Interference between $E1$ and $M1$ transition amplitudes on the $H$ to $C$ transition in ThO

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Calculations of Stark interference between $E1$ and $M1$ transition amplitudes on the $H^3\Delta_1$ to $C^1\Pi$ transition in ThO is performed. Calculations are required for estimations of systematic errors in the experiment for electron electric dipole (eEDM) moment search due to imperfections in laser beams used to prepare the molecule and read out the eEDM signal.

The current limit for the electron electric dipole moment (eEDM) (ACME II experiment), $|d_e| < 1.1 \times 10^{-29}$ e·cm (90% confidence), was set by measuring the spin precession of thorium monoxide (ThO) molecules in the metastable electronic $H^3\Delta_1$ state [1]. Previous experiment (ACME I) used ThO to place a limit $|d_e| < 9 \times 10^{-29}$ e·cm (90% confidence). In both experiments the measurements were performed on the ground rotational level which has two closely-spaced Ω-doublet levels of opposite parity. It was shown that due to existence of closely-spaced Ω-doublet levels the experiment on ThO is very robust against a number of systematic effects [2,3]. In ACME I the state preparation and the spin precession angle, $\phi$, measurement is performed by optically pumping the $H^3\Delta_1 \rightarrow C^1\Pi$ transition with linearly polarized laser beam [4], whereas in ACME II the $H^3\Delta_1 \rightarrow I^1\Pi$ transition was used. The transitions to ground rotational level of $C^1\Pi$ (ACME I) or $I^1\Pi$ (ACME II) which have similar to $H^3\Delta_1$ Ω-doublet structure (see below) is used. Searching for systematic errors is an important part of the eEDM search experiment. It was found that one of the systematic errors in the ACME I experiment [5] are due to Stark interference between $E1$ and $M1$ transition amplitudes on the $H^3\Delta_1$ to $C^1\Pi$ transition in ThO in laser beams used to prepare the molecule and read out the eEDM signal [6]. The similar systematic error related to $H^3\Delta_1$ to $I^1\Pi$ transition is expected for the ACME II experiment.

The measurement of spin precession is repeated under different conditions which can be characterized by binary parameters being switched from $+1$ to $-1$. The three primary binary parameters are $N_1$, $E_1$, $B_1$. $N_1 = +1(-1)$ means that the measurement was performed for lower (upper) Ω-doublet level of $H^3\Delta_1$. $E_1 = \text{sgn}(\hat{z} E)$ and $B_1 = \text{sgn}(\hat{z} B)$ define the orientation of the external static electric and magnetic fields respectively along the laboratory axis $z$. The measured precession angle $\phi$ can be represented as

$$\phi(N_1, E_1, B_1) = 2\pi n^r + N_1 E_1 B_1 + \tilde{\phi} N_1 E_1 B_1 + \tilde{\phi} E_1 B_1 N_1 E_1 B_1,$$

where notation $\phi^{S_1, S_2, \ldots}$ denotes a component which is odd under the switches $S_1, S_2, \ldots$. $\phi^{nr}$ is a component which is even (unchanged) under any of the switches. The eEDM signal is extracted from the $N_1 E_1$-correlated component of the measured phase, $\phi^{N_1 E_1} = \eta \xi E_1 t_1$, where $\xi E_1 = 79.9 \text{ GV/cm}$ [7] (see also Ref. [10]) is the effective electric field acting on the eEDM in the molecule, $t_1$ is interaction time. In case of ideal experiment only the interaction with the eEDM $d_e \xi E_1$ contributes to $\phi^{N_1 E_1}$. However, as is stated above, Stark interference between $E1$ and $M1$ transition amplitudes leads to an additional contribution to $\phi^{N_1 E_1}$ and gives rise to systematic errors in the eEDM measurement. The aim of the present work is to consider this effect for ACME I experiment. The theory can be applied to ACME II experiment as well but require more complicated electronic structure calculation (see section ) and will be performed in forthcoming work.

