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H2+ Quasi Molecular Line Shape Profiles in Stellar Atmospheres

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Introduction to Quasi Molecules and H2+

Quasi molecules are unbound systems of closely interacting atoms which form in stellar atmospheres. The hot temperatures in a stellar atmosphere prevent stable molecules from forming, but "quasi" molecules can exist for short periods of time during close chance encounters between neighboring atoms, as they quickly pass by each other. Such systems can cause spectral features, or satellites, to appear in emergent spectra, and can contribute significant opacity under certain plasma conditions.

The quasi molecule H2+ is formed by a neutral hydrogen atom and a nearby free proton. H2+ is particularly prevalent in the atmospheres of white dwarf stars and metal-poor A stars. H2+ satellites associated with the Lyman series can be particularly strong in white dwarf stars cooler than about 25,000K, and have been frequently observed in ultraviolet spectra.

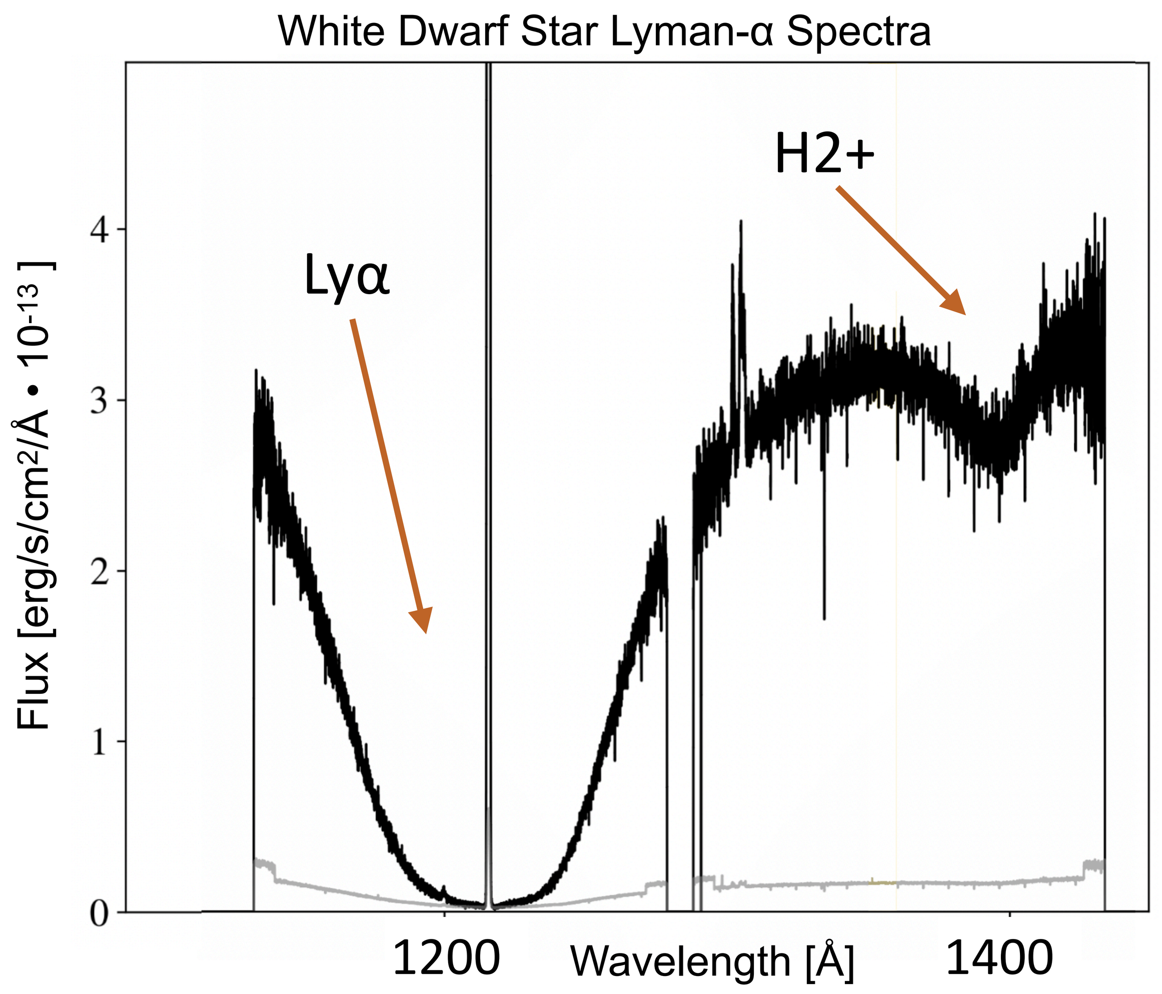

Fig.1: Ultraviolet spectra of DA white dwarf star WD1713+695 from the *Hubble Space Telescope* (HST), illustrating the 1400Å quasi molecular feature associated with the $3d\sigma_g \rightarrow 2p\sigma_u$ transition in H2+

