



# CHORUS

This is the accepted manuscript made available via CHORUS. The article has been published as:

## Magic wavelength for the hydrogen 1S-2S transition: Contribution of the continuum and the reduced-mass correction

C. M. Adhikari, A. Kawasaki, and U. D. Jentschura

Phys. Rev. A **94**, 032510 — Published 20 September 2016

DOI: [10.1103/PhysRevA.94.032510](https://doi.org/10.1103/PhysRevA.94.032510)

# Addendum to: "Magic wavelength for the hydrogen 1S-2S transition"

C. M. Adhikari,<sup>1</sup> A. Kawasaki,<sup>2</sup> and U. D. Jentschura<sup>1</sup>

<sup>1</sup>*Department of Physics, Missouri University of Science and Technology, Rolla MO65409, USA*

<sup>2</sup>*Department of Physics, MIT-Harvard Center for Ultracold Atoms and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

Recently, we have studied the magic wavelength for the atomic hydrogen 1S-2S transition [A.K., Phys. Rev. A **92**, 042507 (2015)]. An explicit summation over virtual atomic states of the discrete part of the hydrogen spectrum was performed to evaluate the atomic polarizability. In this addendum, we supplement the contribution of the continuum part of the spectrum and add the reduced-mass correction. At the magic wavelength, the lowest-order ac Stark shifts of the 1S and 2S states are equal; it is found to be equal to 514.6 nm. The ac Stark shift at the magic wavelength is  $-221.6 \text{ Hz}/(\text{kW}/\text{cm}^2)$ , and the slope of the ac Stark shift at the magic wavelength under a change of the driving laser frequency is  $-0.2157 \text{ Hz}/(\text{GHz kW}/\text{cm}^2)$ .

PACS numbers: 31.15.ap, 32.10.Dk, 32.60.+i, 37.10.Jk

The ac Stark shift is one of the most important perturbations experienced by atoms in external fields. It is induced by any any oscillating electric field, and not restricted to resonant driving. On the one hand, the presence of the ac Stark shift is beneficial when it comes to trapping atoms by a light force in a dispersive region. Optical dipole traps [1] and optical lattices are widely used in the study of ultracold atoms [2]. On the other hand, the ac Stark shift becomes an obstacle in precision measurements aiming to determine transition frequencies in atoms to a level of one Hertz or better. The frequency of narrow two-photon transitions induced by an intense light field, is shifted significantly by the exciting light field [3, 4]. The ac Stark shift due to the black-body radiation is one of the major uncertainties in optical lattice-clock experiments [5], and the ac Stark shift due to the optical lattice light is an essential effect in optical lattice clock experiments [6, 7].

When the optical dipole trap or the optical lattice clock is used for trapping atoms, the resulting ac Stark shift is significantly larger than the target precision for the transition frequency, and furthermore, the ac Stark shift is generally different for the ground state and the excited state of the transition. In order to cancel this shift, one needs to use the light of a special wavelength called the magic wavelength [7].

In order to calculate the magic wavelength, we first evaluate the ac Stark shift for the ground state and the excited state of a transition, and then search the point where the difference is zero. The ac Stark is given for a specific atomic reference state  $|\phi\rangle$  as

$$\delta E_{\text{ac}} = -\frac{I_L}{2\epsilon_0 c} \alpha(\phi, \omega_L), \quad (1)$$

where  $I_L$  is the laser intensity, and  $\alpha(\phi, \omega_L)$ ,  $|\phi\rangle$ , and  $\omega_L$  are the dipole polarizability, the atomic reference state, and the angular frequency of the laser, respectively [8, 9].