**ELECTRONIC STRUCTURE CALCULATIONS**

For molecular calculations the following matrix elements are required:

$$D_{\perp}^0 = \langle \Phi^1 | \hat{D}_z | \Phi^0 \rangle,$$ (2)

$$D_{||}^0 = \langle \Phi^0 | \hat{D}_z | \Phi^1 \rangle,$$ (3)

$$D_{\perp}^r = \langle \Phi^1 | \hat{S}_z | \Phi^1 \rangle,$$ (4)

$$D_{||}^r = \langle \Phi^0 | \hat{S}_z | \Phi^0 \rangle,$$ (5)

where $g_e = 2.0023193$ is the free-electron $g$-factor, $\hat{D}$ is the dipole moment operator, $\hat{J}^r$, $\hat{L}^r$, $\hat{S}^r$ are the total, orbital and spin electronic angular moment operators; $D_{\perp} = D_x + i D_y$ and the same is for other vectors.

To calculate these matrix elements two basis sets were used. The first basis set, LBas, includes 27s, 25p, 23d, 6f, 3g, 2h and 1i (contracted for f, g, h and i-harmonics) Gaussian functions on Th and can be written in the form: $(27s, 25p, 23d, 15f, 10g, 10h, 5i) | [27s, 25p, 23d, 6f, 3g, 2h, 1i]$. LBas corresponds to the aug-cc-pVTZ basis set, $(11s, 6p, 3d, 2f) | [5s, 4p, 3d, 2f]$, [13] [14] for oxygen. The MBas basis set was also used: $(25s, 22p, 21d, 14f, 10g) | [25s, 22p, 21d, 5f, 3g]$ for Th and
aug-cc-pVTZ for O [13, 14]. The technique of constructing natural basis sets, developed in [15] was used for constructing contracted $f - i$ functions. 1s, 4f electrons of thorium were excluded from the explicit electronic calculations using the generalized relativistic effective core potential in its semilocal formulation [16, 17].

The transition matrix elements were calculated using the linear response coupled cluster with single and double cluster amplitudes method, LR-CCSD [18]. 20 electrons ($6s6p6d7s$ of Th and $1s2s2p$ of O) were included in the main correlation calculation which was performed using the LBas basis set. To calculate the correction on the correlation of the $5s5p5d$ outer-core (OC) electrons of Th, the MBas basis set was used. All calculations were performed with R(Th–O) = 3.5107 a.u. which corresponds to the equilibrium geometry of the $H^3\Delta_1$ state.

For the calculations, the DIRAC15 [19] and MRCC [20] codes were used. To calculate matrix elements [21, 22] the code developed in Refs. [10, 21, 22] was used.

**MOLECULAR CALCULATIONS**

The basis set describing the $H^3\Delta_1$ and $C^1\Pi$ states wave functions can be presented as product of electronic and rotational wavefunctions $\Psi_{H(C)\alpha}^\beta M,\Omega(\alpha, \beta)$. Here $\Psi_{H(C)\alpha}^\beta M,\Omega$ is the electronic wavefunction of the $H^3\Delta_1$ ($C^1\Pi$) state, $\beta M,\Omega(\alpha, \beta, \gamma = 0)$ is the rotational wavefunction, $\alpha, \beta, \gamma$ are Euler angles, and $M$ ($\Omega = \pm 1$) is the projection of the molecular angular momentum $J$ on the laboratory $\hat{z}$ (internuclear $\hat{n}$) axis. For short, we will designate the basis set as $|H(C), J, M, \Omega\rangle$. In this paper the $|H, J = 1, \Omega, M = \mp 1\rangle$ and $|C, J = 1, \Omega, M = 0\rangle$ states which are of interest for the eEDM search experiment are considered.

In the absence of the external electric field each rotational level splits into two sublevels, called $\Omega$-doublet levels. One of them is even ($\bar{\Omega} = 1$) and the other one is odd ($\bar{\Omega} = -1$) with respect to change of sign of electronic and nuclear coordinates. The states with $\bar{\Omega} = (-1)^J$ denoted as $e$ and with $\bar{\Omega} = (-1)^{J+1}$ denoted as $f$ are the linear combination of the states with opposite sign of $\Omega$:

$$|H(C)J, \bar{\Omega}, M\rangle = \sqrt{2} |H(C), J, -1, M\rangle. \tag{7}$$

The experimental values of the $\Omega$-doubling, $\Delta(J) = E(|e, J, M\rangle) - E(|f, J, M\rangle)$ are $\Delta_H = 0.181\ J(J + 1)$ MHz for $|H\rangle$ and $\Delta_C = -25 J(J + 1)$ MHz for $|C\rangle$ states correspondingly [23].

