Tune-out wavelength around 413 nm for the helium 2 $^3S_1$ state including relativistic and finite-nuclear-mass corrections

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The tune-out wavelength at 413 nm for the 2 $^3S_1$ state of helium is expected to be sensitive to finite nuclear mass, relativistic, and quantum electrodynamic (QED) corrections, which provides a scheme for testing atomic structure theory [J. Mitroy and L.-Y. Tang, Phys. Rev. A **88**, 052515 (2013)]. In the present work, a large-scale full-configuration-interaction calculation based on both the Dirac-Coulomb-Breit Hamiltonian and the nonrelativistic Hamiltonian is performed for the dynamic dipole polarizabilities of helium in the 2 $^3S_1$ state. The tune-out wavelengths for the magnetic sublevels $M_J = 0$ and $M_J = \pm 1$ are determined to be 413.0801(4) nm and 413.0859(4) nm, respectively, at sub-ppm accuracy, including finite nuclear mass and relativistic corrections. Our value for the $M_J = 1$ sublevel agrees with the measured value of 413.0938(20)(9) nm [B. M. Henson *et al.*, Phys. Rev. Lett. **115**, 043004 (2015)] at the level of 19 ppm. The discrepancy between these two values is mainly due to the uncalculated QED contribution. Our current value confirms quantitatively the prediction of Mitroy and Tang. Also, for the state of 2 $^3S_1$ we find that the corrections due to finite nuclear mass and relativistic effects to the static dipole polarizability of 315.7227(4)a_0^3 are about 600 ppm and 310 ppm, respectively, which are about 1.4 and 5.4 times larger than those for the ground state. A measurement at the level of 10 ppm for the static dipole polarizability of helium in 2 $^3S_1$ can be used to determine the transition matrix element between 2 ^3S and 2 ^3P at the level of 10^{-5}.

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Atomic helium is one of the simplest Coulomb three-body systems. The accurate investigation of its energy levels can be used to determine the fine-structure constant [1,2], to extract the nuclear charge radius [3,4], and to test QED theory [5,6]. For theoretical calculations of energy levels, the most popular approach starts with solving the eigenvalue problem for the nonrelativistic Hamiltonian by using the correlated basis sets; and then relativistic and QED corrections are added by using perturbation theory [7,8]. The current comparison between theory and experimental measurements for the ground-state energy has reached a level of ppb [5,9]. In contrast to this, very few experimental determinations of atomic transition rates have a precision of 0.1% or better [10]. At present, the most precise calculation among atomic properties that are related to atomic transition matrix elements is the static dipole polarizability of helium in the ground state [7,8,11], where the measured precision has reached 9.1 ppm. However, it is difficult to further improve this precision, since a measurement of polarizability depends on modulating precisely the electric field strength.

The tune-out wavelength λ_t is the wavelength at which the dynamic dipole polarizability for a state of interest is zero [12,13], which means that the atom is basically uneffected by the irradiating laser. Since the position of the tune-out wavelength does not depend on the details of laser power or beam profile, a measurement of the tune-out wavelength can have higher accuracy than a measurement of the static dipole polarizability. For example, the tune-out wavelength of potassium has been measured to an accuracy of 2 ppm, which opens the way to determine precisely the oscillator strength ratio for the $4s \rightarrow 4p$ spin-orbit doublet [14,15]. Recently the measurement of the tune-out wavelength for the ground-state hyperfine of rubidium has been reported at a level of sub-ppm [16].

In 2013 Mitroy and Tang [13] pointed out that the tune-out wavelength around 413 nm for the helium metastable 2 $^3S_1$ state can provide a nonenergy test of QED theory. In 2015 Baldwin's group [17] measured the tune-out wavelength of that state at the $M_J = 1$ magnetic sublevel to be 413.0938($9_{\rm stat}$)($20_{\rm syst}$) with the experimental accuracy of 5 ppm. This measured value is more accurate than the theoretical calculation of 413.02(9) nm [13] by two orders of magnitude. Recently we used the nonrelativistic configuration interaction (NRCI) method to obtain the tune-out wavelength of 413.038 28(3) nm [18] for the case of infinite nuclear mass. Compared to the experimental result, there exists a discrepancy of 134 ppm for the NRCI value [18], which has motivated us to do more detailed theoretical investigation on the finite nuclear mass (FNM), relativistic, and QED effects in the tune-out wavelength more rigorously.