The dipole polarizability for a reference state  $|\phi\rangle$ ,

whose energy is denoted as  $E$ , reads as

$$\begin{aligned} \alpha(\phi, \omega_L) &= \frac{e^2}{3} \sum_{\pm} \left\langle \phi \left| \vec{r} \left( \frac{1}{H_A - E \pm \hbar\omega_L} \right) \vec{r} \right| \phi \right\rangle \\ &= P_{\phi}(\omega_L) + P_{\phi}(-\omega_L), \end{aligned} \quad (2)$$

where  $\vec{r}$  is the electron position operator (the scalar product is implied by the repeated occurrence of the vector). Furthermore,  $H_A$  is the atomic (Schrödinger) Hamiltonian. The  $P$  matrix elements are implicitly defined as the terms that emerge from the sum over virtual states.

We have already discussed [10] that Optical trapping with light of the magic wavelength corresponding to the hydrogen 1S-2S transition could be important for the improvements in Doppler-free two-photon spectroscopy. The calculation described in Ref. [10] included the contribution from the discrete virtual states. With the formalism of Eq. (2), we include the effect of the continuous part of the spectrum as well. Based on Ref. [11], we know that the latter effect can be large for the dc Stark shift of the hydrogen ground state. It is known that matrix elements of the form (2) can be summed in close analytic form [12–17]. Angular components are calculated separately from the radial components [18]. As for the radial component, one first performs the Sturmian decomposition of the Schrödinger Green function [19], then does the radial integrations, and finally carries out the summations over the discrete and continuous spectra.

In the approximation of an infinite nuclear mass, the calculation for the hydrogen 1S state results in

$$\begin{aligned} P_{1S}(\omega_L) &= -\frac{e^2 a_0^2}{E_h} \left[ \frac{2t^2}{3(1-t)^5(1+t)^4} (38t^7 + 26t^6 \right. \\ &\quad \left. + 19t^5 - 19t^4 - 12t^3 + 12t^2 + 3t - 3) \right. \\ &\quad \left. - \frac{256 t^9}{3(t-1)^5(t+1)^5} {}_2F_1 \left( 1, -t, 1-t, \left( \frac{1-t}{1+t} \right)^2 \right) \right], \\ t &= \left( 1 + \frac{2\hbar\omega_L}{E_h} \right)^{-1/2}, \end{aligned} \quad (3a)$$

whereas one obtains for  $2S$ ,

$$P_{2S}(\omega_L) = \frac{e^2 a_0^2}{E_h} \left[ \frac{16\tau^2}{3(\tau-1)^6(1+\tau)^4} (1181\tau^8 - 314\tau^7 - 16\tau^6 - 166\tau^5 + 14\tau^4 + 138\tau^3 - 48\tau^2 - 42\tau + 21) - \frac{16384\tau^9(4\tau^2-1)}{3(\tau-1)^6(\tau+1)^6} {}_2F_1\left(1, -2\tau, 1-2\tau, \left(\frac{1-\tau}{1+\tau}\right)^2\right) \right],$$

$$\tau = \left(1 + \frac{8\hbar\omega_L}{E_h}\right)^{-1/2}. \quad (3b)$$

Here,  $a_0 = \hbar/(\alpha m_e c)$ ,  $m_e$ , and  $E_h = \alpha^2 m_e c^2$  are the Bohr radius, the electron mass, and the Hartree energy, respectively. The complete (Gaussian) hypergeometric function is denoted as  ${}_2F_1$ .

The magic angular frequency  $\omega_M$  is determined by the condition  $f(\omega_L = \omega_M) = 0$ , where

$$f(\omega_L) = \alpha(2S, \omega_L) - \alpha(1S, \omega_L). \quad (4)$$

An evaluation using the Newton-Raphson technique with a starting value of  $\hbar\omega_M \approx 0.09 E_h$ , which is a one-significant-digit approximation the magic wavelength inspired by our previous calculation [10], converges to a value of  $\hbar\omega_M \approx 0.088\,581\,526 E_h$ . We employ quadruple precision arithmetic (32 decimals) in intermediate steps.

