 S_{0} \) and \( B = 3 P_{1} \). Then, \( J_{\alpha} = 0, J_{\beta} = 1 \), and \( \Omega = M_{\beta} = 0, 1 \).

For \( k = 1 \), we have \( J_{\alpha} = 1 \) and \( J_{\beta} = 1 \). The coefficients \( A_{1}^{J_{\beta}}(\Omega) \) are listed in Table [Table]. The quantities \( X_{1}^{J_{\beta}} \) are given by

\[ X_{1}^{J_{\beta}} = \frac{45}{2\pi} \int_{0}^{\infty} \alpha_{A}^{1}(i\omega) \alpha_{B}^{2}(i\omega) d\omega + \delta X_{1}^{J_{\beta}}, \]

\[ \delta X_{1}^{J_{\beta}} = \frac{3}{2} |\langle 3P_{1}|d|1S_{0}\rangle|^{2} \alpha_{A}^{1}(0). \]

For \( k = 2 \), we have \( J_{\alpha} = 2 \) and \( J_{\beta} = 0, 1, 2 \). The coefficients \( A_{2}^{J_{\beta}}(\Omega) \) are listed in Table [Table]. The quantities \( X_{2}^{J_{\beta}} \) are given by

\[ X_{2}^{J_{\beta}} = \frac{45}{2\pi} \int_{0}^{\infty} \alpha_{A}^{2}(i\omega) \alpha_{B}^{1}(i\omega) d\omega + \delta X_{2}^{J_{\beta}}, \]

\[ \delta X_{2}^{J_{\beta}} = 2 |\langle 1S_{0}|d|3P_{1}\rangle|^{2} \sum_{n} \frac{(E_{n} - E_{1S_{0}})(|n|S_{0})^{2}}{(E_{n} - E_{1S_{0}})^{2} - \omega_{0}^{2}}. \]

where \( \omega_{0} = E_{3P_{1}} - E_{1S_{0}} \).

For \( k = 3 \), we find that \( J_{\alpha} = 1 \) and \( J_{\beta} = 1 \). For all other \( J_{\alpha} \) and \( J_{\beta} \) this expression turns to zero. Then,

\[ A_{3}^{1J_{\beta}}(\Omega_{p} = 0) = (-1)^{p} \frac{3}{5}, \]

\[ A_{3}^{1J_{\beta}}(\Omega_{p} = 1) = (-1)^{p} \frac{1}{5}. \]

(3)

\[ X_{3}^{1J_{\beta}} = \sum_{n,k} \frac{\langle 1S_{0}|d|n|3P_{1}\rangle\langle n|3P_{1}|Q|3P_{1}\rangle}{E_{n} - E_{1S_{0}} + E_{k} - E_{3P_{1}}}. \]

(4)

For \( k = 4 \), we have \( J_{\alpha} = 2 \) and \( J_{\beta} = 2 \). Then

\[ A_{4}^{2J_{\beta}}(\Omega_{p} = 0) = (-1)^{p} \frac{9}{25}; \]

\[ A_{4}^{2J_{\beta}}(\Omega_{p} = 1) = (-1)^{p} \frac{3}{25}. \]

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