The tune-out wavelength is extracted from the calculation of dynamic dipole polarizabilities, which depend on the fundamental atomic structure information of energies and wave functions. Recently Piszezatowski *et al.* computed the dynamic dipole polarizability of 1.391 811 41 a_0^3 at the He-Ne laser wavelength for the ground state of helium by using the perturbation method [19]. The accuracy of their result is 0.1 ppm. Since the He-Ne laser wavelength of 632.9908 nm is far from any 1 $^1S \rightarrow n$ ^1P resonance transition lines, the dynamic dipole polarizability can be efficiently calculated from a power series expansion in terms of the laser wavelength [20]. However, for the 2 $^3S_1$ state of He, the tune-out wavelength around

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413 nm is very near the excitation threshold of 389 nm relative to the $1s3p\ ^3P$ state. Therefore the power series expansion method of Refs. [19,20] cannot be applied. Thus in the present work, we carry out the relativistic configuration-interaction (RCI) calculations for the dynamic dipole polarizabilities of He in the $2\ ^3S_1$ state by using the full-configuration-interaction method based on B-spline functions to solve the eigenvalue problems of the Dirac-Coulomb-Breit (DCB) Hamiltonian. FNM correction to the tune-out wavelength is extracted from the NRCI calculation. Combining the RCI and NRCI results, we can determine the FNM and relativistic corrected tune-out wavelength around 413 nm and the static dipole polarizability.

The RCI calculation is performed to solve the eigenvalue problem of the DCB Hamiltonian:

$$H_{\rm DCB} = \sum_{i=1}^{2}\left[c\boldsymbol{\alpha}_i\cdot\mathbf{p}_i + \beta m_e c^2 - \frac{2}{r_i}\right] + \frac{1}{r_{12}} + H_{\rm B} \quad (1)$$

with

$$H_{\rm B} = -\frac{1}{2r_{12}}[\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2 + (\boldsymbol{\alpha}_1\cdot\hat{\mathbf{r}}_{12})(\boldsymbol{\alpha}_2\cdot\hat{\mathbf{r}}_{12})], \quad (2)$$

where m_e is the electron mass, c is the speed of light [21], $\mathbf{p}_i$ is the momentum operator, $\boldsymbol{\alpha}_i$ and β are 4×4 Dirac matrices, $\hat{\mathbf{r}}_{12}$ is the unit vector of the electron-electron distance $\mathbf{r}_{12}$, and $H_{\rm B}$ is the Breit operator with the retardation effect excluded. When $H_{\rm B}$ is neglected from Eq. (1), the Hamiltonian of Eq. (1) becomes the Dirac-Coulomb (DC) Hamiltonian.

The wave function $\psi_{ij}(JM_J)$ of helium is expanded as a linear combination of the configuration-state wave functions $\phi_{ij}(JM_J)$, which are constructed by single-electron wave functions with the orbital quantum numbers ℓ_i and ℓ_j less than the maximum number of partial wave $\ell_{\rm max}$. The configuration-state wave functions are constructed by using the Notre Dame basis set [22,23] with N B-spline functions to solve the single-electron Dirac equation. The exponential knot distribution for the B splines is the same as Eq. (24) of our previous paper [18]. Different from the most of RCI calculations [24,25], we do not impose any truncation for the CI basis sets.

The NRCI calculation is performed by applying the B-spline method to solve the eigenvalue problem for the following nonrelativistic Hamiltonian:

$$H = -\sum_{i=1}^{2}\left[\frac{\nabla_i^2}{2\mu} + \frac{2}{r_i}\right] + \frac{1}{r_{12}} - \frac{1}{m_0}\boldsymbol{\nabla}_1\cdot\boldsymbol{\nabla}_2, \quad (3)$$

where $\mu = m_e m_0/(m_e + m_0)$ is the reduced mass of the electron and $m_0 = 7294.2995361 m_e$ is the nucleus mass of ^{4}He [21]. We adopt the same computational procedure as our previous work [18] except that the mass-polarization term $-\boldsymbol{\nabla}_1\cdot\boldsymbol{\nabla}_2/m_0$ is included here.

