Effects on Atomic Spectra: Updates of Line-Shape Models

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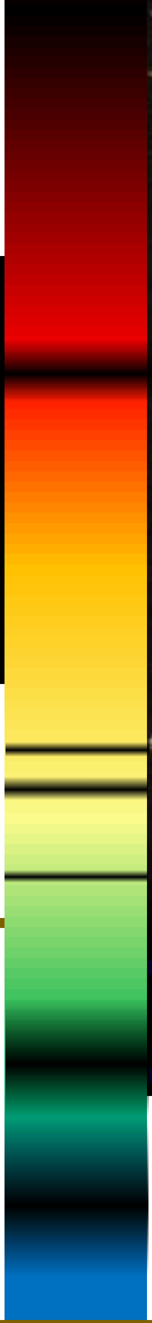
[2]National Solar Observatory

[3]University of Texas at Austin

[4]George Ellery Hale Fellow



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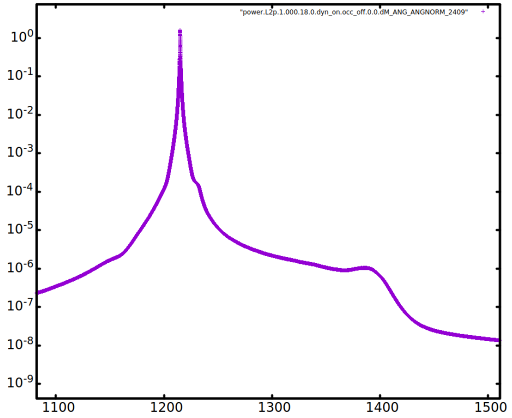
U.S. DEPARTMENT OF ENERGY

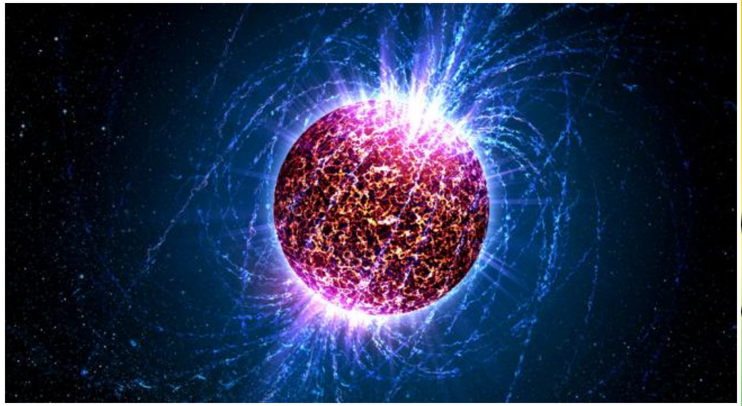
National Nuclear Security Administration

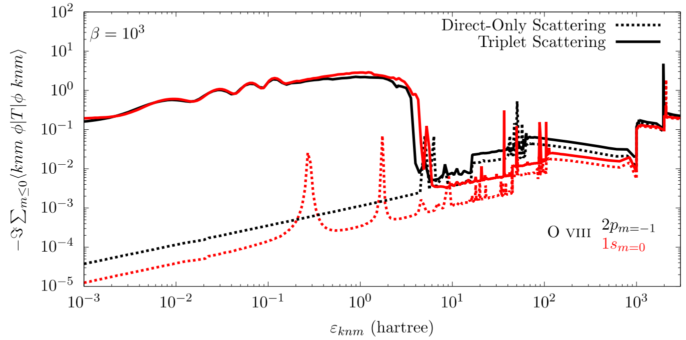
Outline

- Introduction of the WCAPP team
- Line shape primer
- Recent updates by students
  - Penetrating collisions of Ions
  - Carbon line shapes with Simulations

- Magnetic Collisions and Line Shapes
  - Neutron Stars







WCAPP also represents a collaboration among a large number of scientists from national labs and academia.

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R. Heeter, R. Shepherd, D. Liedahl, C. Iglesias, B. Wilson
Lawrence Livermore National Laboratory

T. Perry, C. Fontes, D. Kilcrease, D. Saumon, M. Sherrill, J. Colgan
Los Alamos National Laboratory

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Prism Computational Sciences

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The WCAPP TEAM

The University Team

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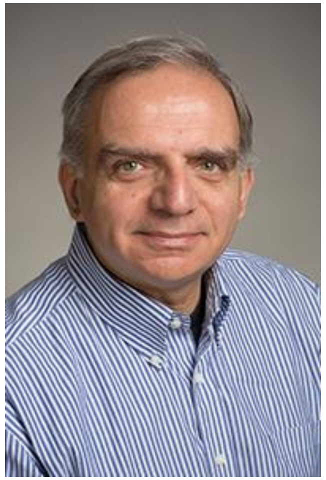

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The WCAPP TEAM

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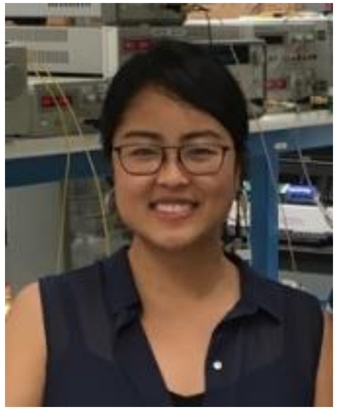
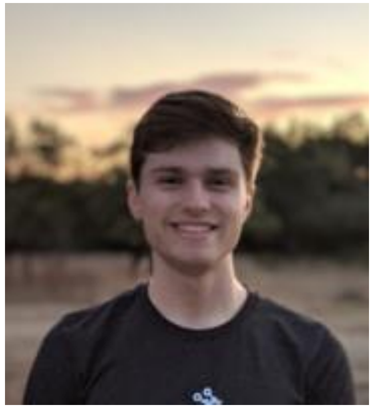

Patty Cho*


Kyle Swanson*


Bryce Hobbs


Malia Kao


Jackson White


Zethran Berbel


Harold Johnson

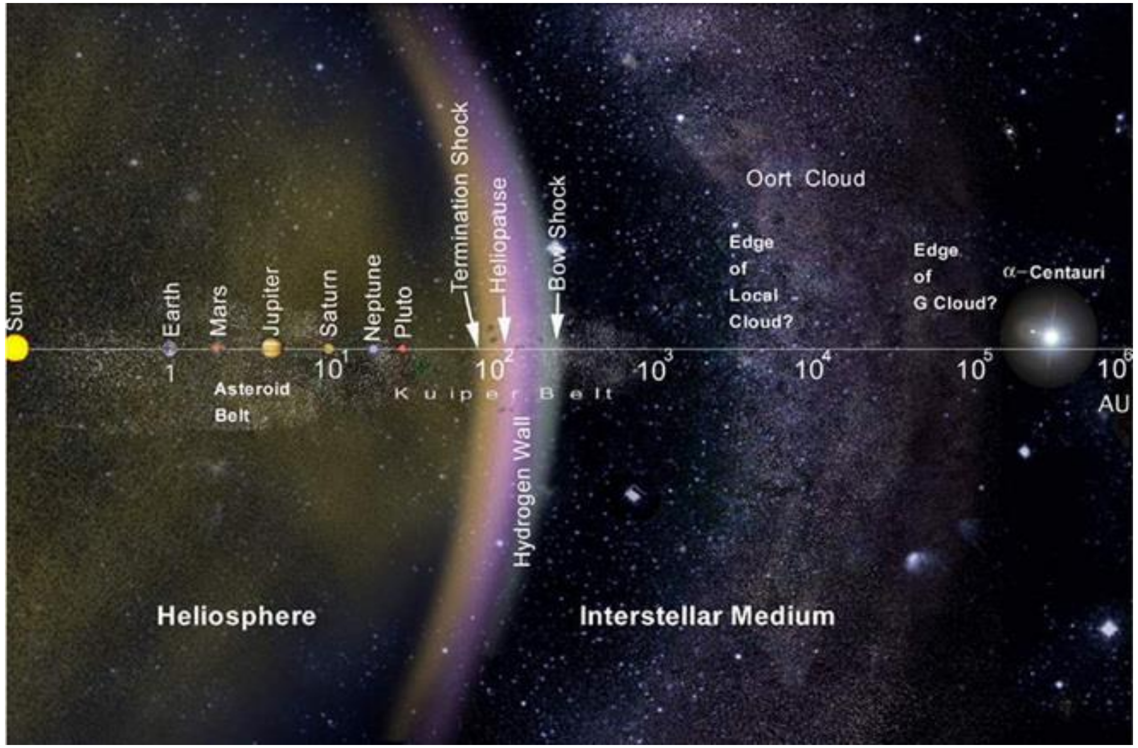

Isaac Huegel

Grad school applications have *increased* by ~ 10 over first 2 years of WCAPP

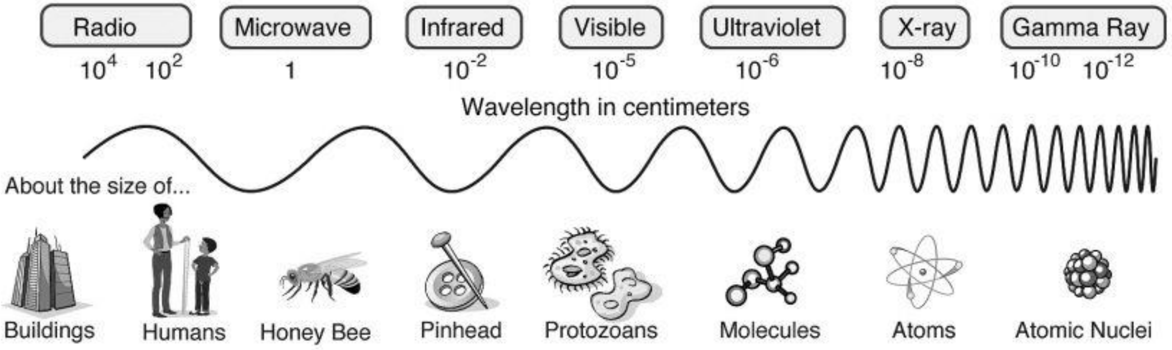
*Patty-Maxwell Award/Fellowship, *Kyle - (Ph.D.).

