Atomic and molecular spectral line shapes in laboratory and selected astrophysical plasma

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Abstract. This work elaborates on laboratory measurements of hydrogen Balmer series lines and diatomic molecular species in laser-plasma. Comparisons with astrophysical white dwarf spectra, recorded at various observatories and the Hubble space telescope, point out direct applications of experimental results. The recorded general relativity gravitational- or Einstein-shift of the atomic lines allows one to infer the ratio of mass and radius. The Stark-effect redshifts of hydrogen alpha and hydrogen beta lines investigated with time-resolved emission spectroscopy are usually one order of magnitude larger than the gravitational shift. In view of white dwarf atmospheres dominated by hydrogen and the associated absorption spectra, averaging the laser-induced plasma data reveals spectral line shapes that mask the redshift caused by the Stark effect. The available white dwarf data indicate that the collected radiation propagated through regions of different density in the star’s atmosphere. Diatomic spectra are typically recorded as white dwarfs further progress in their transformation.

1. Introduction

The Montreal database [1] holds 40,000 entries on white dwarfs as of May 2018, including about 5000 that show a hydrogen atmosphere. And of course there is the companion to the brightest star visible from the earth, Sirius B, radiating at about 26 kK in the constellation canis majoris. Sirius B reveals several lines in absorption of the Balmer series of hydrogen. The “nearby” Procyon B white dwarf from canis minoris with an atmosphere at about 8 kK shows carbon Swan spectra in absorption [2]. And of course there are several white dwarf data sets that are publicly available from the Keck observatory archives (KOA) [3].

Comparisons of spectra from laboratory plasma and astrophysical white dwarf (WD) stars has been the subject of research and documented communications for several decades or about 50 years. Noteworthy are the discussions from the 1970’s regarding the Stark-effect caused redshifts that may contribute [4, 5, 6] to the gravitational- or Einstein- redshifts [7], casting doubt on the determination of the white dwarf ratio of mass over radius. Radiative-transfer and error margin considerations [9] conclude that the pressure shifts are well within error margins of the determined gravitational shifts. A recent re-discussion in 2015 [10] indicates that line profiles from white dwarf stars are composed of contributions from different atmospheric layers, and the recorded integrated spectra mask the Stark-effect or pressure shifts.

Aspects of this work include the determination of hydrogen beta line, H β, central dip-shifts [11] for an electron density, N e, in the range 2 - 20 x 10¹⁷ cm⁻³, superposition of recorded time-resolved data [12] in order to interpret measured white dwarf spectral line shapes, and discussion of results for the spectral appearance of H β for N e of the order of 60 x 10¹⁷ cm⁻³. In other words, hydrogen beta line profiles are elaborated for η = N e/n₀ ≃ 0.24 amg, where n₀ = 268.68 x 10¹⁷ cm⁻³. Selected white dwarf spectra display absorption profiles from...
atmospheres with electron densities of \( \sim 1 - 5 \times 10^{17} \text{cm}^{-3} \), or \( \eta = 0.004 - 0.02 \text{ amg} \). Self-absorption in H\(_\alpha\) laser-plasma experiments become noticeable at \( \eta = 0.1 \text{ amg} \)\[19\].

2. Experimental details
The experimental arrangement for laboratory measurements of laser-induced plasma includes a Q-switched Nd:YAG laser device typically generating 6 ns laser pulses with an energy of 150 mJ per pulse at the fundamental wavelength of 1064 nm. Radiation is tightly focused to a spot size of the order of 10 \( \mu \)m to achieve a peak irradiance above 1 TW/cm\(^2\), or well above optical breakdown in laboratory air at standard ambient temperature and pressure (SATP), and well above optical breakdown of gaseous hydrogen slightly above or below 1 atmosphere. The emanating light from the micro-plasma is recorded with a Czerny-Turner type spectrometer that shows a resolution of 0.02 nm when using a 3600 groves/mm holographic grating and the scanning spectrometer-photomultiplier or linear diode array option, or an intensified two-dimensional detector for time-resolved spectroscopy.

