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Helium tune-out wavelength: Gauge invariance and retardation corrections

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Abstract The problem of calculating the tune-out wavelength for an atom interacting with a plane electromagnetic wave is formulated as a zero in the Rayleigh scattering cross section, rather than a zero in the dynamic polarizability. Retardation (finite wavelength) corrections are discussed in the velocity gauge, and possible gauge transformations to a length form are investigated. For the special case of S-states, it is shown that a pure length form exists for the leading $p_x z$ retardation correction, even though one does not exist in general. The results of high-precision calculations in Hylleraas coordinates are presented for the tune-out wavelength of helium near the $2\,^3S - 3\,^3P$ transition at 413 nm.

Keywords tune-out wavelength · gauge transformation · retardation · helium

1 Introduction

The tune-out wavelength is the wavelength at which the interaction of an atom with an incident laser field vanishes. Recent high-precision measurements in helium [1] are sensitive to relativistic and quantum electrodynamic corrections. The effect has traditionally been formulated as a zero in the ac Stark shift for an atom trapped in an optical lattice formed by counter-propagating laser beams [2,3], and detailed relativistic configuration-interaction (CI) calculations have been carried

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out [4]. However, an optical lattice corresponds to an electric potential that is fixed in space and oscillates in time such that the interaction with an atom depends on its location relative to the nodes of the potential. Calculations are usually done in the long-wavelength approximation for the dipole and higher multipole terms generated by the optical lattice. The Baldwin experiment [1] involves instead the interaction of an atom with a single laser beam corresponding to traveling transverse plane wave with a vector potential of the form

$$\mathbf{A} = A_0 \hat{\boldsymbol{e}} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega t} \tag{1}$$

In this case, it is more appropriate to think of the tune-out wavelength as a zero in the Rayleigh scattering cross section, rather than a zero in the frequency-dependent polarizability. In other words, the tune-out wavelength is the wavelength at which the atom no longer scatters photons, and so it becomes "invisible." The ac Stark shift does not take into account the photon nature of the interaction. The two pictures are equivalent in lowest order, but not when retardation corrections are taken into account; i.e., corrections to the long wavelength approximation.

The purpose of this paper is to reformulate the tune-out wavelength as a zero in the Rayleigh scattering cross section, and to investigate its calculation in the velocity form of the interaction, as well as the length form. We also investigate the calculation of the leading retardation correction. Some of the numerical results have been previously presented [5].

2 Rayleigh scattering formalism

Following the derivation of Akhiezer and Berestetskii [6] from QED, the normalization factor is $eA_0 = ce\sqrt{\hbar/(2\omega\mathcal{V})}$, normalized to unit photon energy $\hbar\omega$ in a volume $\mathcal{V}$, the effective interaction energy is

$$U_{i\to f} = \frac{2\pi\hbar c^2 e^2}{\mathcal{V}\sqrt{\omega_i\omega_f}} \sum_{n\pm} \left[\frac{\langle f \mid \hat{\boldsymbol{e}}_f e^{-i\mathbf{k}_f\cdot\mathbf{r}} \mid n\rangle\langle n \mid \hat{\boldsymbol{e}}_i e^{i\mathbf{k}_i\cdot\mathbf{r}} \mid i\rangle}{E_n - E_i - \hbar\omega_i} \right.$$
$$\left. + \frac{\langle f \mid \hat{\boldsymbol{e}}_i e^{i\mathbf{k}_i\cdot\mathbf{r}} \mid n\rangle\langle n \mid \hat{\boldsymbol{e}}_f e^{-i\mathbf{k}_f\cdot\mathbf{r}} \mid i\rangle}{E_n - E_f + \hbar\omega_i} \right] \tag{2}$$

summed over both positive and negative energy states. In terms of the Dirac γ-matrices, $\hat{\boldsymbol{e}}$ is defined by $\hat{\boldsymbol{e}} = \gamma_\mu e_\mu$, and $\mathbf{e}$ is the polarization vector such that $\mathbf{k}\cdot\mathbf{e} = 0$. For the case of coherent Rayleigh scattering, $E_i = E_f$, $\mathbf{k}_i = \mathbf{k}_f$, and $\omega_i = \omega_f = \omega$. Let us assume for the sake of definiteness that the propagation vector $\mathbf{k}$ points in the z-direction, and the wave is plane-polarized in the x-direction. (The results are easily generalized to the case of arbitrary directions of propagation and polarization.) The expression for $U_{i\to f}$ then becomes

