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Magic Wavelengths for the $1S$–$2S$ and $1S$–$3S$ Transitions in Hydrogen Atoms *

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The dynamic dipole polarizabilities for $1S$, $2S$ and $3S$ states of the hydrogen atom are calculated using the finite B-spline basis set method, and the magic wavelengths for $1S$–$2S$ and $1S$–$3S$ transitions are identified. In comparison of the solutions from the Schrödinger and Dirac equations, the relativistic corrections on the magic wavelengths are of the order of 10^{-2} nm. The laser intensities for a 300-E_r-deep optical trap and the heating rates at 514 and 1371 nm are estimated. The reliable prediction of the magic wavelengths would be helpful for the experimental design on the optical trapping of the hydrogen atoms, and in turn, it would be helpful to improve the accuracy of the measurements of the hydrogen $1S$–$2S$ and $1S$–$3S$ transitions.

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The magic trapping of atoms with laser was proposed by Katori *et al.* in 2003.[1] The laser is at the special wavelength, called the magic wavelength, and the light shift of the concerned transition in the atom is zero in such a laser field. Taking advantage of this unique character, the optical lattice clocks with cold neutral atoms are built at the 10^{-18} fractional accuracy and serve as a platform for the precision measurements and quantum information processing.[2,3]

The precision spectroscopy of the simplest atom, hydrogen, is of great importance in development of fundamental physics, which yields information of the fundamental constants such as the Rydberg constant R_∞ and the proton charge radius r_p, and also acts as a good example to test quantum electrodynamics.[4,5] With the development of the Doppler-free two-photon spectroscopy technique and the absolute frequency measurements via frequency comb, the fractional frequency uncertainty of the $1S$–$2S$ transition in the atomic hydrogen has been of the order of 10^{-15}.[6,7] The $1S$–$3S$ transition of the hydrogen atom has also been measured and the frequency uncertainty reaches to the order of 10^{-12}.[8] The frequency measurements on both transitions are the most precise experimental results in hydrogen and the combination of both frequencies could be helpful to improve the uncertainties of R_∞ and r_p.[8] These measurements were carried out on the hydrogen beam and the temperatures of the atomic beam are 5.8 K in the $1S$–$2S$ measurements[6,7] and the room temperature in the $1S$–$3S$ measurement.[8] The second-order Doppler effect is one of the main sources of the uncertainty of the frequency. It was pointed out that one must measure the $1S$–$3S$ transition frequency with a relative uncertainty lower than 5.5×10^{-13} to significantly contribute to the proton radius puzzle.[9]

It would be feasible to measure the $1S$–$2S$ and $1S$–$3S$ transitions by using the trapped cold hydrogen atoms. Actually, the Bose–Einstein condensation of hydrogen atoms was realized at 50 μK.[10] Taking advantage of the magic trapping technique used in the state-of-art optical lattice clocks, the cold hydrogen atoms could be loaded in the optical lattice. The precision of the measurements on the $1S$–$2S$ and $1S$–$3S$ transitions could be improved. The key point to realize this idea is to identify the magic wavelengths for the $1S$–$2S$ and $1S$–$3S$ transitions of hydrogen. Recently, Kawasaki calculated the magic wavelengths for the hydrogen $1S$–$2S$ transition using the analytical radial wave functions of the hydrogen atoms.[11] The sum-over-states formula of the polarizability was adopted in his work, while only the bound states were taken into account in his calculations.

In this Letter, we perform the calculations on the dynamic dipole polarizabilities for the $1S$, $2S$ and $3S$ states of hydrogen atoms using the finite B-Spline basis set method[12–15] and the magic wavelengths for the $1S$–$2S$ and $1S$–$3S$ transitions are identified. Both the Schrödinger and Dirac equations are solved to obtain the radial wave functions. A basis set of 200 $k = 9$ order B-spline functions defined in a finite region of 0–2000 a.u. is used. The nuclear mass is set to be infinite, and the point nucleus model is adopted. Atomic units are used throughout unless stated otherwise.