The dynamic dipole polarizability for the magnetic sublevel M_{J_g} at the laser frequency ω can be expressed as

$$\alpha_1(\omega) = \alpha_1^S(\omega) + \left(3M_{J_g}^2 - 2\right)\alpha_1^T(\omega), \quad (4)$$

where $\alpha_1^S(\omega)$ and $\alpha_1^T(\omega)$ are, respectively, the dynamic scalar and tensor parts of the polarizability, which can be expressed as the sum over all intermediate states, including the continuum:

$$\alpha_1^S(\omega) = \sum_{n\neq g}\frac{f_{gn}^{(1)}}{(\Delta E_{gn})^2 - \omega^2}, \quad (5)$$

$$\alpha_1^T(\omega) = 3\sum_{n\neq g}(-1)^{1+J_n}\begin{Bmatrix}1 & 1 & 2\\ 1 & 1 & J_n\end{Bmatrix}\frac{f_{gn}^{(1)}}{(\Delta E_{gn})^2 - \omega^2}. \quad (6)$$

In the above, the dipole oscillator strength $f_{gn}^{(1)}$ is

$$f_{gn}^{(1)} = \frac{2\Delta E_{gn}|\langle 2\ ^3S_1\|T_1\|N_nJ_n\rangle|^2}{9}, \quad (7)$$

where $T_1 = \sum_{i=1}^{2} r_i C^{(1)}(\hat{\mathbf{r}}_i)$ is the electronic dipole transition operator, $|N_nJ_n\rangle$ is the nth intermediate eigenfunction with principal quantum number N_n, angular momentum quantum number J_n, and energy E_n, and $\Delta E_{gn} = E_n - E_g$ is the transition energy between the initial state and the intermediate state.

Table I presents the RCI energies for some low-lying states, which are relevant to the dynamic dipole polarizability of the

TABLE I. Comparison of energies from the RCI and NRCI calculations for some low-lying states. The FNM column is the finite nuclear mass corrections extracted from the NRCI values of $^\infty$He and ^{4}He, and the QED column lists the QED corrections adopted from Ref. [27]. The seventh column lists the total energies, which include the FNM, relativistic, and QED corrections. The experimental data are taken from the National Institute of Standards and Technology (NIST) tabulation [28]. The numbers in parentheses are computational uncertainties. In atomic units.

State	RCI	NRCI for $^\infty$He	NRCI for ^{4}He	FNM	QED [27]	Total	Experiment
$2\ ^3S_1$	−2.175 344 5(2)	−2.175 229 36(2)	−2.174 930 17(2)	0.000 299 19(4)	0.000 016 72	−2.175 028 6(2)	−2.175 028 942
$2\ ^3P_2$	−2.133 269 4(2)					−2.132 969 9(2)	−2.132 970 359
$2\ ^3P_1$	−2.133 269 1(2)	−2.133 164 17(2)	−2.132 880 60(2)	0.000 283 57(4)	0.000 015 91	−2.132 969 6(2)	−2.132 970 010
$2\ ^3P_0$	−2.133 264 6(2)					−2.132 965 1(2)	−2.132 965 509
$3\ ^3P_2$	−2.058 187 4(4)					−2.057 891 8(4)	−2.057 891 998
$3\ ^3P_1$	−2.058 187 3(4)	−2.058 081 08(2)	−2.057 801 48(2)	0.000 279 60(4)	0.000 016 05	−2.057 891 7(4)	−2.057 891 898
$3\ ^3P_0$	−2.058 186 1(5)					−2.057 890 5(5)	−2.057 890 665
$4\ ^3P_2$	−2.032 430 8(5)					−2.032 137 2(5)	−2.032 137 409
$4\ ^3P_1$	−2.032 430 8(5)	−2.032 324 35(2)	−2.032 046 81(2)	0.000 277 54(4)	0.000 016 08	−2.032 137 2(5)	−2.032 137 368
$4\ ^3P_0$	−2.032 430 3(5)					−2.032 136 7(5)	−2.032 136 865
$2\ ^1P_1$	−2.123 947(2)	−2.123 841 6(2)	−2.123 544 2(1)	0.000 297 4(3)	0.000 016 11	−2.123 634(2)	−2.123 638 389
$3\ ^1P_1$	−2.055 252(2)	−2.055 145 9(2)	−2.054 862 2(2)	0.000 283 7(4)	0.000 016 10	−2.054 952(2)	−2.054 954 059
$4\ ^1P_1$	−2.031 176(2)	−2.031 069 4(2)	−2.030 790 2(2)	0.000 279 2(4)	0.000 016 10	−2.030 881(2)	−2.030 881 359

TABLE II. Comparison of reduced matrix elements for some transitions of $2\ ^3S_1 \rightarrow n\ ^{1,3}P$ of helium. The values in the FNM column are extracted from the NRCI calculations for both $^\infty$He and ^{4}He, and they represent the finite nuclear mass corrections to the reduced matrix elements, and the sixth column lists the total reduced matrix elements with the FNM and relativistic corrections included. The values from perturbation theory (PT) for the dipole allowed and forbidden transitions are respectively from Refs. [29] and [30]. The numbers in parentheses represent computational uncertainties. In atomic units.