The astrophysical data sets are preferably recorded with a high resolution spectrometer, for instance the so-called HIRES instrument \[14\] at the Keck observatory that utilizes an echelle grating. The spectral resolving power, \( R = \lambda/\Delta \lambda \), i.e., the ratio of wavelength, \( \lambda \), and of the spectral resolution, \( \Delta \lambda \), typically is of the order of 40,000.

At H\(_\beta\), the spectral resolution equals \( \Delta \lambda = 0.012 \text{ nm} \). In terms of the average gravitational redshift, \( v_g = c/R \), with \( c \) the speed of light, the velocity resolution amounts to 7.5 km/s. For comparison, the Sirius B gravitational redshift \[7, 15\] is \( 89 \pm 16 \text{ km/s} \), or \( \Delta \lambda_{\text{Sirius B}} = 0.14 \text{ nm} \).

From the gravitational shift \[10\], \( v_g = 0.64 M/R \), with \( M \) and \( R \) denoting the white dwarf (WD) mass and radius in solar units, respectively, and using thermodynamic cooling models, the WD parameters are inferred, namely gravitational constant, \( g \), temperature, \( T \), mass, \( M \), and radius, \( R \). Typical values for WD’s with a hydrogen atmosphere \( g, T, M, \) and \( R \) amount to \( 10^6 \text{ m/s}^2 \), 30 kK, mass of the sun, and size of the earth, respectively.

3. Laboratory results
Figures 1 and 2 illustrate recent measurements \[11\] of laser plasmas in hydrogen gas. In these experiments, the laser beam propagates parallel to the slit, from top to bottom.

![Figure 1. H\(_\beta\) spectra for a time delay of 175 ns. (a) H\(_\beta\) map, (b) scaled average indicating an electron density \( N_e = 3.5 \times 10^{17} \text{cm}^{-3} \).](image-url)
Figure 2. $\text{H} \alpha$ spectra for a time delay of 175 ns. (a) $\text{H} \alpha$ map, (b) scaled average indicating an electron density $N_e = 3.7 \times 10^{17} \text{cm}^{-3}$.

Time-resolved spectroscopy data yield the full-width at half-maximum for the determination of electron densities as a function of time delay. Electron densities from $\text{H} \beta$ agree with those from $\text{H} \alpha$, while Ref. [12] debates comparisons of the standard [17] with the advanced Stark-broadening [18] theory. The recorded maps reveal expected variations along the slit dimension. Averages of the spatially resolved data along the slit yield spectra that appear similar to those recorded with a linear diode array [12].

In the laboratory data, there are pressure shifts that are larger than the gravitational- or Einstein-shift. Figure 3(a) exhibits the hydrogen beta line with the expected two peaks, one blue-shifted and one red-shifted due to pressure broadening [19]. The illustrated data represent a re-examination of the previously recorded data [12] in view of the dip-shift dependency and comparison with WD spectra.

Figure 3. Line shapes (a) $\text{H} \beta$ for various time delays. For near zero time delay, the arrows indicate the peak separation that implies an electron density of $N_e \simeq 60 \times 10^{17} \text{cm}^{-3}$. The encircled area suggests $\text{H} \beta$ self-absorption. (b) Sum of spectra and Lorentzian overlay.
The appearance of the \( \text{H}_\beta \) line shape is illustrated for electron densities of the order of up to \( 60 \times 10^{17} \text{ cm}^{-3} \), i.e., \( n \simeq 0.24 \text{ amg} \), or for electron density inferences from \( \text{H}_\beta \) near the estimated Inglis-Teller limit \[20\]. For \( \tau = 2 \text{ ns} \), it is difficult to speak of a traditional line shape because only the central portion can be demarcated. The 2-ns line-of-sight data are recorded near the tail of the laser pulse, consequently, experimental variations are expected for the accumulated averages. Figure \( 3(\text{a}) \) illustrates \( \text{H}_\beta \) close to the Inglis-Teller limit \[20\] for \( \tau = 0.02 \text{ ns} \). From Fig. \( 3(\text{b}) \) one clearly recognizes that the peak-separation is significantly modified or masked by contributions from lower density lines, and Fig. \( 3(\text{b}) \) also shows an overlay of a single Lorentzian with the same full-width-half-maximum (FWHM) as the summed profile.