$$U = \frac{2\pi c^2 e^2\hbar}{\omega\mathcal{V}} \sum_{n\pm} \left[\frac{\langle i \mid \alpha_x e^{-ikz} \mid n\rangle\langle n \mid \alpha_x e^{ikz} \mid i\rangle}{E_n - E_i - \hbar\omega} + \frac{\langle i \mid \alpha_x e^{ikz} \mid n\rangle\langle n \mid \alpha_x e^{-ikz} \mid i\rangle}{E_n - E_i + \hbar\omega} \right] \tag{3}$$

where $k = \omega/c$. For convenience, let us write this in the form

$$U = \frac{2\pi c^2 e^2\hbar}{\omega\mathcal{V}} \sum_{n\pm} \left| \langle i \mid \alpha_x e^{ikz} \mid n\rangle \right|^2 \left(\frac{1}{\Delta E_n + \bar{\omega}} + \frac{1}{\Delta E_n - \bar{\omega}} \right) \tag{4}$$

where $\Delta E_n = E_n - E_i$ and $\bar{\omega} = \hbar\omega$. For a many-electron atom, the transition operator $\alpha_x e^{ikz}$ is understood to be summed over the N atomic electrons.

The contribution from negative energy states in Eq. (4) makes an important contribution, even in the nonrelativistic limit. It could be handled directly without approximation by introducing a complete basis set of relativistic Sturmian functions [7–9]. However, our aim here is to obtain equivalent nonrelativistic operators. As discussed by Akhiezer and Berestetskii [6], in the nonrelativistic limit $\hbar\omega << mc^2$, the denominators in Eq. (4) can be replaced by a constant $E_n \simeq -2mc^2$. The sum over n^- can then be extended to a sum over all $n^{\pm}$ with the introduction of negative energy projection operators, and the sum completed by closure. In this approximation, the contribution from negative energy states is proportional to the matrix element $\langle f \mid \mathbf{e}_i \cdot \mathbf{e}_f \exp[i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}] \mid i \rangle$, which just reduces to $N\delta_{if}$ for the case of coherent scattering with $\mathbf{k}_f = \mathbf{k}_i$, and N is the number of electrons. Then U^- becomes

$$U^- = -\frac{2N\pi c^2 e^2 \hbar}{\omega \mathcal{V}} \left(\frac{1}{2mc^2 + \bar{\omega}} + \frac{1}{2mc^2 - \bar{\omega}} \right)$$
$$\simeq -\frac{2N\pi e^2 \hbar}{m\omega \mathcal{V}} \left[1 + \left(\frac{\bar{\omega}}{2mc^2} \right)^2 + \cdots \right] \tag{5}$$

There are of course other binding-energy corrections, which are known in the one-electron case from Lamb shift calculations [10], but the second term in Eq. (5) is certainly one of the frequency-dependent terms that should be included.

U^- can now be combined with the remaining sum over positive energies to obtain the total

$$U = \frac{2\pi c^2 e^2 \hbar}{\omega \mathcal{V}} \left\{ \sum_{n^+} \left| \langle i \mid \alpha_x e^{ikz} \mid n \rangle \right|^2 \left(\frac{1}{\Delta E_n + \bar{\omega}} + \frac{1}{\Delta E_n - \bar{\omega}} \right) \right.$$
$$\left. - \frac{N}{mc^2} \left[1 + \left(\frac{\hbar\omega}{2mc^2} \right)^2 + \cdots \right] \right\} \tag{6}$$

The usual procedure at this point is to make the long wavelength approximation and assume that $kz << 1$ for values of z within the dimensions of the atom, and to insert the retardation expansion

$$e^{ikz} = 1 + ikz - \frac{1}{2}(kz)^2 + \cdots \tag{7}$$

This is rapidly convergent for nonrelativistic frequencies $\omega = k/c$, and so only the leading three terms will be considered for now.