Light is the Best Tool We Have to Study the Universe

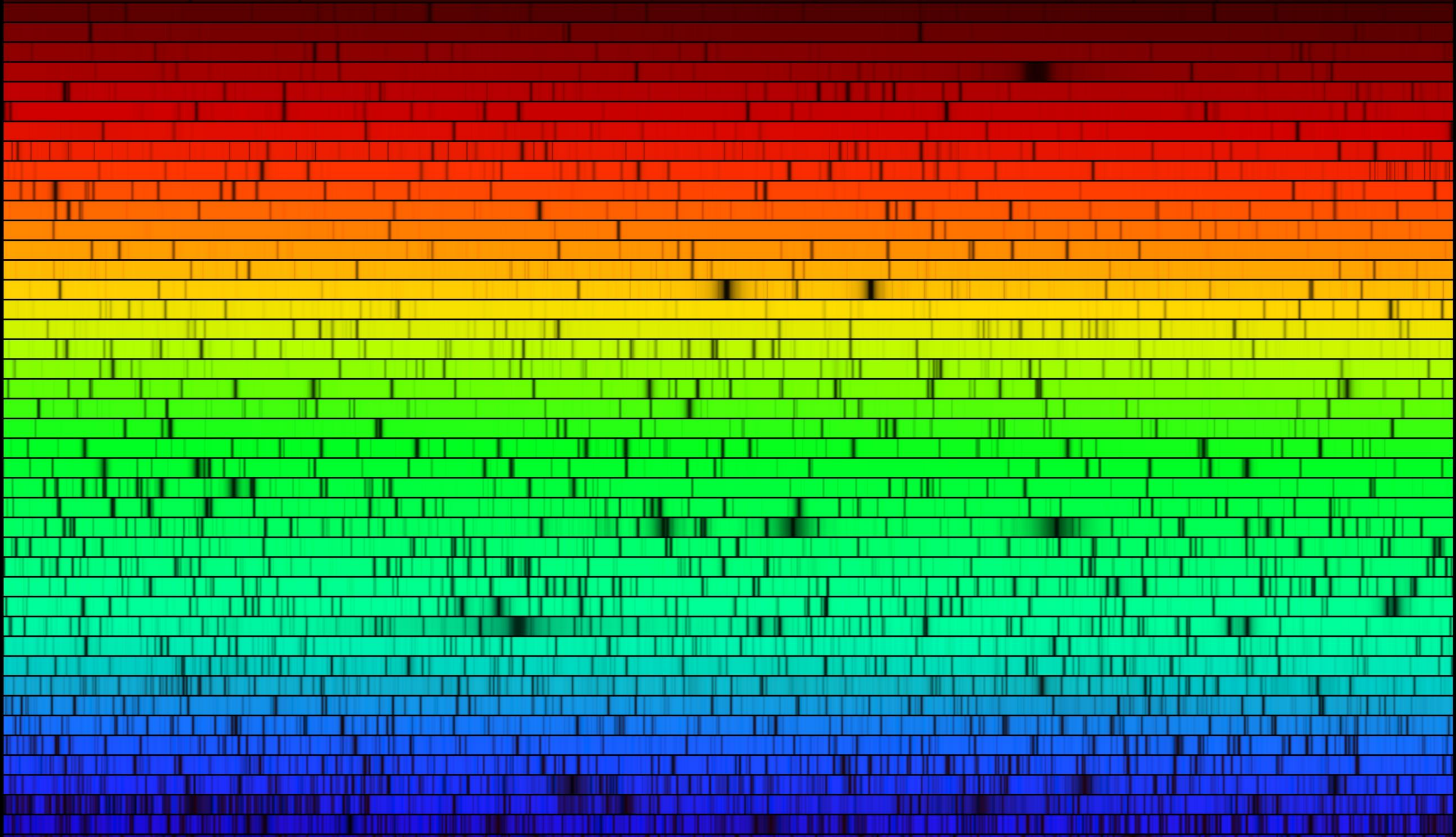
- The solar system contains the only objects that we can visit
- Therefore, the vast majority of what we know about the universe is by analyzing its light
- We also need to be able to probe the full electromagnetic spectrum



Credit: phys.org/news/2015-08-oort-cloud.html

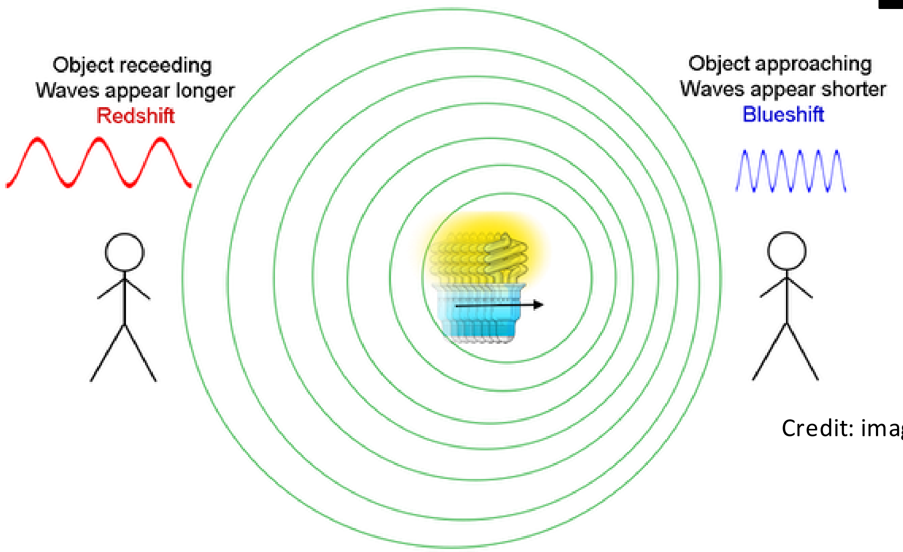


Credit: https://education.nationalgeographic.org/resource/7sun

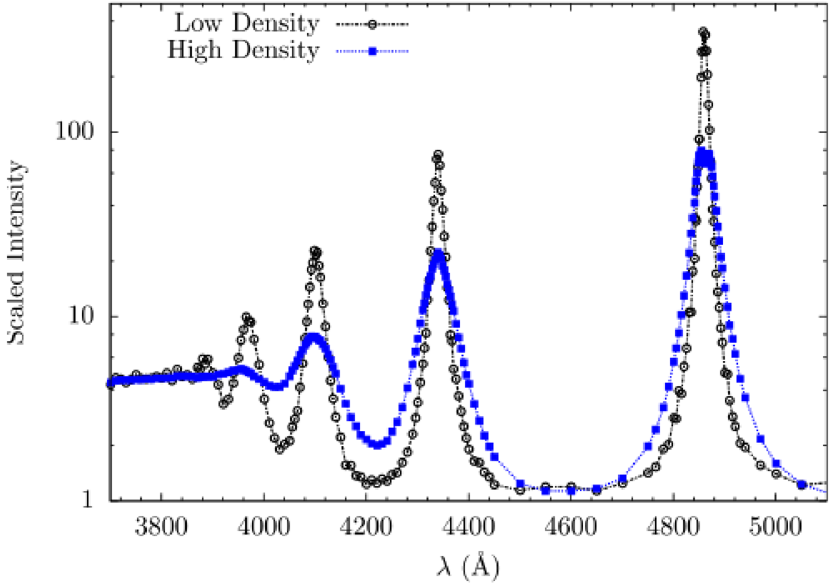


What Information Can Spectral Lines Give Us?