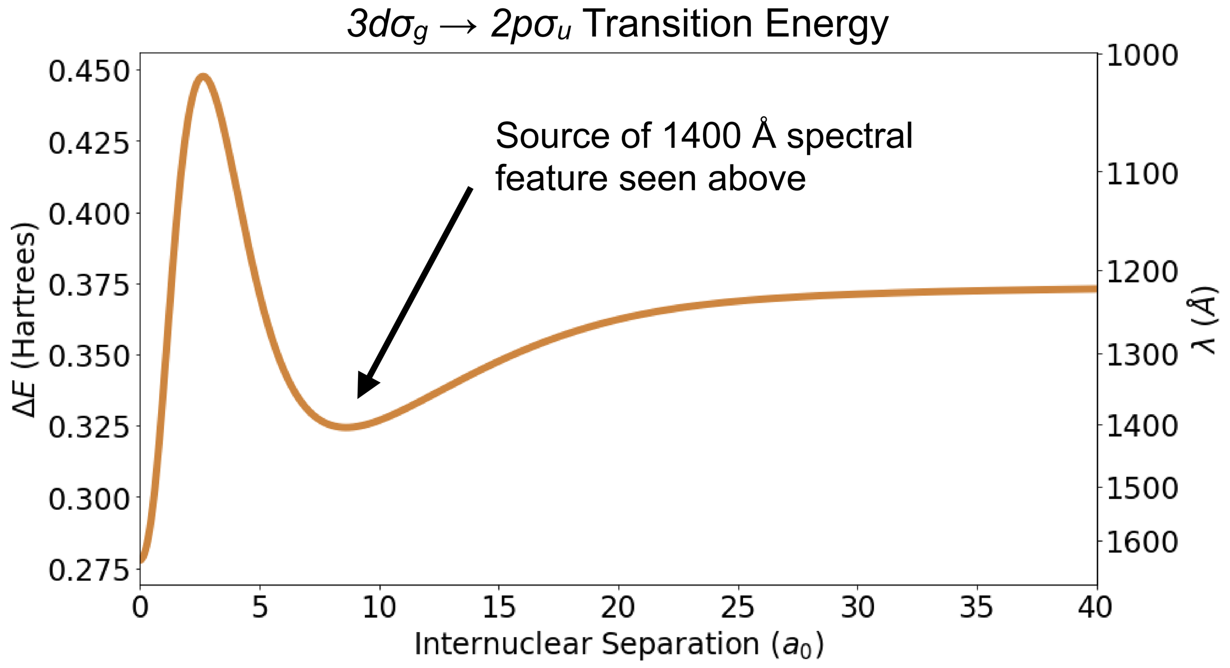

Fig. 2: Transition energy curve for the $3d\sigma_g \rightarrow 2p\sigma_u$ H2+ transition, which reduces to a Lyman-α atomic transition at infinite internuclear separation. The large 1400Å H2+ satellite seen in the above HST spectra is caused by the local minima in the transition energy curve at internuclear separations between 7-11 a_0.

Quasi Molecular H2+ Satellites in Model White Dwarf Star Spectra

Synthetic white dwarf star spectra, with and without H2+ quasi molecular features, show substantial differences in the ultraviolet wavelengths. In the spectra shown on the right, the black curves include Ly-α, Ly-β, and Ly-γ H2+ quasi molecular features, while the orange curves do not. The UV satellites also affect the flux distribution into the visible wavelengths, as seen in the adjacent plot of the Balmer series. Both spectra were calculated with the model atmosphere code Tlusty [1], for a white dwarf star with an effective temperature of 20000K, and log surface gravity of 8.