Let us first consider the nonretarded limit where only the first term of the right-hand-side of Eq. (7) is kept. In that case, the transition matrix element is simply $\langle i \mid \alpha_x \mid n \rangle$, evaluated in terms of Dirac wave functions. In the nonrelativistic limit, we can make the replacement

$$\alpha \cdot \mathbf{A} \to \frac{\mathbf{p} \cdot \mathbf{A}}{mc} + \boldsymbol{\mu} \times \mathbf{A} \tag{8}$$

where $\boldsymbol{\mu} = (e\hbar/2mc)\boldsymbol{\sigma}$ is the spin magnetic moment of the electron. Neglecting for now the spin-dependent part, Eq. (6) then simplifies to

$$U = \frac{2\pi e^2 \hbar}{\omega m \mathcal{V}} \left\{ \frac{1}{m} \sum_{n^+} |\langle i \mid p_x \mid n \rangle|^2 \left(\frac{1}{\Delta E_n + \bar{\omega}} + \frac{1}{\Delta E_n - \bar{\omega}} \right) - N \right\} \tag{9}$$

Equation (9) corresponds to the "velocity" (or momentum) form of the interaction. Calculations of tune-out wavelengths are typically done in the equivalent "length" form involving matrix elements of x in place of p_x. The transformation can be accomplished by making use of the commutation relation

$$[H, x] = \frac{i\hbar}{m} p_x \tag{10}$$

together with $(E_n - E_i)\langle i \mid x \mid n\rangle = -\langle n \mid [H, x] \mid i\rangle$, where x is a short-hand notation for $\sum_{k=1}^{N} x_k$. An interesting feature is that the summation term in Eq. (9) tends to N in the limit $\omega \to 0$ (analogous to the Thomas-Reiche-Kuhn oscillator strength sum rule) and so the two terms cancel. To see this more clearly, it is useful to expand the energy denominators in the form

$$\frac{1}{\Delta E_n + \bar{\omega}} + \frac{1}{\Delta E_n - \bar{\omega}} = \frac{2}{\Delta E_n} \left(1 + \frac{\bar{\omega}^2}{\Delta E_n^2} + \cdots\right) \tag{11}$$

and correspondingly expand $U = U^{(0)} + U^{(2)} + \cdots$. The leading two terms are then

$$U^{(0)} = \frac{2\pi e^2 \hbar}{\omega m \mathcal{V}} \{N - N\} = 0 \tag{12}$$

and

$$U^{(2)} + \cdots = \frac{2\pi e^2 \hbar}{\omega m \mathcal{V}} \left\{ 2\omega^2 m \sum_{n^+} \frac{\langle i \mid x \mid n\rangle\langle n \mid x \mid i\rangle}{\Delta E_n} \left(1 + \frac{\bar{\omega}^2}{\Delta E_n^2} + \cdots\right) \right\} \tag{13}$$

The infinite series in $(\omega/\Delta E_n)^2$ can then be resummed to infinity to obtain the final length form

$$U = \frac{2\pi e^2 \bar{\omega}}{\mathcal{V}} \sum_{n^+} \langle i \mid x \mid n\rangle\langle n \mid x \mid i\rangle \left(\frac{1}{\Delta E_n + \bar{\omega}} + \frac{1}{\Delta E_n - \bar{\omega}}\right)$$

$$\equiv \frac{2\pi \bar{\omega}}{\mathcal{V}} \alpha_d(\omega) \tag{14}$$

where $\alpha_d(\omega)$ is the frequency-dependent dipole polarizability. At this level, it makes no difference whether one identifies the tune-out wavelength as a zero in $\alpha_d(\omega)$, or a zero in the effective interaction energy $U(\omega)$ responsible for Rayleigh scattering. However, it does make a difference when retardation corrections are considered, as discussed in the following section. There is a further qualitative difference in the interaction energy in limit $\omega \to 0$. In this limit, $U(\omega)$ vanishes, but the static dipole polarizability α_d remains constant.

3 Retardation Corrections

Retardation (finite wavelength) corrections to the results in the previous section come from the higher-order terms in Eq. (7). They must be calculated in the velocity form of the interaction because, in general, a length form as usually defined does not exist beyond the lowest-order term for any given multipole [11]. The following paragraphs provide a rationale for the nonexistence of a simple length form.