- Bulk motion towards and away from us
  - Doppler shifts
- Temperature
  - Doppler broadening
- Density
  - Broadened spectral lines
  - Shifted spectral lines
  - Lowered continuum



Credit: imagine.gsfc.nasa.gov



Spectral Line Shapes are the Result of a Time-Dependent Ensemble Average of Plasma Perturbations

- In plasmas, atoms are bombarded by collisions and fields from nearby particles
- This will distort and perturb the radiating atom, shifting the energy levels
- The resulting line shape is due from an ensemble average of perturbations

- Perturbation is not mutually exclusive between upper and lower states
  - Cancellation if the states are perturbed in the same way

Physics Needed

- Atomic Structure
- Radiation Physics
- Collision Physics
- Plasma Dynamics
- Statistical Mechanics

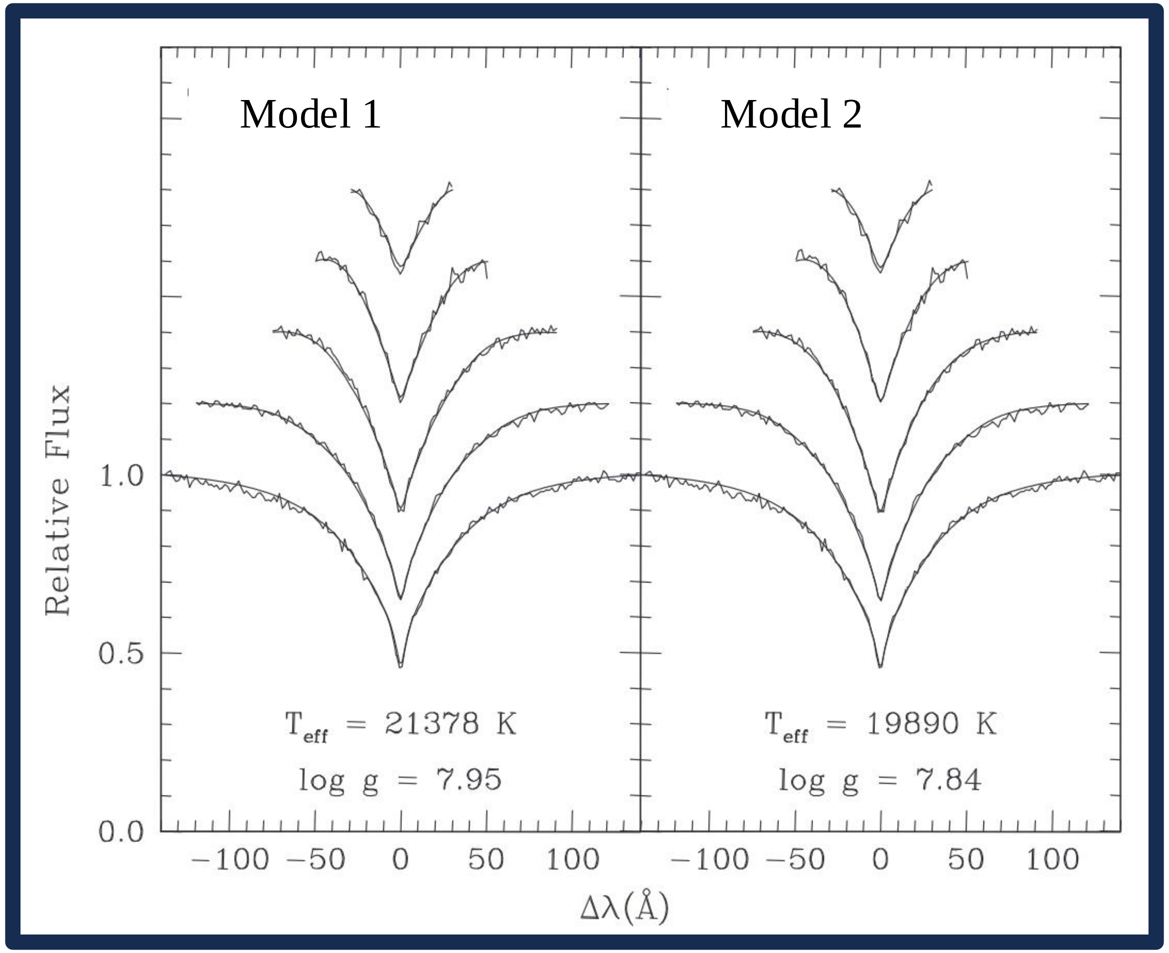
Penetrating Collisions due to Ions

Jackson White’s Master’s Thesis

Interned at LANL and was awarded SSGF graduate Fellowship

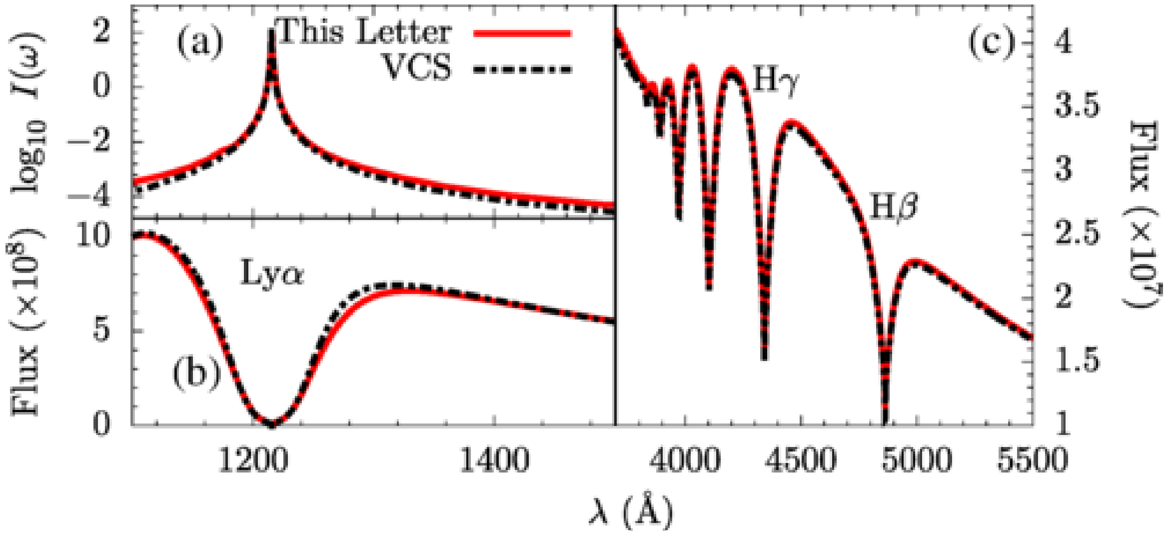
Information from Spectral Line Fitting

- The primary quantity we determine from line fitting is the gravity
  - Bergeron [1] Came up with the technique in 1992
- Without this information, it would be extremely difficult to determine mass and evolution of white dwarfs
  - Still some refinements to be made…
- We want to apply this technique to other systems, including carbon white dwarfs



White Dwarf Intensities are Dependent on Lyα Line Broadening

- Most white dwarf flux emerges from the star in the Lyman regime
- Improved quantum mechanical treatment of Lyα line broadening [1] led to an increase in the wing opacity
- This increase caused a re-distribution of flux of the white dwarf star
  - Greater than the error estimates that are used to calibrate HST/STIS [2,3]
- More work is needed to properly include the quasi-H_2^+ resonances
  - Currently-used models [4] do not properly include the combined effect of ion and electron perturbations



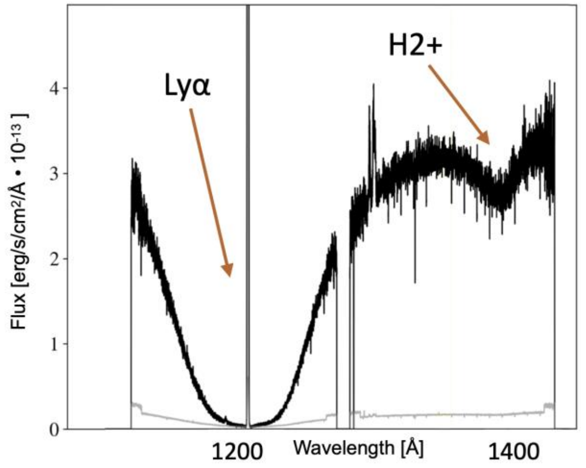
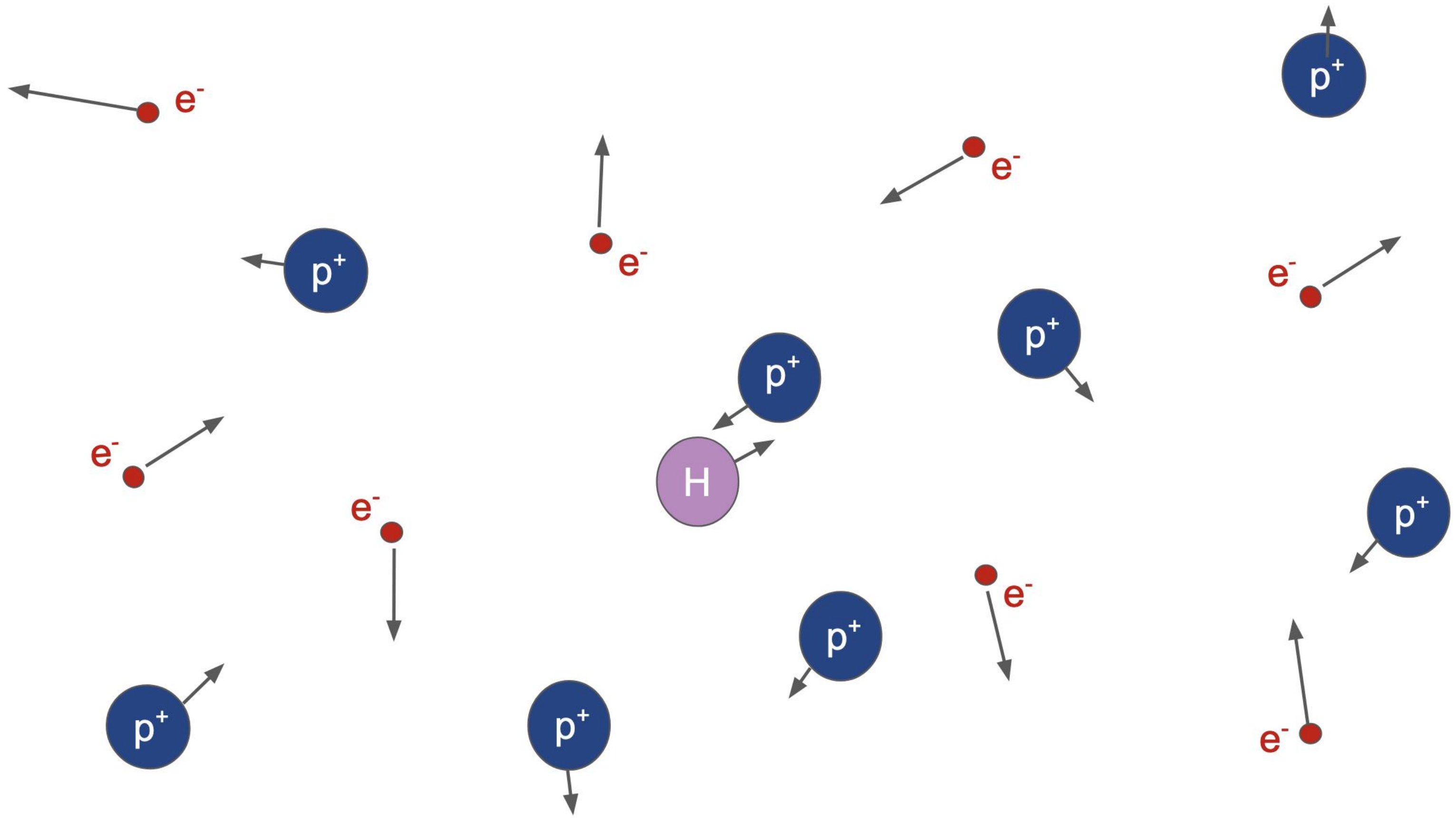