The laboratory measurements \[11\] are analyzed using empirical formulae \[21\] for \( \text{H}_\alpha \) and \( \text{H}_\beta \). In addition, the data reveal the central dip-shifts as function of electron density of \( \text{H}_\beta \),

\[
\Delta \delta_{\text{ds}}[\text{nm}] = 0.14 \left( \frac{N_e[\text{cm}^{-3}]}{10^{17}} \right)^{0.67 \pm 0.03}.
\] (1)

For an electron density, \( N_e \), of \( 1 \times 10^{17} \text{ cm}^{-3} \), the central dip-shift equals the Sirius B gravitational redshift of 0.144 nm, yet Sirius B shows an electron density of \( \simeq 5 \times 10^{17} \text{ cm}^{-3} \).

Figure \( 4 \) illustrates results from fitting the summed profile using one or two Lorentzians. With impact broadening \[22\] the dominant process in the wings, it appears reasonable to consider Lorentzians for fitting of the spectra.

**Figure 4.** Fitting to summed \( \text{H}_\beta \) profiles. (a) Two Lorentzians of 4.9 and 17.6-nm widths indicating electron densities of 1.1 and \( 5.8 \times 10^{17} \text{ cm}^{-3} \), respectively. (b) Single Lorentzian fit of 6.9-nm width and \( N_e = 1.8 \times 10^{17} \text{ cm}^{-3} \), but with discrepancies near the wings and at center.

The double Lorentian fit, Fig. \( 4(\text{a}) \), simulates the summed profile as a superposition from two regions that show different electron density. As the plasma expands spatially and temporally, and if one were to record continuously, one would expect several regions of different density contributing to the recorded signal. There are deficiencies in the single fit, Fig. \( 4(\text{b}) \), similar to the mentioned concerns when discussing Fig. \( 3(\text{b}) \) yet there are subtle differences between measured and single-Lorentzian fitted spectra.

Adding the original spectra \[12\], recorded in the first 2.5 \( \mu \text{s} \) temporal window with 6-ns gate-widths, yields a result similar to using a longer gate-width in the measurement. Strictly speaking, use of gate-widths and gate-delays that entirely cover the first 2.5 \( \mu \text{s} \), and then adding the results would be equivalent to using a 2.5 \( \mu \text{s} \) gate. Nevertheless, Fig. \( 3(\text{b}) \) is an acceptable representation of continuous recording as was the case for the collection of WD spectra.
4. Astrophysical white dwarf spectra

Collection of spectra from white dwarf stars preferably occurs with a resolving power sufficient for determination of the gravitational shift. Recent data for the star GD 394, recorded with an echelle spectrometer on November 15, 2015, with KOA-ID: HI.20151115.19364 \[3\], shows a resolving power of \( R = 38000 \), or a resolution of \( \Delta \lambda = 0.013 \) nm. Figure 5 displays the composite Echelle spectra of \( \text{H}_\beta \) using the extracted ”green” charge coupled device data, and it also shows the fitted, broad and narrow Lorentzian profiles. The extracted spectra are publicly available \[3\]. Fig. 5(b) illustrates the expanded region that indicates asymmetric data and the fitted, 0.12-nm redshifted symmetric Lorentzian. Data from the same day with KOA-ID: HI.20151115.16693 and HI.20151115.17054 show fitted redshifts of 0.19 nm and 0.15 nm, respectively. The gravitational redshift of 0.043 nm (26.77 km/s) and the photospheric component of 0.047 nm (29.3 km/s) \[23\] account for a 0.09-nm redshift. In view of Fig. 5(b) improvements in fitting with possibly asymmetric line-shapes or adjustments to the background slope could very well confirm an overall redshift of 0.09 nm within error bars.