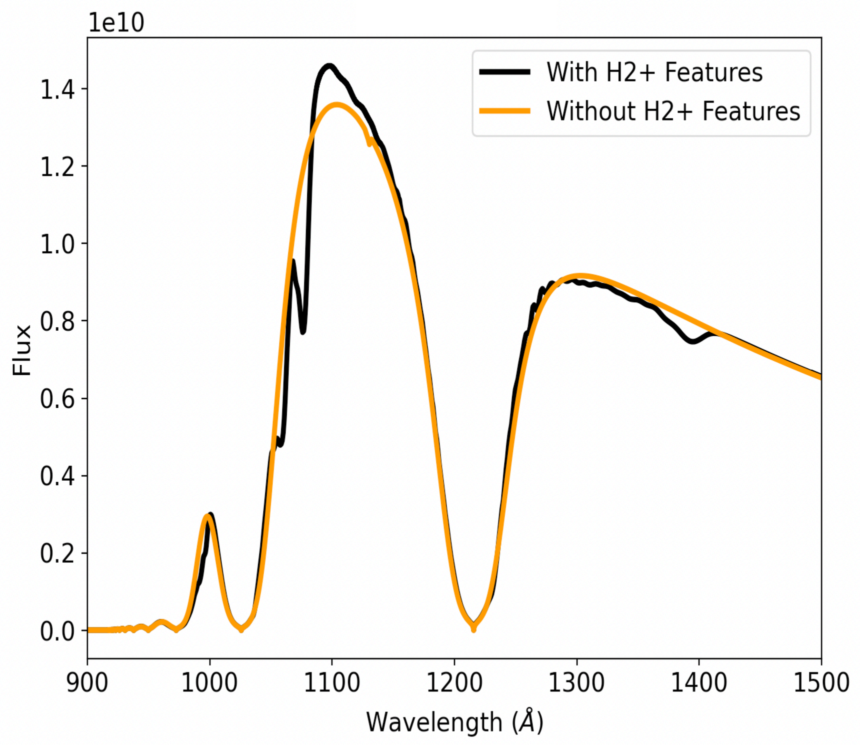

Fig 3: Lyman series in white dwarf star model spectra

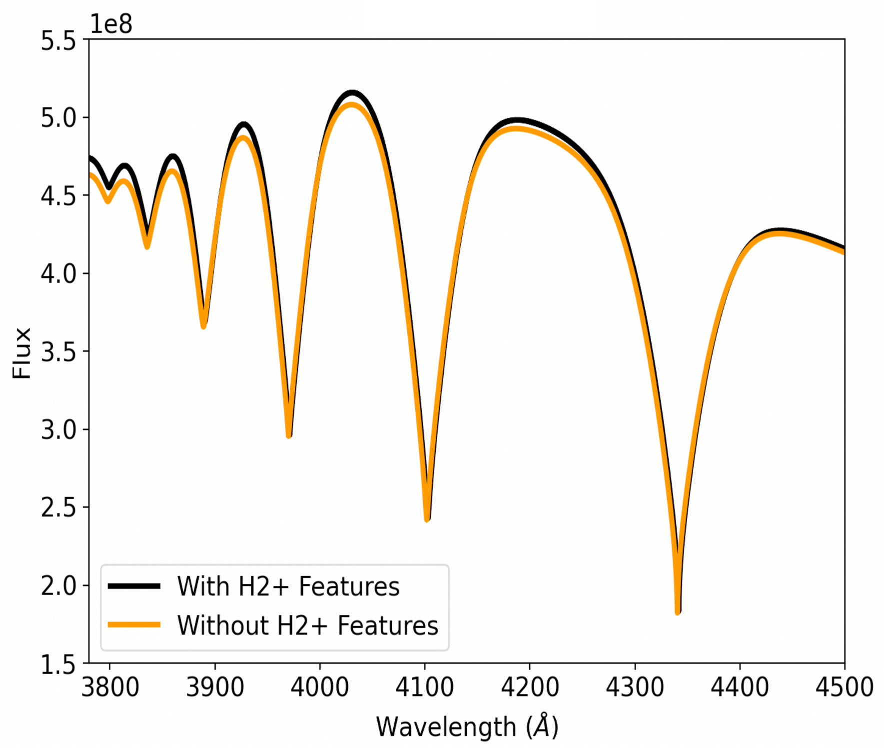

Fig 4: Balmer series in white dwarf star model spectra

Deficiencies in Current Theoretical Quasi Molecular Line Shapes

Past modeling of the H2+ quasi-molecular features, led by Nicole Allard, considered theoretical profiles generated solely by ion Stark broadening [2]. In the Allard models, perturbing ions move along rectilinear paths around a stationary radiating hydrogen atom. However, Allard profiles do not account for electron Stark broadening, and do not include any screening effects. These physical effects are typically significant for Stark broadened line shape profiles.