Fig.3: Ultraviolet spectra of DA white dwarf star WD1713+695 from the *Hubble Space Telescope* (HST), illustrating the 1400Å quasi molecular feature associated with the $3d\sigma_g \rightarrow 2p\sigma_u$ transition in H2+

[1] Gomez et al. PRL (2021); [2] Narayan et la. (2019); Bohlin et al. (2020); [4] Allard & Koester (1992)

Quasi-Molecules are Transient unbound Close Collisions Between Plasma Particles that Occur due to Random Stochastic Motion



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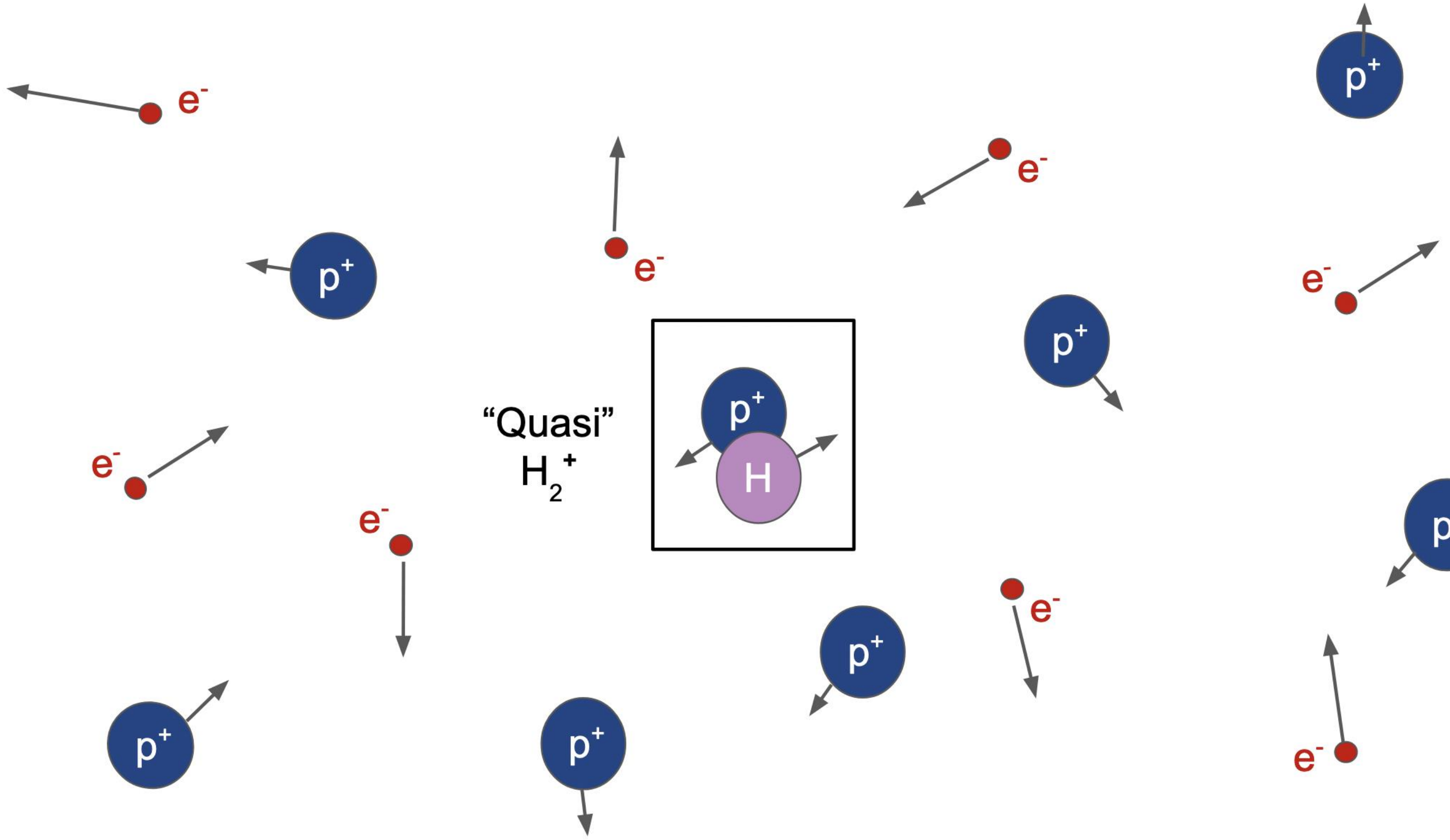
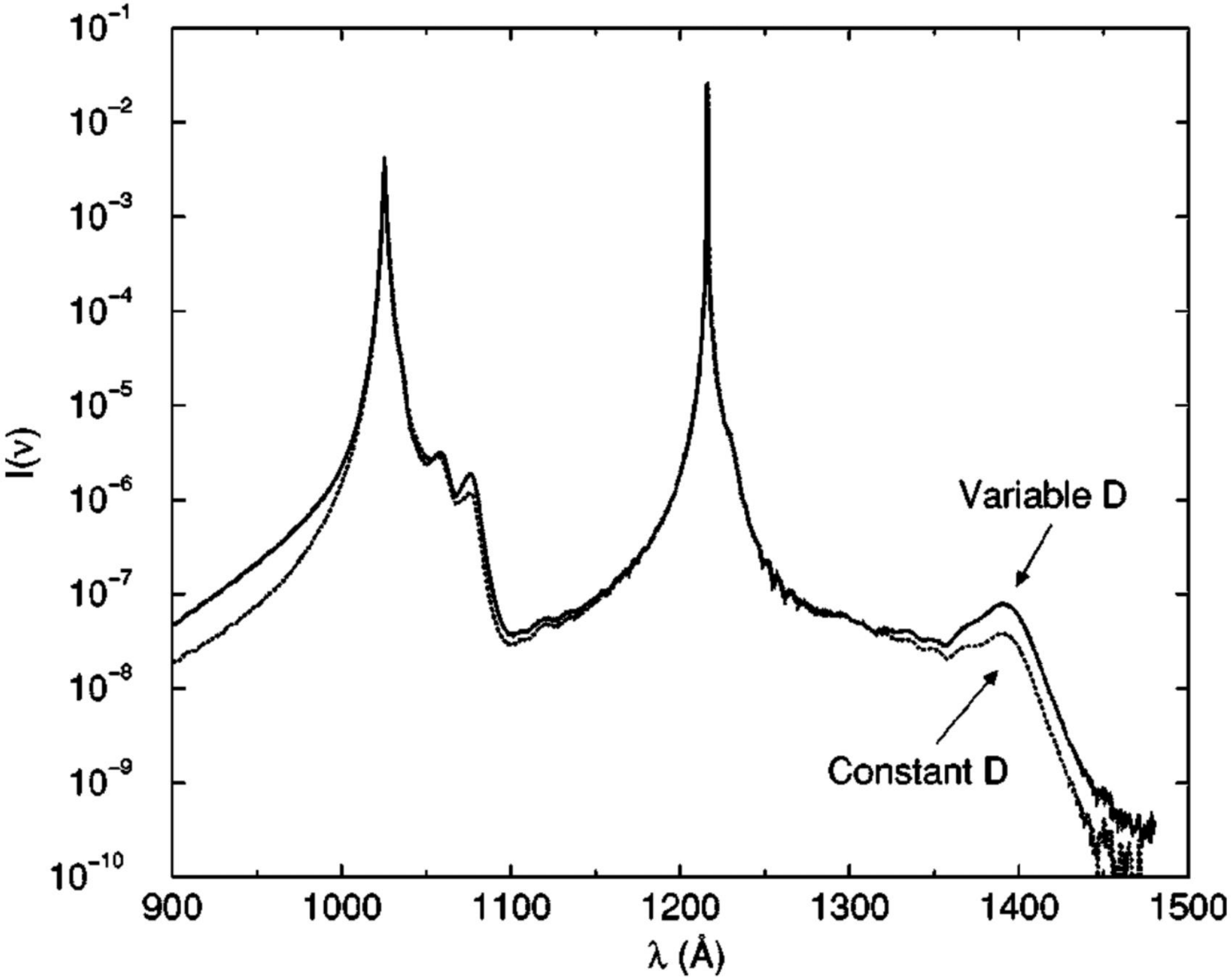
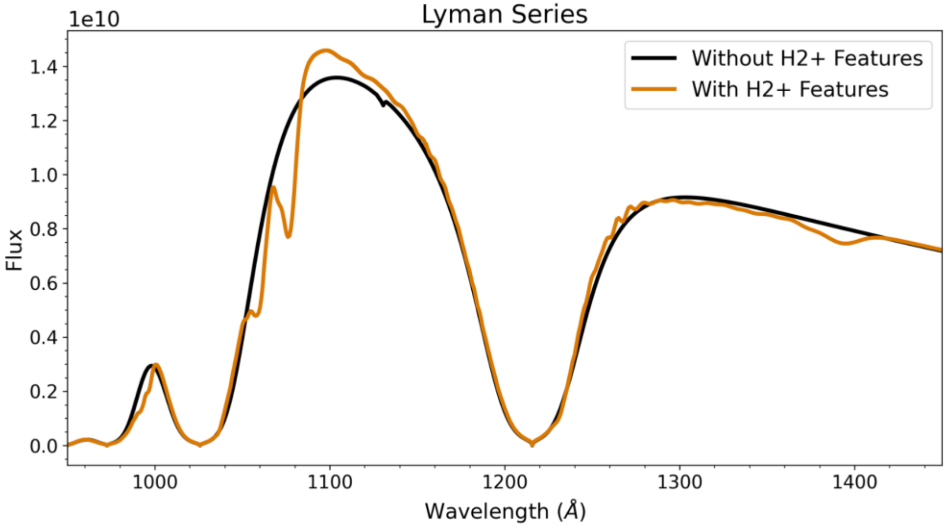
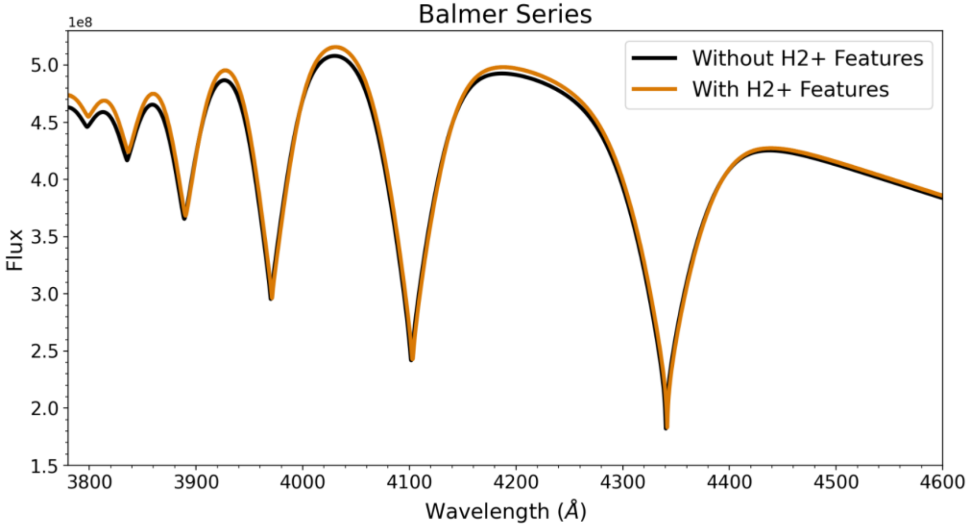