The first reduced-mass correction is taken into account by observing that the hydrogen transition frequencies, and transition matrix elements, scale with the reduced mass of atomic hydrogen,

$$m_r = \frac{m_e m_p}{m_e + m_p}, \quad (5)$$

where  $m_p$  is the proton mass. The result for the magic angular frequency thus receives an additional correction factor  $m_r/m_e$  and reads as

$$\omega_M = 2\pi \times 5.825\,211 \times 10^{14} \text{ Hz}, \quad (6)$$

which corresponds to a frequency of  $\nu_M = 5.825\,211 \times 10^{14} \text{ Hz}$ . The magic wavelength thus is

$$\lambda_M = 514.646 \text{ nm}. \quad (7)$$

The difference of result for the magic wavelength obtained here [Eq. (7)] and our previous calculation [10] is larger than the reduced-mass correction. This implies that the effect of the continuous part of the spectrum is not negligible. This is consistent with observations made in the calculation of the dc Stark shift of the hydrogen ground state, and Bethe logarithms in other simple atomic systems like helium [20]. As evident from Fig. 1 of Ref. [10], the wavelength (7) lies in between the  $2S$ – $3S$  and  $2S$ – $4S$  transitions. We note that the vertical bars in the cited figure correspond to the sign changes of the ac Stark shift near resonant frequencies of the hydrogen atom; these resonances formally induce poles as they correspond to zeros of the propagator denominator in Eq. (2).

In order to evaluate the absolute value of the ac Stark shift at the magic wavelength numerically, the series representation [21, 22] of the hypergeometric function is sufficient. The result is

$$\Delta E_M = \Delta E_{ac}(1S, \omega_M) = \Delta E_{ac}(2S, \omega_M) = -221.584 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}. \quad (8)$$

In obtaining Eq. (8), we have taken into account that the polarizability matrix elements in Eqs. (3a) and (3b) receive reduced-mass corrections in the form of factors  $(m_e/m_r)$ , which multiply the Bohr radius and the energy denominator, resulting in an overall prefactor  $(m_e/m_r)^3$ . Finally, the slope of the ac Stark shift within the improved formulation of the problem presented in this Addendum is

$$\eta = \left. \frac{\partial}{\partial \omega_L} (\Delta E_{ac}(2S, \omega_M) - \Delta E_{ac}(1S, \omega_M)) \right|_{\omega_L = \omega_M} = -0.215\,748 \frac{\text{Hz}}{\text{GHz (kW/cm}^2)}. \quad (9)$$

Relativistic corrections to the polarizability can be taken into account, if desired, by perturbing the Hamiltonian, wave function, and the energy of the reference state, in the following way,

$$H_A \rightarrow H_A + H_R, \quad (10a)$$

$$E \rightarrow E + \langle H_R \rangle, \quad (10b)$$

$$|\phi\rangle \rightarrow |\phi\rangle + \left( \frac{1}{E - H_A} \right)' H_R |\phi\rangle. \quad (10c)$$

Here, the Schrödinger Hamiltonian  $H_A$  and the relativistic correction term  $H_R$  are

$$H_A = \frac{\vec{p}^2}{2m_e} - \frac{\alpha \hbar c}{r} \quad (11)$$

$$H_R = -\frac{\vec{p}^4}{8m_e^3 c^2} + \frac{1}{2} \alpha \left( \frac{\hbar^2 g_s}{2m_e^2 c} \right) \frac{\vec{L} \cdot \vec{S}}{|\vec{r}|^3} + \frac{\hbar^3}{8m_e^2 c} 4\pi\alpha \delta^{(3)}(\vec{r}), \quad (12)$$

where  $g_s \approx 2$  is the spin  $g$  factor. These relativistic effects shift the transition frequencies in hydrogen, and the magic wavelength, by a relative correction of order  $\alpha^2 \sim 10^{-4}$ . The relative accuracy of the results given in Eqs. (7), (8) and (9) thus is of the order of  $10^{-4}$ . The reduced-mass correction, by contrast, is of the order of  $m_e/m_p \sim 10^{-3}$  and is the dominant correction to the nonrelativistic one-particle approximation.