Transition	RCI	NRCI for $^\infty$He	NRCI for ^{4}He	FNM	Total	PT for ^{4}He
$2\ ^3S_1 \rightarrow 2\ ^3P_0$	2.531 323(2)				2.531 782(2)	2.531 375
$2\ ^3S_1 \rightarrow 2\ ^3P_1$	4.384 31(2)	4.384 432 5(4)	4.384 891 3(3)	0.000 458 8(7)	4.384 77(2)	4.384 692
$2\ ^3S_1 \rightarrow 2\ ^3P_2$	5.660 13(2)				5.660 59(2)	5.660 605
$2\ ^3S_1 \rightarrow 3\ ^3P_0$	0.524 23(2)				0.524 78(2)	0.524 549
$2\ ^3S_1 \rightarrow 3\ ^3P_1$	0.908 17(2)	0.908 502 9(3)	0.909 049 1(2)	0.000 546 2(5)	0.908 72(2)	0.908 546
$2\ ^3S_1 \rightarrow 3\ ^3P_2$	1.172 46(2)				1.173 01(2)	1.172 934
$2\ ^3S_1 \rightarrow 4\ ^3P_0$	0.300 14(2)				0.300 39(2)	0.300 281
$2\ ^3S_1 \rightarrow 4\ ^3P_1$	0.519 93(2)	0.520 078 8(3)	0.520 328 0(2)	0.000 249 2(5)	0.520 18(2)	0.520 103
$2\ ^3S_1 \rightarrow 4\ ^3P_2$	0.671 24(2)				0.671 49(2)	0.671 450
$2\ ^3S_1 \rightarrow 2\ ^1P_1$	0.001 27(2)					0.001 262
$2\ ^3S_1 \rightarrow 3\ ^1P_1$	0.000 12(2)					0.000 121

$2\ ^3S_1$ state. The NRCI energies for $^\infty$He and ^{4}He are also listed in the third and fourth columns. For the RCI energies, our values for the triplet states have seven significant digits. For the singlet states, the present RCI energies have converged to the sixth significant digit. For the NRCI energies, our results have eight and seven significant digits for the triplet and singlet states, respectively. From the RCI energies of $2\ ^3P_{0,1,2}$ state, we can obtain the fine-structure splittings of $\nu_{01} = 29\,609$ MHz and $\nu_{02} = 31\,582$ MHz, which may compare to the values of 29 564 MHz and 31 881 MHz [26] that include the leading-order relativistic correction. By comparing the results for $^\infty$He and ^{4}He, we can extract the FNM corrections to the energies listed in the fifth column. Finally by adding the QED corrections [27] listed in the sixth column and the FNM to our RCI values we obtain the total energies listed in the seventh column. We can see that our total energies are in good agreement with the NIST energies [28].

Table II lists some reduced matrix elements for $2\ ^3S_1 \rightarrow n\ ^{1,3}P$ transitions in helium. The last column contains the perturbation values of Refs. [29,30] where both the FNM and the leading-order relativistic corrections are included. In the last column, the results for the dipole allowed transitions are derived from Ref. [29], and the values for the dipole forbidden transitions are converted by using the oscillator strengths f_α and the transition energies $\Delta\epsilon_\alpha$ in Table 6 of Ref. [30]. It is seen that our NRCI results for $^\infty$He and ^{4}He have six to seven significant digits, and our RCI values have four to six significant digits. If we add the FNM correction of 0.0004588(7) to the RCI value of 4.38431(2) for the $2\ ^3S_1 \rightarrow 2\ ^3P_1$ transition, we obtain a value 4.38477(2), which has five significant digits compared to the value 4.384692 [29] using perturbation theory. The detailed comparison for the energies and matrix elements listed in Tables I and II has shown that the present RCI and NRCI calculations for the dynamic dipole polarizability and the tune-out wavelength of helium are reliable.