Close Collisions Form Molecular Resonances in Line Shapes



Quasi-Molecular Features affect Flux Distribution

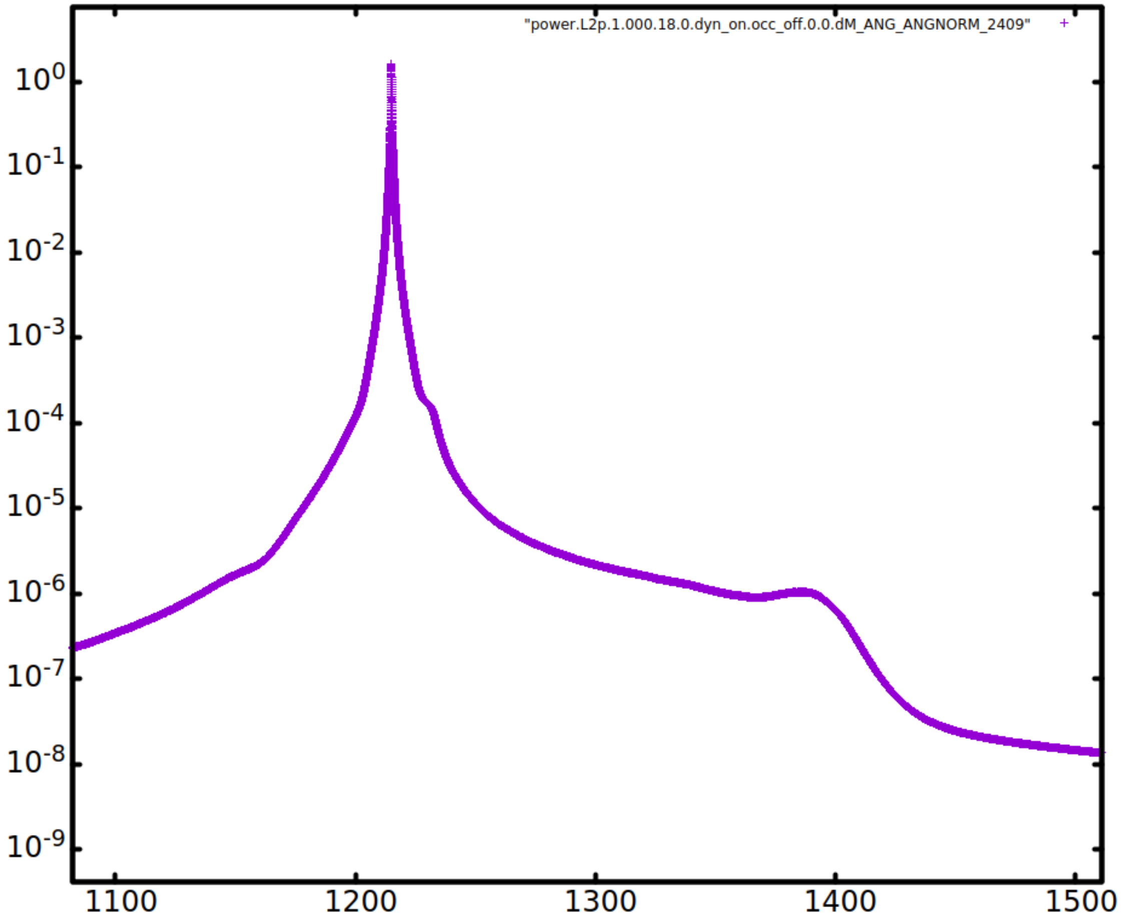




Hubeny & Lanz (1995)

New Xenomorph Calculation with Penetrating Ions

- The update successfully removed:
  - Binary Collision Approximation
  - Field Angle Approximation
  - Single-velocity Approximation
  - Ion Screening