There is, in addition, a field-configuration dependent shift of the transition frequency, due to the following term in the long-wavelength quantum electrodynamic Hamiltonian [16, 24].

$$H_{LW} = -e \vec{r} \cdot \vec{E}(t, \vec{0}) - \frac{e}{2} r^i r^j \frac{\partial E^i(t, \vec{r})}{\partial r^j} \Big|_{\vec{r}=\vec{0}} - \frac{e}{6} r^i r^j r^k \frac{\partial^2 E^i(t, \vec{r})}{\partial r^j \partial r^k} \Big|_{\vec{r}=\vec{0}}. \quad (13)$$

TABLE I. Influence of the reduced-mass correction (RMC) on the magic wavelength  $\lambda_M$ , ac Stark shift  $\Delta E_M$ , and slope  $\eta$  of the ac Stark shift, with results indicated in Eqs. (7), (8), and (9). The  $1S-3S$  and  $1S-4S$  results are obtained using a generalization of the result given in Eq. (3b) to higher excited states, using techniques familiar from analytic Lamb shift calculations [23].

Quantity	Without RMC	With RMC
$1S-2S$ Transition		
$\lambda_M$	514.366 nm	514.646 nm
$\Delta E_M$	$-221.222 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}$	$-221.584 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}$
$\eta$	$-0.215396 \frac{\text{Hz}}{\text{GHz}(\text{kW/cm}^2)}$	$-0.215748 \frac{\text{Hz}}{\text{GHz}(\text{kW/cm}^2)}$
$1S-3S$ Transition		
$\lambda_M$	1371.11 nm	1371.85 nm
$\Delta E_M$	$-212.307 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}$	$-212.654 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}$
$\eta$	$-3.20679 \frac{\text{Hz}}{\text{GHz}(\text{kW/cm}^2)}$	$-3.21203 \frac{\text{Hz}}{\text{GHz}(\text{kW/cm}^2)}$
$1S-4S$ Transition		
$\lambda_M$	2811.24 nm	2812.77 nm
$\Delta E_M$	$-211.249 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}$	$-211.594 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}$
$\eta$	$-28.4676 \frac{\text{Hz}}{\text{GHz}(\text{kW/cm}^2)}$	$-28.5142 \frac{\text{Hz}}{\text{GHz}(\text{kW/cm}^2)}$

Let us assume, for definiteness, a plane standing wave of linearly  $z$ -polarized light with wave vector  $\vec{k}$  aligned along the  $x$ -direction. In this case, the electric field is given by

$$\vec{E}(t, x) = \hat{e}_z \mathcal{E}_L \cos(\omega_L t) \cos(k_L x), \quad (14)$$

where  $k_L = \omega_L/c$ . We assume that atoms are at antinodes of the standing wave, i.e., that we have  $\cos(k_L x) = 1$  at the position of the atom. In this case, the first and third terms in (13) contribute, and we obtain

$$H_{LW} \approx -e z \mathcal{E}_L \cos(\omega_L t) + \frac{e}{6} k_L^2 x^2 z \mathcal{E}_L \cos(\omega_L t). \quad (15)$$

The leading field-configuration dependent correction to the dynamic polarizability of state  $|\phi\rangle$  therefore reads

$$\delta\alpha(\phi, \omega_L) = -\frac{e^2 k_L^2}{6} \sum_{\pm} \left\langle \phi \left| z \frac{1}{H_0 - E_\phi \pm \hbar\omega_L} x^2 z \right| \phi \right\rangle, \quad (16)$$