Table III shows a convergence study for the static dipole polarizability and the tune-out wavelength for the $M_J = 0$ sublevel of $2\ ^3S_1$ obtained from the RCI calculations under the DC Hamiltonian. The numbers of configurations for the $^3S_1$,

TABLE III. Convergence of the static dipole polarizability $\alpha_1(0)$ (in a_0^3) and the tune-out wavelength λ_t (in nm) under the DC Hamiltonian for the $2\ ^3S_1(M_J = 0)$ state of helium as the number of B-splines N increases and the number of partial wave $\ell_{\max}$ is fixed at 5, and as the number of partial wave $\ell_{\max}$ increases and the number of B splines N is fixed at 30. $N_{^3S_1}$, $N_{^3P_0}$, $N_{^{1,3}P_1}$, and $N_{^3P_2}$ are the numbers of configurations for the $^3S_1$, $^3P_0$, $^{1,3}P_1$, and $^3P_2$ symmetries, respectively. The numbers in parentheses in the extrapolated values represent computational uncertainties.

	$\ell_{\max} = 5$		
N	$(N_{^3S_1}, N_{^3P_0}, N_{^{1,3}P_1}, N_{^3P_2})$	$\alpha_1(0)$	λ_t
30	(9285, 4500, 12 600, 15 300)	315.542 767 16	412.990 357 56
35	(12 670, 6125, 17 150, 20 825)	315.542 477 89	412.990 248 23
40	(16 580, 8000, 22 400, 27 200)	315.542 403 44	412.990 219 55
Extrap.		315.542 38(2)	412.990 21(1)
	$N = 30$		
$\ell_{\max}$	$(N_{^3S_1}, N_{^3P_0}, N_{^{1,3}P_1}$, and $N_{^3P_2})$	$\alpha_1(0)$	λ_t
5	(9285, 4500, 12 600, 15 300)	315.542 767 26	412.990 357 60
6	(11 055, 5400, 15 300, 18 900)	315.543 805 18	412.991 398 79
7	(12 825, 6300, 18 000, 22 500)	315.544 149 55	412.991 768 97
Extrap.		315.5443(2)	412.9919(2)

TABLE IV. Convergence study of the tune-out wavelength λ_t (in nm) under the DCB Hamiltonian for the $2\,^3S_1$ state of He as the number of partial wave $\ell_{\max}$ increases and the number of B splines N is fixed at 30. $N_{^3S_1}$, $N_{^3P_0}$, $N_{^{1,3}P_1}$, and $N_{^3P_2}$ are the numbers of configurations for the $^3S_1$, $^3P_0$, $^{1,3}P_1$, and $^3P_2$ symmetries, respectively. The numbers in parentheses of the extrapolated values represent computational uncertainties from finite $\ell_{\max}$. The last line lists the recommended values where the uncertainties are doubled due to finite sizes of CI basis sets.

$\ell_{\max}$	$(N_{^3S_1}, N_{^3P_0}, N_{^{1,3}P_1}, N_{^3P_2})$	$2\,^3S_1(M_J=0)$	$2\,^3S_1(M_J=\pm1)$
3	(5745, 2700, 7200, 8100)	412.957 203 22	412.963 070 12
4	(7515, 3600, 9900, 11 700)	412.974 017 84	412.979 876 96
5	(9285, 4500, 12 600, 15 300)	412.977 620 94	412.983 476 59
6	(11 055, 5400, 15 300, 18 900)	412.978 662 92	412.984 516 96
7	(12 825, 6300, 18 000, 22 500)	412.979 032 83	412.984 886 06
Extrap.		412.9792(2)	412.9850(2)
Rec.		412.9792(4)	412.9850(4)

$^3P_0$, $^{1,3}P_1$, and $^3P_2$ symmetries are also listed as $N_{^3S_1}$, $N_{^3P_0}$, $N_{^{1,3}P_1}$, and $N_{^3P_2}$, respectively. It is seen that both the static dipole polarizability and the tune-out wavelength converge more rapidly as the number of B splines N increases and at the same time the number of partial-wave $\ell_{\max}$ is fixed at five, than the case when $\ell_{\max}$ increases and N is fixed at 30. When $\ell_{\max}$ is fixed, the extrapolated values of $\alpha_1(0)$ and λ_t are, respectively, $315.54238(2)a_0^3$ and 412.990 21(1) nm, which are one order of magnitude more accurate than the extrapolated results of $315.5443(2)a_0^3$ and 412.9919(2) nm when N is fixed. Thus in the following calculations, we will fix N at 30 and increase $\ell_{\max}$ to test convergence for the dynamic dipole polarizability and the tune-out wavelength. The incompleteness of the basis sets due to the truncation of N will be combined with the truncation of $\ell_{\max}$ to estimate the uncertainties in the final recommended values. The same convergence style exists for the $M_J=\pm1$ sublevels, and the same extrapolated values of $\alpha_1(0)=315.5443(2)a_0^3$ and $\lambda_t=412.9919(2)$ nm with $N=30$ are obtained for the $M_J=\pm1$ sublevels, since the tensor part of the polarizability makes small contribution to the total dynamic polarizability in Eq. (4).