When immersed in an electromagnetic field, the dominant contribution to the energy shift of a given

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state n in an atomic system is given by

$$\Delta E \approx -\frac{1}{2}\alpha_1(\omega)F^2, \tag{1}$$

where F is a measure of the strength of the ac electromagnetic field, and $\alpha_1(\omega)$ is the dynamic electric dipole polarizability of the atomic state n at frequency ω, which can be written as

$$\alpha_1(\omega) = \sum_n \frac{f_{gn}^{(1)}}{E_{gn}^2 - \omega^2}. \tag{2}$$

Here $f_{gn}^{(1)}$ is the oscillator strength for an electric dipole transition from the state g to n, and in the form of the length gauge, it is written as

$$f_{gn}^{(1)} = \frac{2|\langle\psi_g\|rC^{(1)}(\hat{r})\|\psi_n\rangle|^2 E_{gn}}{3(2l_g+1)}, \tag{3}$$

where $\langle\psi_g\|rC^{(1)}(\hat{r})\|\psi_n\rangle$ is the reduced matrix element, and $E_{gn} = E_g - E_n$ is the transition energy between the initial state g and the intermediate state n. It is noted that Eq. (3) is in the nonrelativistic form. The orbital angular momentum l_g in Eq. (3) should be replaced by the total angular momentum j_g when the wave functions are obtained from the Dirac equation.[16]

Table 1. The static dipole polarizabilities $\alpha_1(0)$ (in a.u.) of the $1S$, $2S$ and $3S$ states. NR represents the nonrelativistic calculations and all of the intermediate states including the continuous states are considered. NRB represents the nonrelativistic calculations and only the bound states of the intermediate states are considered. RE represents the relativistic calculations, and all of the eigenvectors including the continuous states are considered.

Method	$\alpha_1^{1S}(0)$	$\alpha_1^{2S}(0)$	$\alpha_1^{3S}(0)$
NRB	3.6632	110.79	976.20
NR	4.499999999998	120.000000000	1012.500000001
RE	4.499751495177	119.990228572	1012.409740959
Exact NR results	4.5[17,18]	120[17,18]	1012.5[18]
Other RE results	4.499751495177639 2674[19]	119.99022857241[19]	

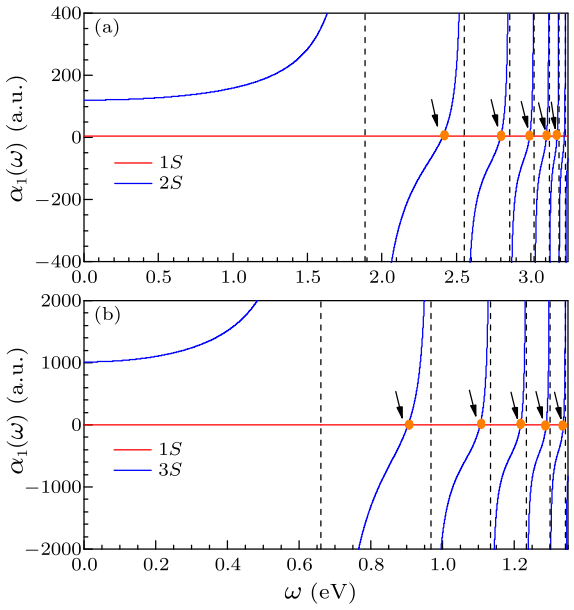

Fig. 1. (Color online) Dynamic electric dipole polarizabilities $\alpha_1(\omega)$ (in a.u.) of the hydrogen atom, (a) for the $1S$ and $2S$ states, and (b) for the $1S$ and $3S$ states. The crossing points noted by the solid circles and pointed out by the arrows indicate the positions of the magic wavelengths. Only the five lowest magic wavelengths are shown in the figures. The vertical dashed lines are the resonance transition positions.

The dynamic polarizability in the limit of $\omega \to 0$ is the static polarizability. Table 1 presents the results of our calculations on the static dipole polarizabilities of the $1S$, $2S$ and $3S$ states in hydrogen atoms. Our nonrelativistic and relativistic results have a good agreement with other results from literature. It gives a good start for the reliable dynamic polarizability and magic wavelength calculations. It is noted that we also test the sum-over-states calculations on the polarizabilities including only the bound states of all intermediate states. The contributions of the continuous states to the static dipole polarizability are 18.6% for the $1S$ state, 7.7% for the $2S$ state and 3.6% for the $3S$ state. The results show that the contribution from the continuous states could not be ignored. The comparison of the nonrelativistic and relativistic results of our calculations show that the relativistic correction to the $1S$, $2S$ and $3S$ dipole polarizabilities is on the fifth significant digit.