Jackson Implemented a Change-of-Basis Procedure

- Initial Change of Basis

$$U_m(t_i) = \sum_{a,a'} P_{a'} U_a(t_i) P_a$$

- Time Evolution in Molecular Basis

$$U_m(t + \Delta t) = U_m(\Delta t) U_m(t)$$

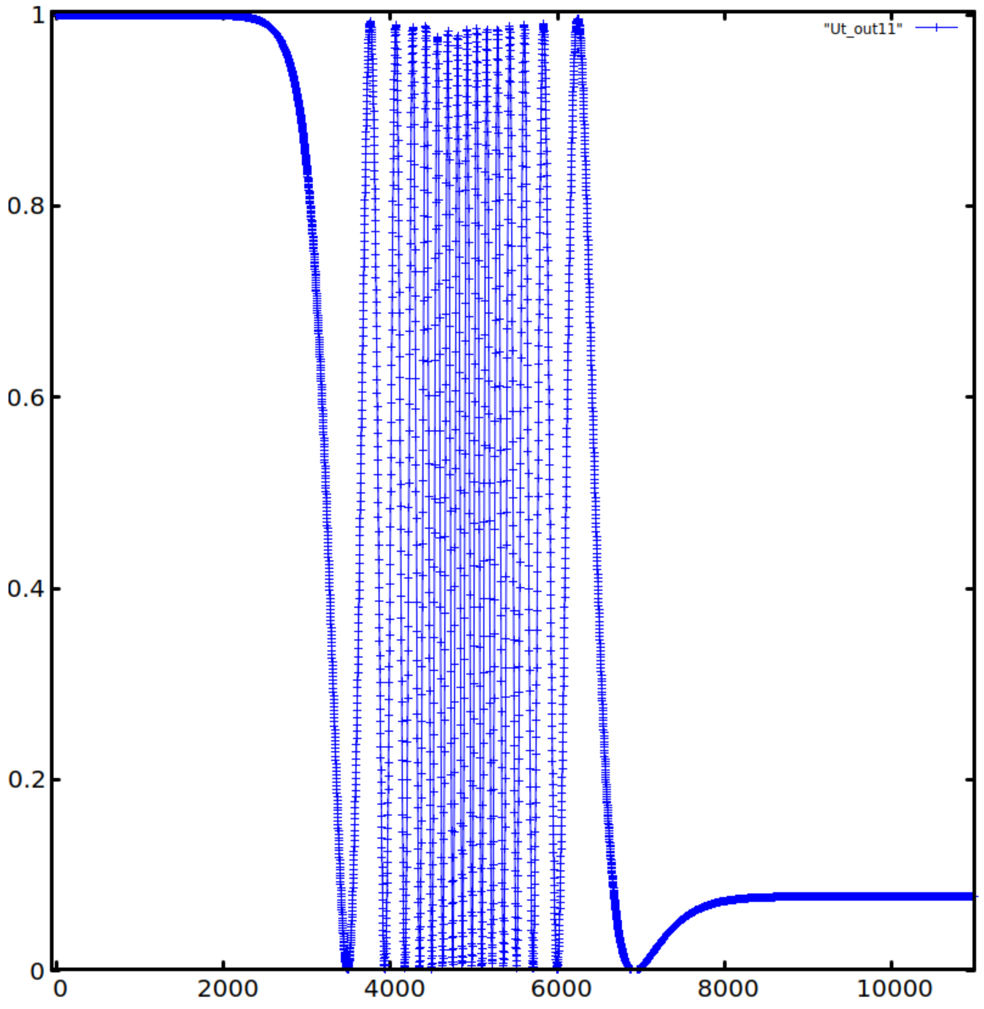
$$U_m(\Delta t) = e^{-i\Delta t H_m}$$

- Change of Basis back to Atomic Basis

$$U_a(t) = \sum_{m,m'} P_{m'} U_m(t) P_m$$

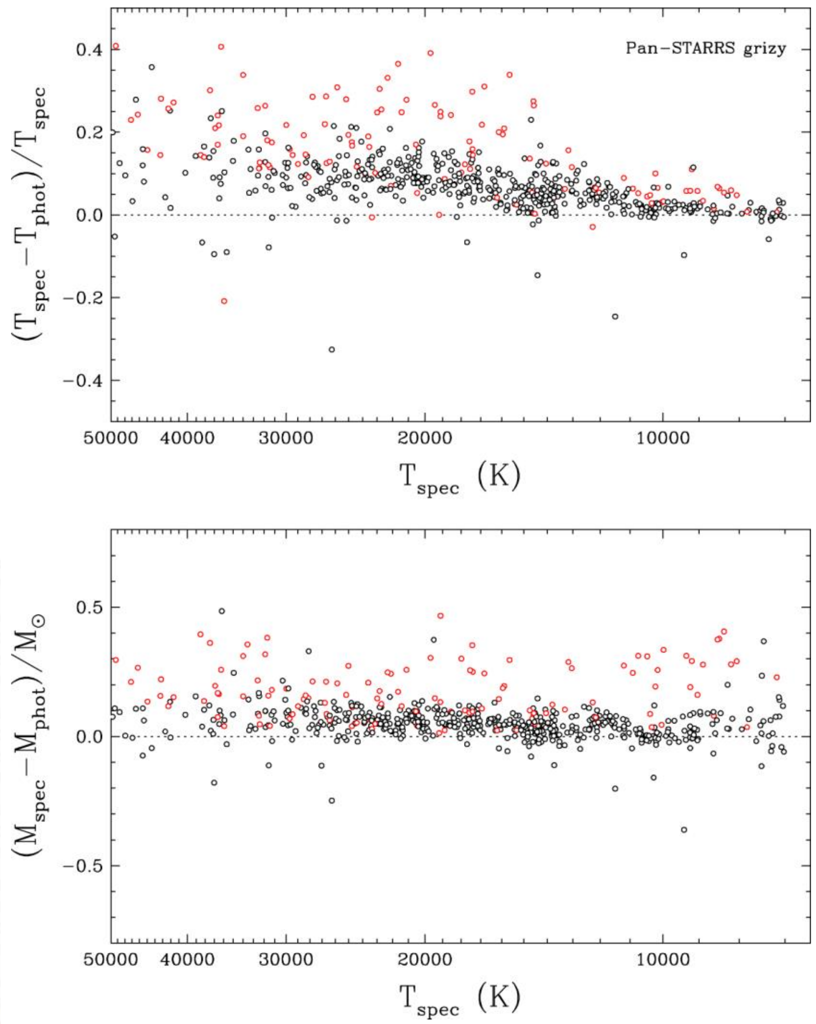
Future Implications?

- With this technique, we are able to calculate the quasi-molecular features
- We can also simulate charge exchange process in detail
- How does charge exchange affect spectra beyond affecting populations?
  - Opacity?

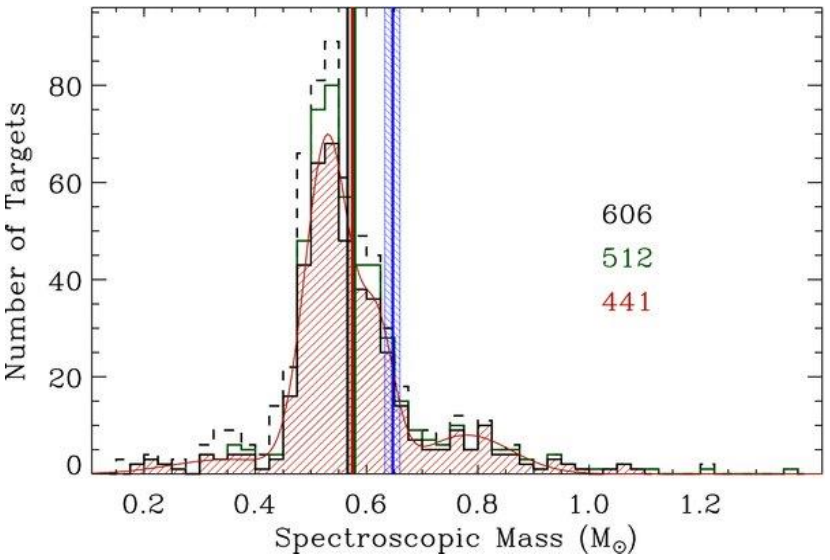


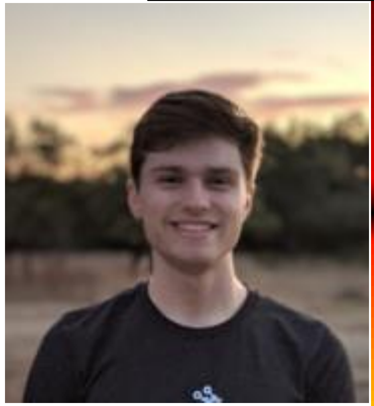
Implications on White Dwarf Astronomy

- White dwarf parameters can now be obtained from photometry from GAIA [1]
  - Changes in the model intensities can change our interpretation of spectra
- May go some way to resolve the mass estimates from gravitational redshifts and spectroscopy [2]



- This work is essential for understanding white dwarf evolution, stellar evolution
- WD cooling times affect cosmochronology