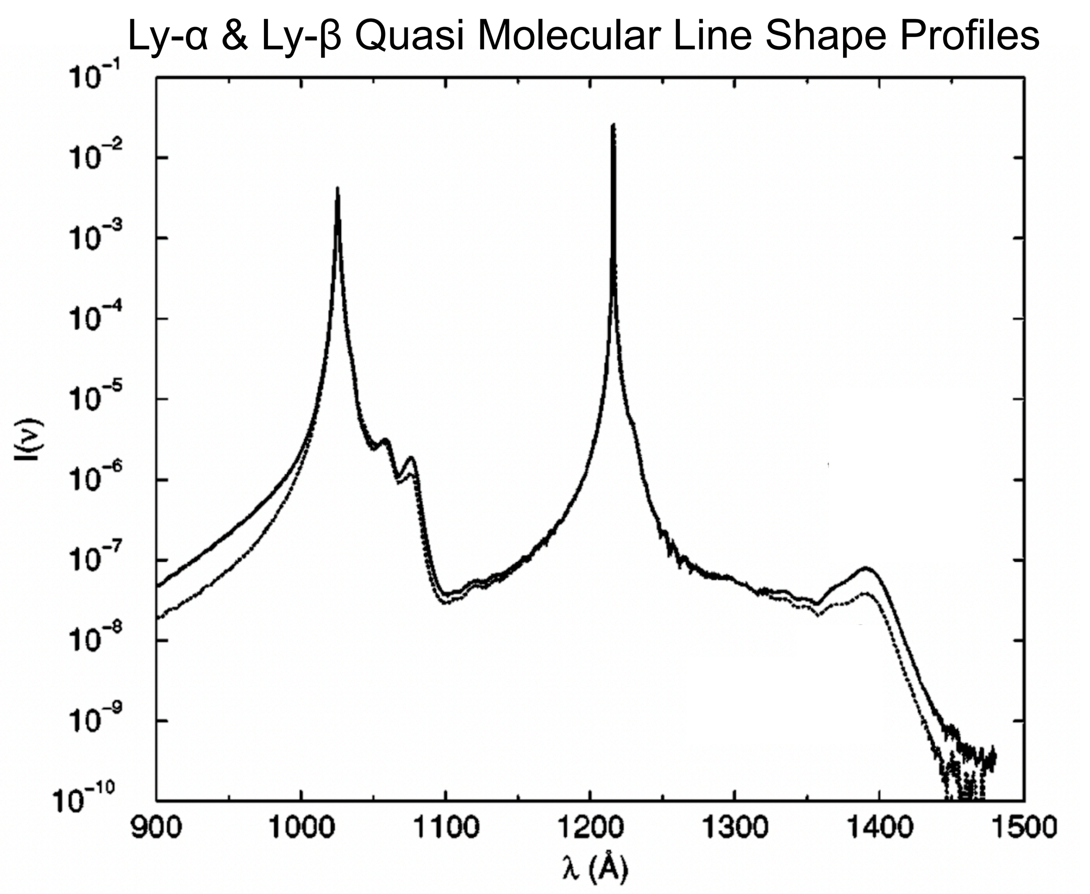

Fig 5: Ly-α and Lyman-β ion-only line shape profile with strong quasi molecular features visible at 1050, 1070, and 1400 Å [3].

Currently, quasi molecular profiles are incorporated into model atmosphere codes by simply adding them to Stark broadened profiles such as the VCS line shapes. This combination of different profiles fails to account for simultaneous ion and electron Stark broadening and may be introducing significant errors, as seen in figure 6.