According to the usual argument, the equivalence of the length and velocity forms can be viewed as a gauge transformation of the electromagnetic fields E and B which satisfy Maxwell's equations

$$\mathbf{E} = -\nabla V - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} \tag{15}$$

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{16}$$

The physical fields $\mathbf{E}$ and $\mathbf{B}$ are invariant under an arbitrary transformation of the scalar and vector potentials V and A according to

$$\mathbf{A} \longrightarrow \mathbf{A} + \nabla f(\mathbf{r}, t) \tag{17}$$

$$V \longrightarrow V - \frac{1}{c}\frac{\partial f(\mathbf{r}, t)}{\partial t} \tag{18}$$

where $f(\mathbf{r}, t)$ is an arbitrary differentiable function of $\mathbf{r}$ and t. For a wave propagating in the z-direction and polarized in the x-direction, choose

$$\mathbf{A} = A_0 \hat{\mathbf{e}}_{\mathbf{x}}\, e^{ikz - i\omega t} \tag{19}$$

$$f(\mathbf{r}, t) = \mathcal{C}\, e^{ikz - i\omega t} \tag{20}$$

where $\mathcal{C}$ is an arbitrary constant. Then the gauge transformation yields

$$\mathbf{A} \to A_0 \hat{\mathbf{e}}_{\mathbf{x}}\, e^{ikz - i\omega t} + \mathcal{C} ik\hat{\mathbf{e}}_{\mathbf{z}}\, e^{ikz - i\omega t} \tag{21}$$

$$V \to V + \mathcal{C}\frac{i\omega}{c}\, e^{ikz - i\omega t} \tag{22}$$

where $k = \omega/c$. Define a new arbitrary constant $\mathcal{C}' = ik\mathcal{C}$. Then

$$\mathbf{A} = A_0 \hat{\mathbf{e}}_{\mathbf{x}}\, e^{ikz - i\omega t} + \mathcal{C}' \hat{\mathbf{e}}_{\mathbf{z}}\, e^{ikz - i\omega t} \tag{23}$$

$$V = V_0 + \mathcal{C}'\, e^{ikz - i\omega t} \tag{24}$$

Thus the gauge transformation introduces a longitudinally polarized component $\mathcal{C}' \hat{\mathbf{e}}_{\mathbf{z}}\, e^{ikz - i\omega t}$ counterbalanced by an additional contribution $\mathcal{C}'\, e^{ikz - i\omega t}$ to the scalar potential V, while leaving the physical $\mathbf{E}$ and $\mathbf{B}$ fields unchanged.

Quantum mechanical matrix elements are also unchanged, provided that the wave functions are exact, and this leads to the "length" form of the transition operator, at least in lowest order, as follows. Equating matrix elements of the $\mathcal{C}'$-dependent parts of $-(\mathbf{p} \cdot \mathbf{A} + \mathbf{A}) \cdot \mathbf{p}/(2mc)$ and V between arbitrary orthogonal states $\mid a \rangle$ and $\mid b \rangle$ yields

$$\frac{1}{2mc}\langle a \mid p_z e^{ikz} + e^{ikz} p_z \mid b \rangle = -\langle a \mid e^{ikz} \mid b \rangle \tag{25}$$

where, by conservation of energy, $k = \omega_{ab}/c$. This equation is satisfied term-by-term to all orders in the expansion $e^{ikz} = 1 + ikz + \cdots$, provided that the wave functions are exact and orthogonal. This can easily be seen by making the substitution

$$\begin{aligned}
\langle a \mid (ikz)^{n+1} \mid b \rangle &= i\omega_{ab}\frac{(ik)^n}{c}\langle a \mid z^n \mid b \rangle \\
&= i\frac{(ik)^n}{\hbar c}\langle a \mid [H_0, z^n] \mid b \rangle
\end{aligned} \tag{26}$$

and evaluating the commutator with the field-free Hamiltonian H_0. The leading nonvanishing terms give

$$\frac{1}{mc}\langle a \mid p_z \mid b \rangle = -\frac{i\omega_{ab}}{c}\langle a \mid z \mid b \rangle \tag{27}$$

This is the usual equivalence of the length and velocity forms. However, the correct velocity operator for our assumed plane wave is $\boldsymbol{p_x}e^{ikz}$, not $\boldsymbol{p_z}e^{ikz}$. In general, there is no equivalent length form valid beyond leading order [11].

3.1 Gauge invariance of multipole expansions

A similar argument applies to each partial wave if the plane wave discussed so far with definite direction of propagation $\mathbf{k}$ and direction of polarization $\hat{\mathbf{e}}$ in terms of definite angular momentum L and parity. It is always possible to write

$$\bar{\omega}_{ab}\langle a \mid r^L Y_L^M \mid b \rangle = \langle a \mid [H, r^L Y_L^M] \mid b \rangle \tag{28}$$

where Y_L^M is a spherical harmonic. Furthermore, since $\nabla^2 r^L Y_L^M(\theta, \phi) = 0$, it follows that (in atomic units)

$$[H, r^L Y_L^M] = -\frac{1}{2}[\nabla^2, r^L Y_L^M] \tag{29}$$

$$= -\nabla r^L Y_L^M \cdot \nabla \tag{30}$$

$$= -i\nabla r^L Y_L^M \cdot \mathbf{p} \tag{31}$$

which is the correct velocity form of the operator. However, this works only to lowest order. The function r^L is just the leading term in the power series expansion of the spherical Bessel function $j_L(kr) = j_L(\omega r/c)$ [14], and in general $\nabla^2 r^K Y_L^M(\theta, \phi) \neq 0$ unless $K = L$.