The curves of the dynamic electric dipole polarizabilities of the hydrogen $1S$, $2S$ and $3S$ states, obtained from the nonrelativistic calculations, are shown in Fig. 1. The crossing points in Figs. 1(a) and 1(b) represent that the dynamic electric dipole polarizabilities of the different atomic states are the same and indicate that the locations of the magic wavelengths are identified. In Table 2, the lowest five magic wavelengths for both the $1S$–$2S$ and $1S$–$3S$ transitions are listed.

In comparison of the data in Table 2 obtained from the nonrelativistic and relativistic calculations, it can be found that the relativistic effect makes the dynamic polarizabilities at the magic wavelengths deduced about 2–3×10^{-4} a.u. It makes the magic wavelengths blue shift about 1–2×10^{-2} nm. It is noted that our nonrelativistic results of the lowest three magic wavelengths for the $1S$–$2S$ transition are 514.366, 442.971 and 414.257 nm, respectively, which

do not agree with Kawasaki's results 512.64, 441.8 and 413.7 nm.[11] Although a large enough upper limit $n_{\max} = 4000$ was used in his summation calculations on the polarizability, the contribution from the continuous states was ignored. We take the similar procedure and make the summation over only the bound states obtained from our nonrelativistic calculations, the lowest magic wavelength for the $1S$–$2S$ transition is 512.00 nm, which is consistent with Kawasaki's result. Though the number of the bound states in our calculations is not as great as Kawasaki's, it is believed that the continuous states cannot be ignored in the reliable polarizability calculations using the sum-over-states formula. The theoretical contributions to the energy levels of hydrogen atoms,[20] including relativistic, quantum electrodynamic, recoil, and nuclear size effects, correspond to a fractional amount of 5.4×10^{-4} at most. The variations of the nonrelativistic results of the magic wavelengths caused by these corrections are less than 1.0 nm. Therefore, the magic wavelengths predicted in this work have three significant digits reliable at least.

Table 2. The lowest five magic wavelengths in both units of eV and nm, and the corresponding dynamic dipole polarizabilities at the magic wavelengths for the $1S$–$2S$ and $1S$–$3S$ transitions of the hydrogen atom. The results obtained from both the NR and RE calculations are given. All of the intermediate states including the continuous states are taken into account.

$\omega^{\rm NR}_{\rm magic}$ (eV)	$\lambda^{\rm NR}_{\rm magic}$ (nm)	$\alpha_1^{\rm NR}(\omega_{\rm magic})$	$\omega^{\rm RE}_{\rm magic}$ (eV)	$\lambda^{\rm RE}_{\rm magic}$ (nm)	$\alpha_1^{\rm RE}(\omega_{\rm magic})$
$1S$–$2S$ transition					
2.410426	514.3663	4.719786	2.410474	514.3561	4.719528
2.798923	442.9710	4.802007	2.798977	442.9627	4.801744
2.992925	414.2576	4.849032	2.992979	414.2501	4.848767
3.105555	399.2337	4.878281	3.105610	399.2266	4.878014
3.177064	390.2478	4.897622	3.177119	390.2409	4.897355
$1S$–$3S$ transition					
0.904264	1371.1065	4.529568	0.904279	1371.0829	4.529318
1.105082	1121.9454	4.544316	1.105100	1121.9275	4.544066
1.218064	1017.8789	4.553967	1.218083	1107.8634	4.553715
1.289188	961.7231	4.560549	1.289207	961.7089	4.560297
1.337105	927.2584	4.565206	1.337124	927.2450	4.564954