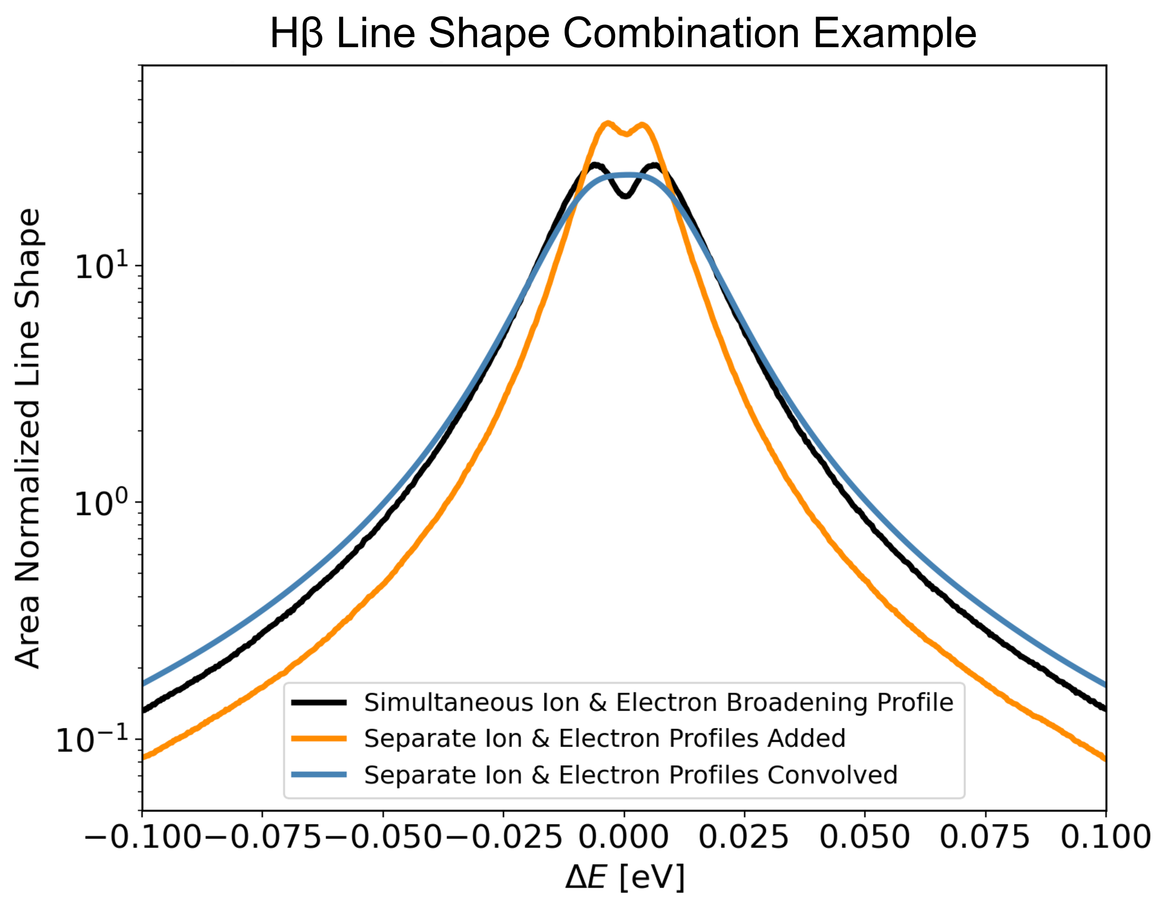

Fig 6: A demonstration of trying to combine separate Stark broadened line shapes for the case of Hβ. A simple addition artificially decreases the expected line width, and a convolution fails to reproduce the correct line shape. Each line shape is calculated with the Xenomorph code [4], at a temperature of 10000K and a density $n_e = 10^{17}$.

Calculating New Quasi Molecular Line Shapes

We are currently developing new quasi molecular line shape profiles which incorporate simultaneous electron and ion broadening. Following the relaxation theory, this can be accomplished analytically by calculating electron broadening from collision amplitudes for electron scattering induced transitions. These new profiles will remove the need to preform imprecise combinations with separate Stark broadened line shape profiles, allow for the incorporation of a screening procedure, and will provide a benchmark for evaluating the accuracy of the ion-only approximations currently in use.

Spectral Impact on Stellar Fits

Modifications to the quasi molecular line shape profiles will affect the fits to observed white dwarf stars and will systematically modify their derived characteristics, such as temperature, mass, and luminosity. These fits are done by either matching observed Balmer lines to theoretical spectra, or by comparing visible bandpass magnitudes to theoretical models. Small changes to line profiles in the ultraviolet are influential to these fits because they cause flux to be redistributed into the visible wavelengths, as seen in figure 4.

We have previously observed this sensitivity between ultraviolet line shape profiles and stellar fits through the implementation of new all-order full-coulomb profiles, developed by Thomas Gomez [5]. Improvements to the quasi molecular line shape profiles will further modify our estimates of stellar parameters for white dwarf stars, and may help resolve observed discrepancies between different fitting procedures [6].

Possible Future Laboratory Testing

A powerful test of the quasi molecular line shapes would be to compare current theoretical profiles against laboratory data. With the development of the WCAPP hydrogen gas cell experiment [7], which can reproduce the conditions of a white dwarf star photosphere using the Z machine, the plasma environment needed to produce these H2+ satellites is already being reached experimentally. The primary barrier to preforming these laboratory tests is the development of ultraviolet spectral diagnostic tools for usage on the Z-machine, which would allow us to observe the spectral range where these satellites are most prominent.

Acknowledgments

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