External electric field $\hat{E} = \hat{E}\hat{E} \hat{z}$ does not couple the $|C, J = 1, \bar{\Omega} = -1, M = 0\rangle$ and $|C, J = 1, \bar{\Omega} = +1, M = 0\rangle$ states, whereas the $|H, J = 1, \bar{\Omega} = -1, M = \mp 1\rangle$ and $|H, J = 1, \bar{\Omega} = +1, M = \pm 1\rangle$ states are coupled. Neglecting the interaction between different rotational and electronic states

$$|H, \hat{E}, \bar{\Omega}, M\rangle = k(-\bar{\Omega}) |H, J = 1, \bar{\Omega} = -1, M = \pm 1\rangle - k(+\bar{\Omega}) |H, J = 1, \bar{\Omega} = +1, M = \pm 1\rangle \tag{8}$$

where

$$k(\pm 1) = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{\Delta_H(J = 1)}{\Delta_H(J = 1)^2 + (\Delta_H)^2}} \tag{9}$$

$\Delta_H = -1.612\ a.u.$ is the dipole moment for the $H$ state [23, 24]. $\hat{E} > 0$ is the magnitude of the electric field, $\hat{E}$ defines direction of electric field.

The dark state (which the preparation laser does not couple to the $C$ state), $|H_D, \hat{E}, \bar{\Omega}, N\rangle$ is the initial state, for the spin precession experiment. Let the preparation laser polarization is exactly linear $\hat{\epsilon}_p = \hat{z}$. Then, neglecting the small contribution from magnetic amplitude, the resulting initial (dark) state under ideal conditions is

$$|H_D, \hat{E}, \bar{\Omega}, N\rangle = \frac{1}{\sqrt{2}} \left(|H, \hat{E}, \bar{\Omega}, +1\rangle + |H, \hat{E}, \bar{\Omega}, -1\rangle\right) \tag{10}$$

Then the molecules enter a spin precession region with presence of electric and magnetic fields which produce a relative energy shift between the two Zeeman sublevels $|H_D, \hat{E}, \bar{\Omega}, N\rangle, \pm 1\rangle$. The final state of the molecule is

$$\Psi(\phi) = \frac{1}{\sqrt{2}} \left(e^{-i\phi} |H, \hat{E}, \bar{\Omega}, +1\rangle + e^{i\phi} |H, \hat{E}, \bar{\Omega}, -1\rangle\right). \tag{11}$$

Then in a detection region $\phi$ is measured by optically pumping on the same $H^3\Delta_1 \rightarrow C^1\Pi$ transition with linearly polarized laser beams with polarizations $\hat{\epsilon}_X, \hat{\epsilon}_Y$ determined by azimuthal angles $\theta_X = 45^\circ, \theta_Y = 135^\circ$ (azimuthal angle for preparation laser $\theta_p = 0^\circ$). Then, neglecting the small contribution from magnetic amplitude, for $\phi \ll 1$, for exact linear polarizations of preparation and readout lasers one can obtain [7]

$$A(\Psi(\phi)) = \frac{F_X - F_Y}{F_X + F_Y} = 2\bar{\Phi}_\psi, \tag{12}$$

where $A$ is asymmetry, $F_{X,Y}$ are the detected in the experiment fluorescence after applying the readout lasers. Then the eEDM sensitive component $\phi^{NE}$ can be calculated as

$$\phi^{NE} = \frac{1}{8} \sum_{\bar{\mathcal{N}}, \bar{\mathcal{B}}, \bar{\mathcal{E}}} \mathcal{N}\mathcal{E}\phi \left(\bar{\mathcal{N}}, \bar{\mathcal{B}}, \bar{\mathcal{E}}\right). \tag{13}$$

Similarly, other components in Eq. [1] can be calculated.
The laser pointing vector \( \hat{k} \) and polarization can be parameterized as

\[
\hat{k} = \cos \varphi \sin \vartheta \hat{x} + \sin \varphi \sin \vartheta \hat{y} + \cos \vartheta \hat{z}
\]  