Table IV is a convergence study for the tune-out wavelength as $\ell_{\max}$ increases under the DCB Hamiltonian for the magnetic sublevels $M_J=0$ and $M_J=\pm1$ in the state of $2\,^3S_1$ of helium. $N_{^3S_1}$, $N_{^3P_0}$, $N_{^{1,3}P_1}$, and $N_{^3P_2}$ represent the total numbers of configurations for the $^3S_1$, $^3P_0$, $^{1,3}P_1$, and $^3P_2$ symmetries, respectively. According to the convergence pattern, we obtain the extrapolated values as $\ell_{\max}$ increases to infinity. In order to estimate the effect from the incompleteness due to truncation of B splines, we double the uncertainties in the recommended values listed in the last line of Table IV. The RCI values under the DCB Hamiltonian for the $M_J=0$ and $M_J=\pm1$ states are, respectively, 412.9792(4) nm and 412.9850(4) nm, which have six significant digits. Compared to the DC value of 412.9919(2) nm in Table III, we can see that the Breit interaction reduces the tune-out wavelength by 13 picometers for $M_J=0$ and by 7 picometers for $M_J=\pm1$.

Table V lists the tune-out wavelength obtained from the NRCI and RCI methods, as well as a comparison with published values. From the NRCI values for $^\infty$He and ^{4}He, the FNM correction to the tune-out wavelength is determined to be 0.10091(5) nm. After adding this correction to the RCI values, we obtain the total tune-out wavelengths of 413.0801(4) nm and 413.0859(4) nm for the sublevels of $M_J=0$ and $M_J=\pm1$, respectively. The averaged value over the magnetic sublevels is $\lambda_t=413.0845(4)$ nm with an accuracy of sub-ppm. Compared to the hybrid value [13], which is obtained by incorporating Hylleraas matrix elements for the $2\,^3P_J$ and $3\,^3P_J$ states and the core-polarization model matrix elements for the rest transitions, our averaged result improves the value of Mitroy and Tang [13] by two orders of magnitude. Compared the present value of 413.0859(4) nm for the $M_J=1$ sublevel with the measured value of $413.0938(9_{\rm stat})(20_{\rm syst})$ nm, the agreement is at the level of 19 ppm. The existing discrepancy between the two values is from the uncalculated QED correction.

In Table V we present a comparison for the static dipole polarizability of helium in the $2\,^3S_1$ state. It is seen that our NRCI value for $^\infty$He is in perfect agreement with the result from the Hylleraas calculations [32] and is more accurate than the NRCI result using Slater basis sets [31]. Comparing our NRCI values for both $^\infty$He [18] and ^{4}He, the FNM correction increases the $\alpha_1(0)$ by $0.1889(4)a_0^3$. After adding this correction to our RCI values, we obtain the values of $315.7165(4)a_0^3$ and $315.7248(4)a_0^3$ for the $M_J=1$ and $M_J=\pm1$ sublevels, respectively. The averaged value of $315.7227(4)a_0^3$ over the magnetic sublevels is also listed

TABLE V. Comparison of the tune-out wavelength (in nm) and the static dipole polarizability $\alpha_1(0)$ (in a_0^3) for the $2\,^3S_1$ state of helium. The numbers in parentheses are computational uncertainties.