but this expression depends on our choice (14) of the laser field configuration and would be different for, e.g., a traveling as opposed to standing wave. The second term on the right-hand side of Eq. (13), which is a lower-order contribution, vanishes for symmetry reasons, and magnetic effects can be neglected [10]. As already stated, the magic angular frequency for the two-photon  $1S-2S$  transition lies in between the frequencies of the single-photon  $2S-3P$  and  $2S-4P$  transitions, and therefore is of the same order-of-magnitude as typical optical transition frequencies; thus, we have  $(k_L x) \sim \mathcal{O}(\alpha^2)$  as a parametric estimate. The correction (16) therefore is of the same order-of-magnitude as the relativistic correction induced by the Hamiltonian (11). Because the former depends on the specific configuration of the light field used in the experiment, we do not pursue the calculation of these effects any further here. If needed, they can be evaluated based on techniques used in Lamb shift calculations [25].

The analysis presented in this Addendum will be important for any future experimental implementation of the proposal presented in Ref. [10]. The main results for the  $1S-2S$  transition are summarized as the magic wavelength at 514.646 nm, the polarizability of  $-221.584 \frac{I_L}{\text{kW/cm}^2} \text{ Hz}$ , and its slope of  $-0.215748 \text{ Hz}/(\text{GHz}(\text{kW/cm}^2))$ . These results are separately indicated in Table I, with a focus on the reduced-mass correction, and results for the magic wavelengths and ac Stark effects of the  $1S-3S$  and  $1S-4S$  transitions are supplemented (cf. Ref. [26]). The theoretical uncertainty of these values is on the level of  $10^{-4}$ . Nevertheless, we have adopted the policy of indicating the numerical results to a nominal accuracy of six decimals, in order to facilitate an independent numerical evaluation. The dominant correction to the nonrelativistic one-particle approximation of the magic wavelength is due to the reduced-mass correction, and the relativistic correction of order  $\alpha^2$  is shadowed by a laser-field configuration dependent correction which has to be individually evaluated for a particular experimental setup.

*Acknowledgments.*—This research was supported by the National Science Foundation under Grant PHY-1403973.

- 
- [1] B. Bederson and H. Walther, “Optical Dipole Traps for Neutral Atoms,” *Adv. At. Mol. Opt. Phys.* **42**, 95–170 (2000).  
 [2] I. Bloch, “Ultracold quantum gases in optical lattices,” *Nat. Phys.* **1**, 23–30 (2005).  
 [3] M. Haas, U. D. Jentschura, C. H. Keitel, N. Kolachevsky, M. Herrmann, P. Fendel, M. Fischer, Thomas Udem, R. Holzwarth, T. W. Hänsch, M. O. Scully, and G. S.

- Agarwal, “Two-photon excitation dynamics in bound two-body coulomb systems including ac stark shift and ionization,” *Phys. Rev. A* **73**, 052501 (2006).  
 [4] C. G. Parthey, A. Matveev, J. Alnis, B. Bernhardt, A. Beyer, R. Holzwarth, A. Maistrou, R. Pohl, K. Predehl, T. Udem, T. Wilken, N. Kolachevsky, M. Abgrall, D. Rovera, C. Salomon, P. Laurent, and T. W. Hänsch, “Improved Measurement of the Hydrogen  $1S-2S$  Transi-