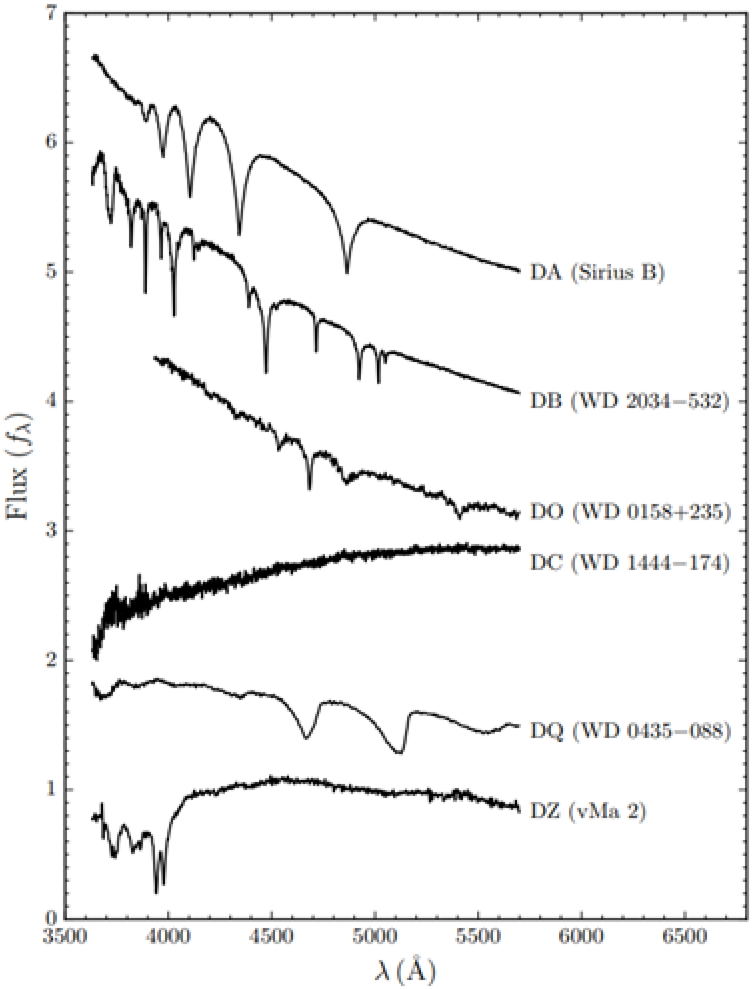


Hyperbolic Trajectories in Xenomorph

Bryce Hobb’s Master’s Thesis

White Dwarfs Have Many Different Spectral Types

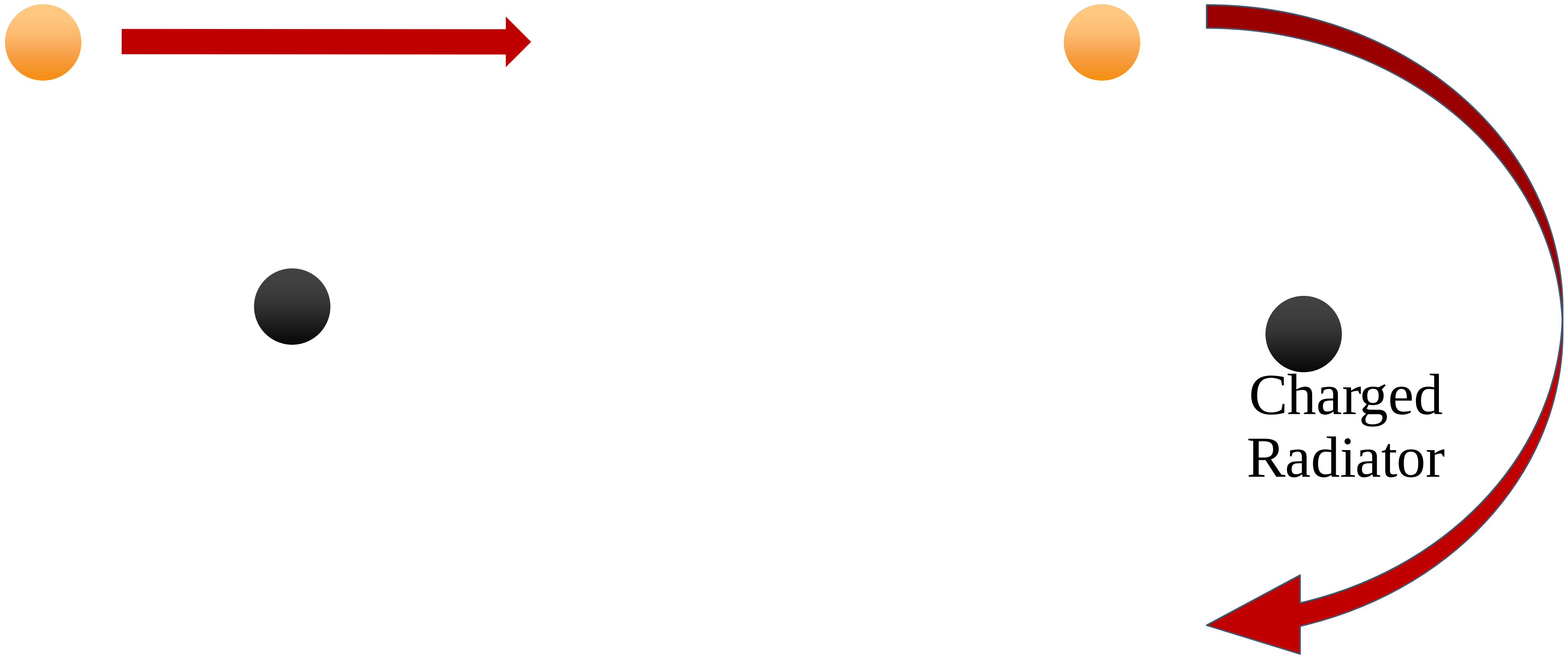
Spectral Type	Atmosphere Characteristics
DA	Hydrogen Lines Only
DB	Helium Lines Only
DO	Singly Ionized Helium Lines
DC	Continuum Only
DQ	Carbon Lines, usually Helium Dominated
DZ	Metal Lines



- The origin of DQ stars is unknown
- Early work indicates that they are more massive than their hydrogen counterparts

Dufour (2009)