Method	λ_t(nm)	$\alpha_1(0)$ (a.u.)
NRCI for $^\infty$He [18]	413.038 28(3)	315.6315(2)
NRCI for ^{4}He	413.139 19(2)	315.8204(2)
Correction from FNM	0.100 91(5)	0.1889(4)
RCI for $2\,^3S_1(M_J=0)$	412.9792(4)	315.5276(2)
RCI for $2\,^3S_1(M_J=\pm1)$	412.9850(4)	315.5359(2)
Total for $2\,^3S_1(M_J=0)$	413.0801(4)	315.7165(4)
Total for $2\,^3S_1(M_J=\pm1)$	413.0859(4)	315.7248(4)
Averaged over M_J	413.0845(4)	315.7227(4)
Hybrid [13]	413.02(9)	315.462
Expt. [17]	$413.0938(9_{\rm stat})(20_{\rm syst})$	
Slater NRCI [31]		315.611
Hylleraas [32]		315.631 468(12)

in the table for a direct comparison. We can see that the present averaged value is 0.023% larger than the hybrid value of $315.462a_0^3$. Compared with previous experimental measurements [33,34], our averaged value is much more accurate than the measured result $322(6.8)a_0^3$ by four orders of magnitude.

Meanwhile, we find that for the metastable $2\ ^3S_1$ state, the FNM and relativistic corrections to $\alpha_1(0)$ are, respectively, 600 ppm and 310 ppm. However, for the ground-state helium, the corresponding corrections are 447 ppm and 58 ppm [7,8]. This means that the FNM and relativistic corrections to the static dipole polarizability of $2\ ^3S_1$ are, respectively, 1.4 and 5.4 times larger than those for the ground state. Therefore a precise measurement of the static dipole polarizability of $2\ ^3S_1$ can test atomic structure theory related to the transition matrix elements.

Furthermore, since the $2\ ^3S \rightarrow 2\ ^3P$ transition contributes about $304.8351a_0^3$ to the static dipole polarizability of $315.8204(2)a_0^3$ for the $2\ ^3S$ state of ^{4}He, the static dipole polarizability can be expressed as

$$\alpha_1(0) = \frac{2X^2}{3\Delta E_{2\,^3S\rightarrow 2\,^3P}} + \alpha_{\rm rem}(0). \tag{8}$$

Here $X = \langle 2\ ^3S\|T_1\|2\ ^3P\rangle$ is the reduced matrix element, $\alpha_{\rm rem}(0)$ is the contribution from all the $2\ ^3S \rightarrow n\ ^3P$ ($n \geqslant 3$) transitions, which can be calculated accurately as $10.9670(8)a_0^3$ by replacing the first nine energies and matrix elements of our RCI values with the NIST energies and Hylleraas matrix elements. Since the accuracy of $\Delta E_{2\,^3S\rightarrow 2\,^3P}$ is better than 0.05 ppb [35], we can derive the following relationship between the relative uncertainty for X and $\alpha_1(0)$ from Eq. (8):

$$\frac{\delta X}{X} \simeq \frac{1}{2}\frac{\delta[\alpha_1(0) - \alpha_{\rm rem}(0)]}{[\alpha_1(0) - \alpha_{\rm rem}(0)]}. \tag{9}$$

At the present precision of $\alpha_{\rm rem}(0)$, we have

$$\frac{\delta X}{X} \simeq \frac{1}{2}\frac{\delta\alpha_1(0)}{\alpha_1(0)} + 10^{-6}. \tag{10}$$

If the experimental measurement accuracy for $\alpha_1(0)$ of the $2\ ^3S$ state can reach 10 ppm, which is possible using modern atom interferometry technique [14], the transition matrix element of $\langle 2\ ^3S\|T_1\|2\ ^3P\rangle$ would be determined at the level of 10^{-5} according to Eq. (10).

In summary, the tune-out wavelengths of 413.0801(4) nm and 413.0859(4) nm for the magnetic sublevels $M_J = 0$ and $M_J = \pm 1$, respectively, in the state of $2\ ^3S_1$ of helium have been determined by combining the RCI and NRCI calculations, including the FNM and relativistic corrections. The present value for the $M_J = 1$ sublevel reduces the discrepancy between the previous theoretical calculation and experimental measurement from 134 ppm to 19 ppm. The existing 19 ppm discrepancy between theory and experiment for the tune-out wavelength calls for further QED calculation. In addition, we have found that the FNM and relativistic corrections to the static dipole polarizability of the $2\ ^3S_1$ state of helium are about 1.4 and 5.4 times larger than those for the ground state. Therefore high-precision measurement of the static dipole polarizability of helium in $2\ ^3S_1$ will not only provide a test on atomic structure theory, but also can determine the transition matrix element of $2\ ^3S \rightarrow 2\ ^3P$ at a level better than 10^{-4}.

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