- tion Frequency,” *Phys. Rev. Lett.* **107**, 203001 (2011).
- [5] I. Ushijima, M. Takamoto, M. Das, T. Ohkubo, and H. Katori, “Cryogenic optical lattice clocks,” *Nat. Photon.* **9**, 185–189 (2015).
- [6] T. L. Nicholson, S. L. Campbell, R. B. Hutson, G. E. Marti, B. J. Bloom, R. L. McNally, W. Zhang, M. D. Barrett, M. S. Safronova, G. F. Strouse, W. L. Tew, and J. Ye, “Systematic evaluation of an atomic clock at  $2 \times 10^{-18}$  total uncertainty,” *Nat. Commun.* **6**, 6896 (2015).
- [7] H. Katori, M. Takamoto, V. G. Pal’chikov, and V. D. Ovsiannikov, “Ultrastable optical clock with neutral atoms in an engineered light shift trap,” *Phys. Rev. Lett.* **91**, 173005 (2003).
- [8] M. Haas, U. D. Jentschura, and C. H. Keitel, “Classical vs. Second-Quantized Description of the Dynamic Stark Shift,” *Am. J. Phys.* **74**, 77–81 (2006).
- [9] U. D. Jentschura and K. Pachucki, “Functional Form of the Imaginary Part of the Atomic Polarizability,” *Eur. Phys. J. D* **69**, 118 (2015).
- [10] A. Kawasaki, “Magic wavelength for the hydrogen  $1S-2S$  transition,” *Phys. Rev. A* **92**, 042507 (2015).
- [11] L. Castillejo, I. C. Percival, and M. J. Seaton, “On the Theory of Elastic Collisions Between Electrons and Hydrogen Atoms,” *Proc. Roy. Soc. London, Ser. A* **254**, 259–272 (1960).
- [12] M. Gavrilă and A. Costescu, “Retardation in the Elastic Scattering of Photons by Atomic Hydrogen,” *Phys. Rev. A* **2**, 1752–1758 (1970).
- [13] R. A. Swainson and G. W. F. Drake, “A unified treatment of the non-relativistic and relativistic hydrogen atom I: the wavefunctions,” *J. Phys. A* **24**, 79–94 (1991).
- [14] R. A. Swainson and G. W. F. Drake, “A unified treatment of the non-relativistic and relativistic hydrogen atom II: the Green functions,” *J. Phys. A* **24**, 95–120 (1991).
- [15] R. A. Swainson and G. W. F. Drake, “A unified treatment of the non-relativistic and relativistic hydrogen atom III: the reduced Green functions,” *J. Phys. A* **24**, 1801–1824 (1991).
- [16] K. Pachucki, “Higher-Order Binding Corrections to the Lamb Shift,” *Ann. Phys. (N.Y.)* **226**, 1–87 (1993).
- [17] U. Jentschura and K. Pachucki, “Higher-order binding corrections to the Lamb shift of  $2P$  states,” *Phys. Rev. A* **54**, 1853–1861 (1996).
- [18] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1974).
- [19] U. D. Jentschura, *Master Thesis: The Lamb Shift in Hydrogenlike Systems, [in German: Theorie der Lamb-Verschiebung in wasserstoffartigen Systemen]*, (University of Munich, 1996, unpublished (see e-print hep-ph/0305065)).
- [20] G. W. F. Drake and S. P. Goldman, “Bethe logarithms for  $\text{Ps}^-$ ,  $\text{H}^-$ , and heliumlike atoms,” *Can. J. Phys.* **77**, 835–845 (1999).
- [21] H. Bateman, *Higher Transcendental Functions*, Vol. 1 (McGraw-Hill, New York, 1953).
- [22] H. Bateman, *Higher Transcendental Functions*, Vol. 2 (McGraw-Hill, New York, 1953).
- [23] U. D. Jentschura, A. Czarnecki, and K. Pachucki, “Non-relativistic QED approach to the Lamb shift,” *Phys. Rev. A* **72**, 062102 (2005).
- [24] J. Evers, U. D. Jentschura, and C. H. Keitel, “Relativistic and Radiative Corrections to the Mollow Spectrum,” *Phys. Rev. A* **70**, 062111 (2004).
- [25] A. Czarnecki, U. D. Jentschura, and K. Pachucki, “Calculation of the One- and Two-Loop Lamb Shift for Arbitrary Excited Hydrogenic States,” *Phys. Rev. Lett.* **95**, 180404 (2005).
- [26] D. Yin, Y.-H. Zhang, C.-B. Li, and X.-Z. Zhang, “Magic Wavelengths for the  $1S-2S$  and  $1S-3S$  Transitions in Hydrogen,” *Chem. Phys. Lett.* **33**, 073101 (2016).