(14)

\[
\hat{\varepsilon} = \epsilon_x \hat{x} + \epsilon_y \hat{y} + \epsilon_z \hat{z},
\]

(15)

where

\[
\epsilon_x = \cos \theta (\cos \Theta + \sin \Theta) + i \sin \theta (\sin \Theta - \cos \Theta)
\]

(16)

\[
\epsilon_y = \sin \theta (\cos \Theta + \sin \Theta) + i \cos \theta (\sin \Theta - \cos \Theta)
\]

(17)

\[
\epsilon_z = \tan \vartheta (\cos (\theta - \varphi) (\cos \Theta + \sin \Theta) + i \sin (\theta - \varphi) (\sin \Theta - \cos \Theta)),
\]

(18)

\( \Theta \) is the ellipticity angle. For an ideal experiment \( \Theta_{p, X, Y} = 45^\circ \), \( \vartheta_{p, X, Y} = 0^\circ \), \( \varphi = 0^\circ \), \( \vartheta_X = 45^\circ \), \( \vartheta_Y = 135^\circ \). Label \( i = p, X, Y \) refer to preparation and readout \( X, Y \) lasers. The deviation of \( \Theta, \vartheta, \varphi \) from their ideal values together with Stark interference between \( E1 \) and \( M1 \) transition amplitudes generates a systematic error in searches for the eEDM according to [8]

\[
\hat{\phi}^{N E} = \frac{a_{M1}}{4} \left[ \hat{\vartheta}_p^2 (-2 S_p c_p + \hat{P}_p (S_X - S_Y)) + \hat{\vartheta}_X^2 (S_{X c_p} + \hat{P}_p c_p s_p) + \hat{\vartheta}_Y^2 (S_{Y c_p} - \hat{P}_p s_p y_p) \right],
\]

(19)

where, \( a_{M1} \) is ratio of \( M1 \) and \( E1 \) amplitudes, \( S_i = -2d \Theta_i, \Theta = \vartheta + \pi/4 \), \( c_i = \cos (\theta_i - \varphi_i) \), \( s_i = \sin (\theta_i - \varphi_i) \). Eq. (19) assumes that ground rotational levels of \( H^3 \Delta_1 \) and \( C^3 \Pi \) states can be written according to Eqs. (7) [9]. However accounting for interaction with other electronic and rotational states, magnetic field, modify Eqs. (7) [9] and give rise to systematic errors for other components of \( \phi \). To take into account the perturbation above the numerical calculation was performed. Following the computational scheme of [8, 9, 22, 26], wavefunctions of \( H \) and \( C \) states in external static electric and magnetic fields are obtained by numerical diagonalization of the molecular Hamiltonian over the basis set of the electronic-rotational wavefunctions. Detailed features of the Hamiltonian are described in [9]. After calculation of wavefunctions the systematic error \( \hat{\phi} \) for precession angle \( \phi \) was calculated as \( A(\Psi(\phi = 0)) = 2 \hat{P} \hat{\phi} \).

RESULTS AND DISCUSSIONS

Table I gives results of electronic calculations of matrix elements [2, 9].

Comparison of numerical calculations and Eq. (19) for \( \hat{\phi}^{N E} \) is given in Table II. Typical values of \( \Theta_{p, X, Y}, \vartheta_{p, X, Y}, \varphi \) are little deviated from ideal values are used in the Table III. Calculations show that accounting for perturbations described above does not lead to notable changes in \( \hat{\phi}^{N E} \). Numerical calculations are in agreement with Eq. (19) within 15% or less. Systematic error for the eEDM due to Stark interference between \( E1 \) and \( M1 \) transition amplitudes is \( \hat{\phi}^{N E} \sim 10^{-8} \text{rad} \). Note that current limits in terms of \( \hat{\phi}^{N E} \) are approximately \( \hat{\phi}^{N E} < 10^{-5} \text{rad} \) for ACME I and \( \hat{\phi}^{N E} < 10^{-6} \text{rad} \) for ACME II. The systematic error can be further suppressed by about factor of ten due to the rotation of the readout polarization basis by \( \Theta_{p, X, Y} \to \Theta_{p, X, Y} + 90^\circ \) and a global polarization rotation of both state preparation and readout lasers \( \Theta_{p, X, Y} \to \Theta_{p, X, Y} + 90^\circ \). The final systematic error \( \hat{\phi}^{N E} \sim 10^{-9} \text{rad} \) substantially less than the current limit for \( \hat{\phi}^{N E} \). Similar systematic error can be expected for ACME II experiment which uses \( H^3 \Delta_1 \) to \( I^1 \Pi \) transition instead of \( H^3 \Delta_1 \) to \( C^3 \Pi \).