Figure 5. White dwarf GD 394 B, \( \text{H}_\beta \) combined absorption profiles, recorded with the HIRES echelle spectrometer \[3\]. (a) Two Lorentzians of 0.39- and 7.3-nm widths. (b) Expanded region showing a 0.12 nm redshift.

Comparisons with the laboratory spectra reveals the absence of the double-peak structure due to averaging of the absorption spectra along the line-of-sight. The combination of two additive line profiles would indicate density gradients in the WD atmosphere. Absorption widths of 0.39- and 7.3-nm would indicate electron densities of 0.032 and \( 2.0 \times 10^{17} \) cm\(^{-3} \), respectively.

Figure 6 displays a WD molecular \( \text{C}_2 \) Swan band absorption spectrum from GJ 841 B \[24\]. Analogous to analysis of \( \text{C}_2 \) emission spectra in laser-induced plasma, the absorption spectrum in Fig. 6(a) is inverted and subsequently analyzed with the well-established diatomic molecular fitting program \[25\]. Fig. 6(b) illustrates fitting results for the strongest band \( \Delta v = 0 \) of the \( \text{C}_2 \) Swan spectra.

Initial analysis indicates a temperature of 5.9 kK and a spectral resolution, \( \delta \lambda \), of 2.5 nm for the entire range. The recorded data are shifted by an overall 0.5 nm to correct for wavelength accuracy. The GJ 841 B spectra are captured with a resolving power of 833, so the 0.5 nm adjustment is of the order of the spectral resolution. The fitting of \( \Delta v = +2 \) and \( + 1 \) indicate best-fit spectral resolutions of 1.5 nm that are about a factor of 2 larger than those for \( \Delta v = -1 \) and \( -2 \) fitting. The effective temperature of the GJ 841 B white dwarf is documented \[1\] to be \( \sim 7.2 \) kK.
Figure 6. White dwarf GJ 841 B [1]. (a) C₂ Swan absorption spectrum. (b) ∆v = 0: T = 7.1 kK, δλ = 1.8 nm.

The analysis of the C₂ absorption spectra suggests deviation from equilibrium due to the significant differences in computed and recorded spectra for the investigated bands. Figure 7 displays further results for the ∆v = -1 and -2 bands. The extracted temperature from fitting these selected bands is lower than that from fitting all bands ∆v = +2, +1, 0, -1, -2. The temperature inferred from ∆v = 0 band is higher than that from the other bands.

Figure 7. (a) ∆v = -1: T = 4.5 kK, δλ = 1.5 nm, (b) ∆v = -2: T = 4.2 kK, δλ = 1.5 nm.

5. Discussion
Expanding laser-induced plasma is usually accompanied by a hypersonic shock wave, including rarefaction waves and associated temperature and density gradient regions that contribute in line-of-sight experiments. One can utilize integral inversion techniques to explore the spatial plasma distribution, or one can investigate line shape details in the data reduction of the spectra. In analogy with laser-ablation, occurrence of density variations can be attributed to formation
of particle clusters [26, 27] that can be studied with flowing gas leading to percolation effects that may cause line shapes that require double-Lorentzian line shape analysis.

The comparison of laboratory and astrophysical spectra implies that different electron density regions in the atmosphere of the investigated hot (∼ 25 kK) white dwarf stars cause absorption contributions that mask Hβ peak separation and central dip-shifts. Molecular spectra display variations across vibrational bands, possibly indicating varying C2 concentrations of cool (∼ 7 kK) white dwarf atmospheres. Fitting of hydrogen spectra reveals broad and narrow profiles that may be caused by local thermodynamic non-equilibrium as WD stars cool [28, 29]. The laser-induced plasma is well-reproduced in consecutive optical breakdown events allowing accumulations of several tens of laser-plasma events for each time delay. Recent laboratory measurements [30] explore white dwarf photospheric spectral lines to elucidate details in WD atmosphere modeling.

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