For the choice of the lasers to build the optical lattice for trapping the atoms, the far-off-resonance wavelength is favorable.[21,22] In the hydrogen atom case, the magic wavelengths of 514.3 nm for the $1S$–$2S$ transition and 1371 nm for the $1S$–$3S$ transition are preferable. The recoil energy $E_{\rm r} = \hbar^2 k_{\rm L}^2/2m_{\rm a}$ is the natural energy unit for the optical trapping dynamics, where $k_{\rm L}$ is the wave vector of the lattice laser, and $m_{\rm a}$ is the atomic mass. The depth of the optical trap $U_{\rm dip}(\boldsymbol{r})$ is related to the intensity of the laser light field,[22] $U_{\rm dip}(\boldsymbol{r}) \propto \alpha(\omega_{\rm L})I(\boldsymbol{r})$. A trap with several hundreds of $E_{\rm r}$ depth would be deep enough for trapping the atoms. The scattering of the lattice photons with the trapped atoms in an optical lattice would cause the heating. The heating rate $\gamma_{\rm h}$ at the magic wavelength is associated with the laser intensity and the dynamic polarizability of the atomic state,[23]

$$\gamma_{\rm h} = \alpha^4 \cdot \frac{32}{3}\omega_{\rm L}^3[\alpha(\omega_{\rm L})]^2 I. \tag{4}$$

Assuming we want to build an optical trap with the potential depth of $300E_{\rm r}$, some of the parameters for the optical trapping of hydrogen atoms are estimated and listed in Table 3, including the recoil energy $E_{\rm r}$, the laser intensity for a 300-$E_{\rm r}$-deep trap and the heating rate in the laser field at the magic wavelength. Our estimation for the laser intensity for the $1S$–$2S$ transition is consistent with the result obtained by Kawasaki.[11] Since the magic wavelength for the $1S$–$3S$ transition is larger than that of the $1S$–$2S$ transition and the recoil energy is lower, the laser intensity to build a 300-$E_{\rm r}$-deep trap is about one order of magnitude lower. Suppose that the laser beam has a waist diameter of 10 μm, 1 W light at 514.3 nm injected to an optical cavity of finesse 3000π would achieve the intensity of 3.1×10^6 kW/cm^2 for the $1S$–$2S$ transition experiment.[11] However, for the $1S$–$3S$ transition experiment using the same optical cavity, a 150 mW laser at 1371 nm would be required. Also, the heating rate in the laser field at 1371 nm is two orders of magnitude lower than in the laser field at 514.3 nm. The lower laser power and heating rate at 1371 nm indicate that the magic optical trapping of the hydrogen atom for the measurement of $1S$–$3S$ transition is more feasible.

Table 3. Some of the parameters for the optical trapping of the hydrogen atom.

Parameter	$1S$–$2S$ transition	$1S$–$3S$ transition
$\lambda_{\rm magic}$ (nm)	514.3	1371
$E_{\rm r}$ (μK)	71.8	10.1
I (kW/cm^2)	3.1×10^6	4.5×10^5
$\gamma_{\rm h}$ (s^{-1})	1.43	0.01

In summary, the dynamic electric dipole polarizabilities of the $1S$, $2S$ and $3S$ states in the hydrogen atom have been calculated via both nonrelativistic and relativistic methods by using the finite B-spline basis set. The magic wavelengths for the hydrogen $1S$–$2S$ and $1S$–$3S$ transitions are identified. The relativistic corrections to the magic wavelengths predicted in

the present work are of the order of 10^{-2} nm. Taking into account higher order effects, such as the quantum electrodynamic, recoil, and nuclear size effects, would be helpful to improve the accuracy of the magic wavelengths. Although the laser intensities for a 300-E_r-deep optical trap and the heating rates are estimated at 514.6 nm and 1371 nm, the real experiments on trapping the hydrogen atoms in an optical lattice are complicated. Further study on the reliability of the magic wavelengths and the impact of the laser intensity fluctuations[24] are needed. It should also be noted that only the electric dipole polarizabilities are included in our theoretical identification of magic wavelengths. Although the contributions of the magnetic dipole and the electric quadrupole interactions are several orders of magnitude smaller than the electric dipole interaction in the laser field at the predicted magic wavelength,[2,11] they have a non-zero contribution to the transition frequency shifts. In general, the contribution of the differential hyperpolarizabilities to the transition frequency shifts, which is proportional to F^4, is not zero at the magic wavelength. Further delicate studies on the dynamic magnetic dipole, electric quadrupole polarizabilities and hyperpolarizabilities would be helpful for the analysis of the frequency shifts of the hydrogen $1S$–$2S$ and $1S$–$3S$ transitions due to the high order Stark effects and multipolar interactions in optical lattice and the evaluation of the systematic error budget of the experimental measurements.

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