Calculations show that \( \hat{\phi}^{NB} \sim 10^{-7} \text{rad} \) and \( \hat{\phi}^B \sim 10^{-8} \text{rad} \) which formally are sources of systematic errors in measurement of g-factor, g-factor difference between the \( \Omega \)-doublets (see for details Ref. [3]), though are several orders of magnitude less than measured \( \hat{\phi}^{NB} \) and \( \hat{\phi}^B \).

CONCLUSION

We have calculated the Systematic error for the eEDM search experiment due to Stark interference between \( E1 \) and \( M1 \) transition amplitudes. We found that the error is about three orders of magnitude less than the current limit for the eEDM obtained in ACME II experiment [1].

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TABLE I. Calculated electric and magnetic transition dipole moments for the ThO molecule.

| X → C | H → C |
|-------|-------|
| $D_{\text{XCE}}^C$ | $G_{\text{XCE}}^C$ | $J_{\text{XCE}}^C$ | $D_{\text{HEC}}^H$ | $D_{\text{HEC}}^H$ |
| 20e | -0.596 | 0.217 | 0.211 | 0.018 | -0.069 |
| OC | 0.071 | -0.013 | -0.015 | -0.002 | -0.002 |
| Total | -0.525 | 0.204 | 0.197 | 0.016 | -0.071 |

TABLE II. Calculated systematic errors $\tilde{\phi}^{\text{NE}}$, $\tilde{\phi}^{\text{NB}}$, $\tilde{\phi}^B$ in $10^{-8}$ rad as functions of $\vartheta$, $\varphi$, $\theta$, $\Theta$ (in degrees) for preparation and readout lasers. Numerical calculations take into account interaction between different rotational and electronic levels.

| $\vartheta_p$ | $\varphi_p$ | $\Theta_p$ | $\vartheta_X$ | $\varphi_X$ | $\Theta_X$ | $\vartheta_Y$ | $\varphi_Y$ | $\Theta_Y$ | $\tilde{\phi}^{\text{NE}}$ | $\tilde{\phi}^{\text{NB}}$ | $\tilde{\phi}^B$ | Eq.19 | numerical calculation |
|--------------|--------------|-------------|--------------|--------------|-------------|--------------|--------------|-------------|----------------|----------------|--------------|-------|---------------------|
| 0.3 20. 1. 46. 0.2 20. 46. 44. 0. 0. | 136. 45. 0.3426 | 0.3423 | 3.621 | 0.4961 |
| 0.3 20. 1. 46. 0.2 20. 46. 44. 0. 0. | 136. 47. -0.1347 | -0.1353 | 10.0857 | 1.488 |
| 0.3 20. 1. 46. 0.2 20. 46. 44. 0. 0. | 136. 44. 0.8199 | 0.8162 | -3.616 | -0.4956 |
| 0.3 20. 1. 46. 0.2 20. 46. 44. 0. 0. | 136. 44. 0.596 | 0.5578 | -3.616 | -0.4956 |
| 0.3 20. 1. 46. 0.3 20. 46. 44. 0.3 0. | 136. 44. 0.4765 | 0.4496 | -3.611 | -0.4949 |
| 0.3 20. 1. 46. 0.1 20. 46. 44. 0. 0. | 134. 44. 0.4224 | 0.4048 | -3.598 | -0.4931 |
| 0.3 20. 1. 46. 0.1 20. 46. 44. 0. 0. | 134. 46. -0.2530 | -0.2978 | 7.207 | 0.9877 |
| 0.3 20. 1. 46. 0.3 20. 46. 44. 0. 0. | 134. 46. -0.0333 | -0.1477 | 7.207 | 0.9877 |
| 0.3 20. 1. 46. 0.1 20. 46. 44. 0. 0. | 134. 46. -0.3835 | -0.3835 | 7.207 | 0.9877 |
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