3.2 The leading retardation term

As an illustrative example, the operator for the leading retardation correction to the velocity form $p_x e^{ikz}$ is $ikp_x z$. In general, there is no corresponding pure length form [11], but for the special case of the interaction energy U for spherically symmetric S-states, the operator can be symmetrized with respect to x and z to obtain, for matrix elements

$$\langle a \mid \frac{ik}{2mc}(p_z x + p_x z) \mid b \rangle = -\frac{k}{2\hbar c}\langle a \mid [H_0, xz] \mid b \rangle$$

$$= -\frac{k^2}{2}\langle a \mid xz \mid b \rangle \tag{32}$$

evaluated at $k = \omega_{ab}/c$. The right-hand-side looks superficially like a quadrupole interaction, but in fact it is a retardation correction. It is a factor of two smaller

than what one might naively expect. Using this equivalence, the velocity and length forms of the xz-retardation correction are

$$\Delta U_{xz}^V = \frac{2\pi e^2 \hbar}{\omega m \mathcal{V}} \left\{ \frac{k^2}{m} \sum_{n^+} |\langle i \mid p_x z \mid n \rangle|^2 \left(\frac{1}{\Delta E_n + \bar{\omega}} + \frac{1}{\Delta E_n - \bar{\omega}} \right) \right\} \quad (33)$$

$$\Delta U_{xz}^L = \frac{2\pi e^2 \bar{\omega}}{\mathcal{V}} \left\{ \frac{k^2}{4} \sum_{n^+} |\langle i \mid xz \mid n \rangle|^2 \left(\frac{1}{\Delta E_n + \bar{\omega}} + \frac{1}{\Delta E_n - \bar{\omega}} \right) \frac{\Delta E_n^2}{\bar{\omega}^2} \right\} \quad (34)$$

The results presented in the following section demonstrate that the above expressions yield identical results to within the accuracy allowed by the variational wave functions. The next $(kz)^2/2$ in Eq. (7) also contributes as a cross-term after squaring. This and other finite mass and relativistic corrections will be discussed separately in a future publication.

4 Calculations and Conclusions

This section presents results of calculations of the tune-out wavelength for helium near the 413 nm transition corresponding to the $2\,^3S - 3\,^3P$ transition. The field-free Hamiltonian for helium in reduced mass atomic units is

$$H_0 = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} - \frac{\mu}{M}\nabla_1 \cdot \nabla_2 \quad (35)$$

where the last term is the mass polarization term, and μ is the electron reduced mass. The transition matrix elements and energies were evaluated in terms of variational solutions to the Schrödinger equation with wave functions expressed in Hylleraas coordinates of the form [15,16]

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{p=1}^{2} \sum_{i,j,k} a_{ijk}^{(p)} \, r_1^i r_2^j r_{12}^k \, e^{-\alpha_p r_1 - \beta_p r_2} \, \mathcal{Y}_{l_1 l_2 L}^M(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \pm \mathbf{1} \leftrightarrow \mathbf{2} \quad (36)$$

with $i + j + k \leq \Omega$, $\Omega = 4,\ 5,\ 6,\ \cdots 15$, and $\mathcal{Y}_{l_1 l_2 L}^M(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$ is a vector-coupled product of spherical harmonics for the two electrons to form a state of total angular momentum L and component M. The sum over p allows for two (or more) individually optimized distance scales as determined by the nonlinear parameters α_p and β_p. The resulting wave functions have exceptional numerical stability so that standard quadruple precision arithmetic (approximately 32 decimal digits) is sufficient.

The infinite sums over intermediate states in the previous section (including an integration over the continua) were replaced by finite sums over variationally determined pseudostates obtained by diagonalizing the Hamiltonian in an N-dimensional basis set of P-states for the nonrelativistic tune-out wavelength, and D-states for the xz-retardation correction.

As an illustrative example, Table 1 shows the convergence with basis set size for the nonrelativistic tune-out wavelength λ_t in both the length (L) and velocity (V) forms. It is significant that the velocity form is more rapidly convergent with basis set size (as controlled by Ω) by more than an order of magnitude, even though it does not yield an accurate value for the static polarizability α_d due to

Table 1 Nonrelativistic tune-out wavelength λ_t near the $2\,^3S - 3\,^3P$ transition of helium at 413 nm for the case of infinite nuclear mass, calculated in both the length (L) and velocity (V) forms. N_S and N_P are the numbers of terms in the S- and P-state basis sets respectively for each $\Omega = (i + j + k)_{\max}$. $\Delta\lambda_t^L$ and $\Delta\lambda_t^V$ are the changes in λ_t^L and λ_t^V for successive values of Ω to show the respective rates of convergence.

Ω	N_S/N_P	λ_t^L (nm)	$\Delta\lambda_t^L$	λ_t^V (nm)	$\Delta\lambda_t^V$
4	35/104	413.140 681 9343		413.031 682 9604	
5	56/164	413.046 812 8503	−0.093 869 0840	413.036 738 3288	0.005 055 3684
6	84/238	413.040 187 6300	−0.006 625 2203	413.038 111 5461	0.001 373 2173
7	120/300	413.038 656 7622	−0.001 530 8678	413.038 278 7252	0.000 167 1791
8	164/371	413.038 394 3741	−0.000 262 3881	413.038 295 0253	0.000 016 3001
9	218/457	413.038 345 3450	−0.000 049 0291	413.038 301 6088	0.000 006 5835
10	281/551	413.038 308 7062	−0.000 036 6388	413.038 304 0087	0.000 002 3999
11	356/660	413.038 305 4303	−0.000 003 2759	413.038 304 3265	0.000 000 3178
12	441/775	413.038 304 5622	−0.000 000 8681	413.038 304 3887	0.000 000 0622
13	540/905	413.038 304 4523	−0.000 000 1099	413.038 304 3817	−0.000 000 0070
14	650/1039	413.038 304 3970	−0.000 000 0553	413.038 304 3859	0.000 000 0042
15	776/1189	413.038 304 3893(35)	−0.000 000 0077	413.038 304 3858(1)	−0.000 000 0001
Other theory		413.038 28(3)[a]			

[a] Zhang et al. [4].

numerical cancellation (cf. Eq. (12).) Also, the length form tends to converge from above while the velocity form converges (predominantly) from below. The result for the finite nuclear mass case for ^{4}He with $\mu/M = 1.370\,745\,665 \times 10^{-4}$ is

$$\lambda_t(^4\text{He}) = 413.082\,590\,5833\, m_e/\mu = 413.139\,221\,4630(1) \text{ nm} \tag{37}$$

where $\mu/m_e = 1 - \mu/M$ is the reduced mass to electron mass ratio, and for the finite nuclear mass case, the factor of $1/m$ in Eq. (9) should be replaced by $(1/m)(1 + \mu/M)$. The numerical result marginally disagrees with the nonrelativistic value $413.139\,19(2)$ nm from Ref. [4].

Finally, the calculated xz-retardation correction is $\delta\lambda_t^{(xz)} = 0.000\,560\,0236$ nm assuming infinite nuclear mass. This is a correction of nominal order α^2, and so is significant relative to other relativistic and QED corrections. It has not been included in previous calculations. A detailed discussion of these other corrections will be given in a future publication. They must also be included before a meaningful comparison can be made with the experimental value $\lambda_t = 413.0938(9_{\text{stat}})((20_{\text{syst}})$ [1], and the most recent theoretical value $\lambda_t = 413.09015(4)$ nm [17].

In conclusion, we have reformulated the tune-out wavelength problem as a zero in the Rayleigh scattering cross section instead of a zero in the frequency-dependent polarizability, and demonstrated how the calculation can be done in the velocity form as well as the length form. The velocity form turns out to be more rapidly convergent for the tune-out wavelength, but not for the static polarizability. In addition, we have shown how retardation corrections can be calculated in the velocity form, even though a pure length form in general does not exist. The choice of which formalism to use depends entirely on the experimental conditions, and in particular whether the atom is interacting with a travelling wave as expressed by Eq. (1) or a standing wave in an optical lattice. In future work, relativistic and QED corrections will be discussed, including corrections to the radiative transition operator [18].

Aclnowledgments

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