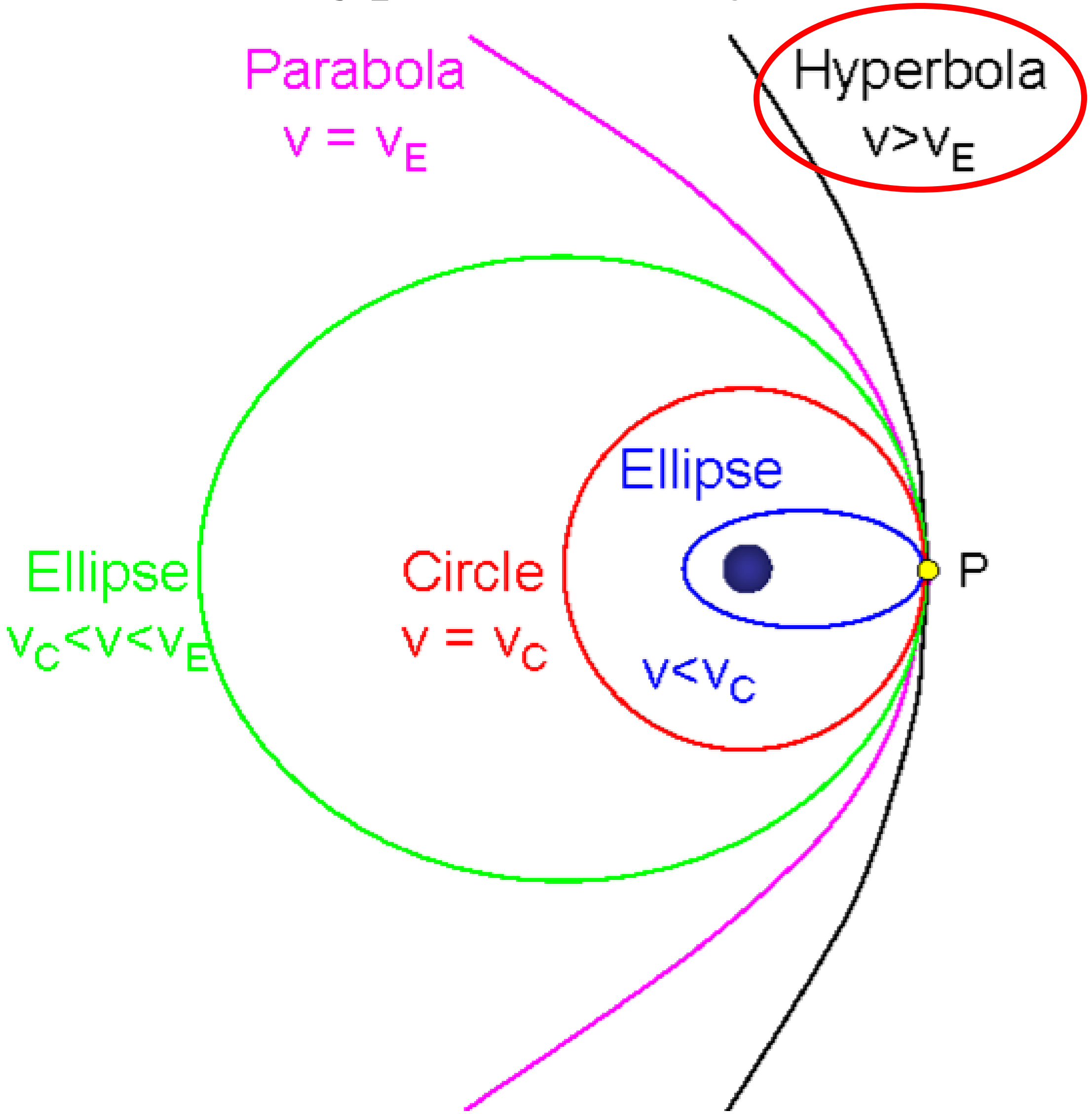
Neutral
Radiator



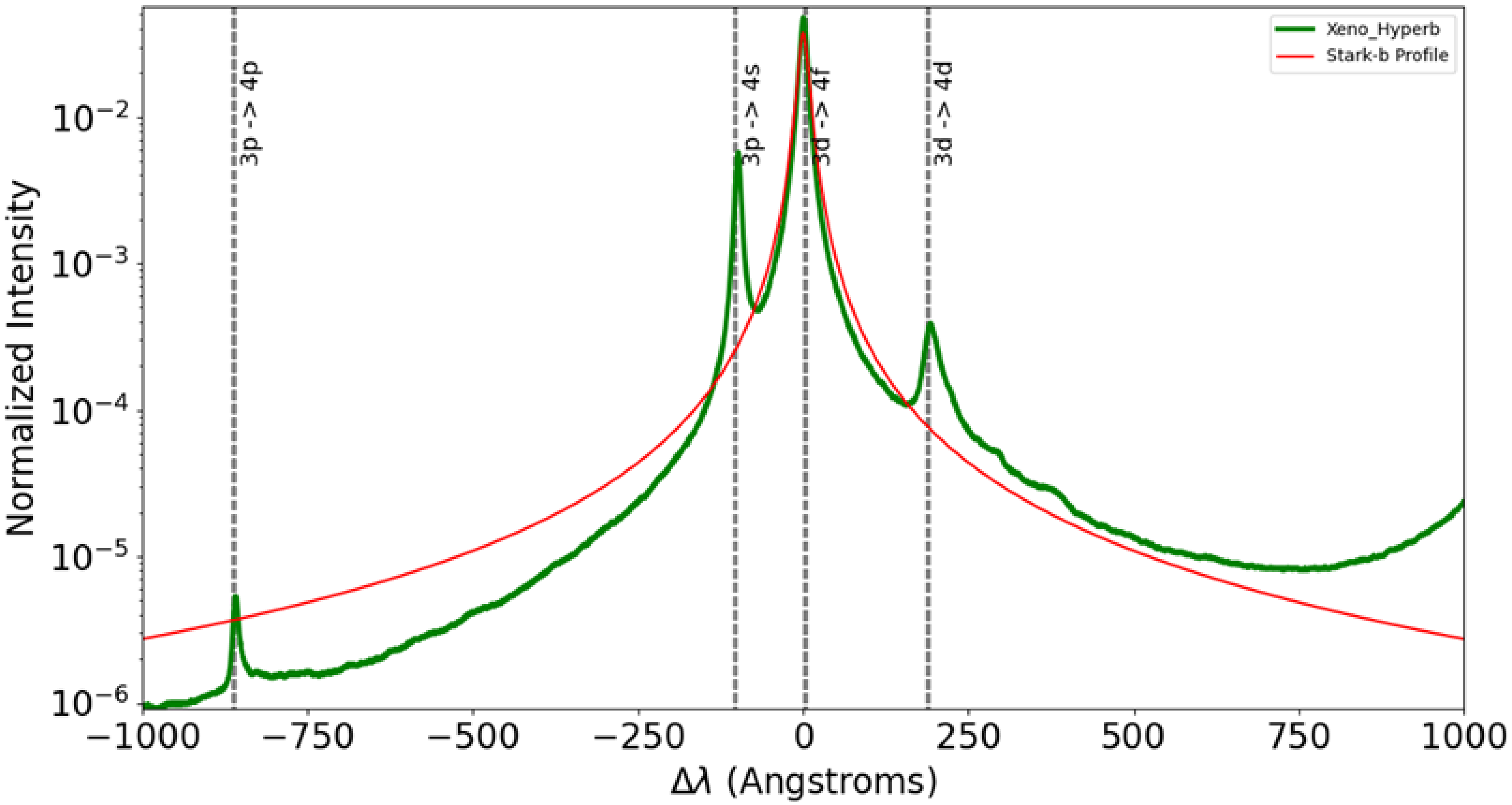
For charged radiators, particles will move on Hyperbolic Trajectories

$$r(\theta) = \left(\frac{-km}{L^2}(1 + e\,cos(\theta) \right)^{-1}$$

$$v_r(\theta, r) = -\frac{L^2}{km^2r^2}\left(\frac{e\,sin(\theta)}{e\,cos(\theta) + 1} \right)^2$$



Xenomorph Predicts Narrower Pines and Additional Features



- Early interpretation states that narrower spectral lines leads to higher density atmospheres
- This would indicate that DQ stars are even more massive than previously thought, progenitor stars for type Ia supernovae?

Atomic Processes in Magnetic Fields

Magnetic Fields are Found Everywhere

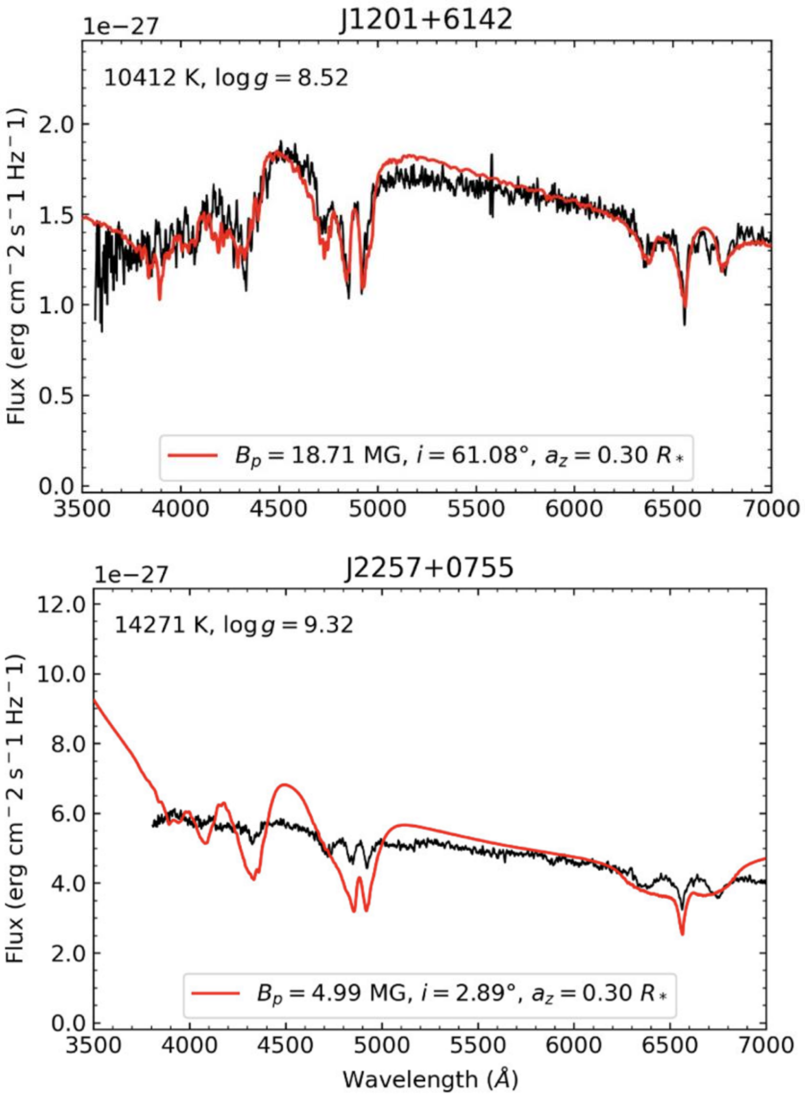
Astrophysics

- The sun
  - Flares/CMEs (T)
- Other main sequence stars
- Compact Objects:
  - White Dwarfs (kT)
  - Neutron Stars (100MT)
- Accretion Disks

Laboratory

- Magnetically Confined Fusion Plasmas
  - MagLIF (10kT)
  - AutoMag (100kT)
- High Intensity Lasers

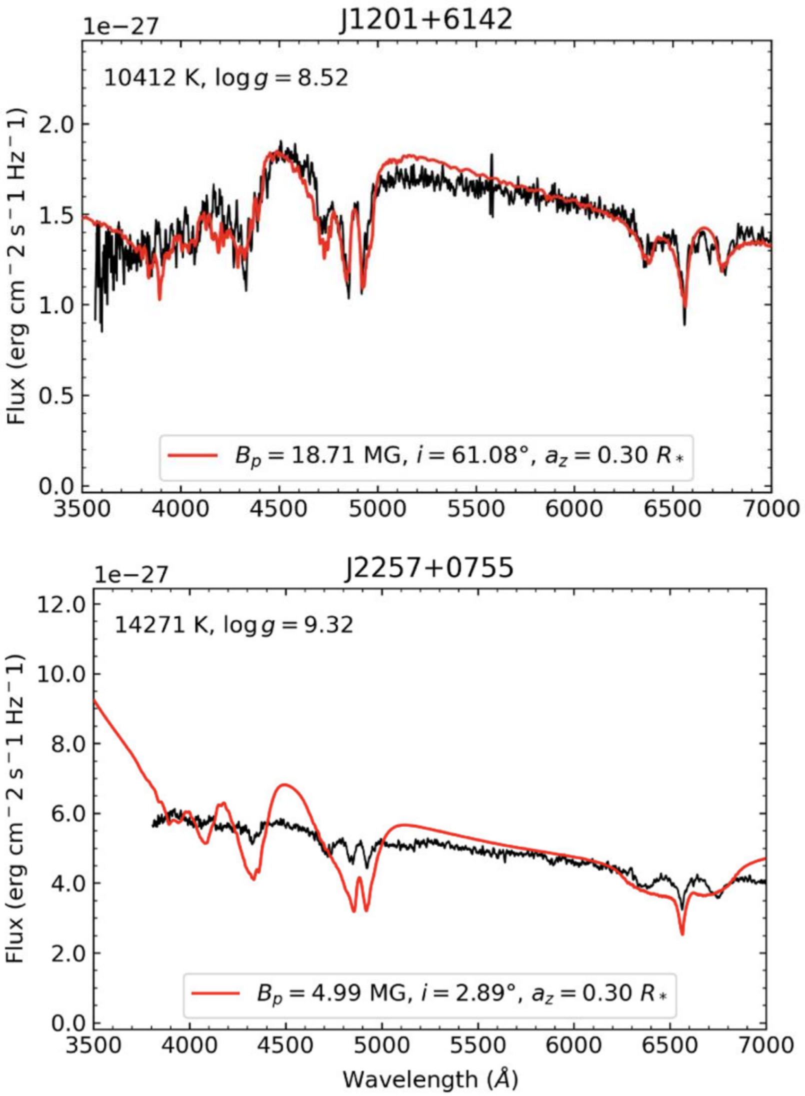
Models That Include Magnetic Fields are Woefully Incomplete



- The Physics is Modified
  - Atomic Structure
  - Free-Free Radiation
  - Radiation Transport
  - Polarization
  - Collisions

Hardy et al. (2023)

Models That Include Magnetic Fields are Woefully Incomplete



- The Physics is Modified
  - Atomic Structure
  - Free-Free Radiation
  - Radiation Transport
  - Polarization
  - ***Collisions***

Models are likely incomplete

DETAILED MODELS DO NOT EXIST!

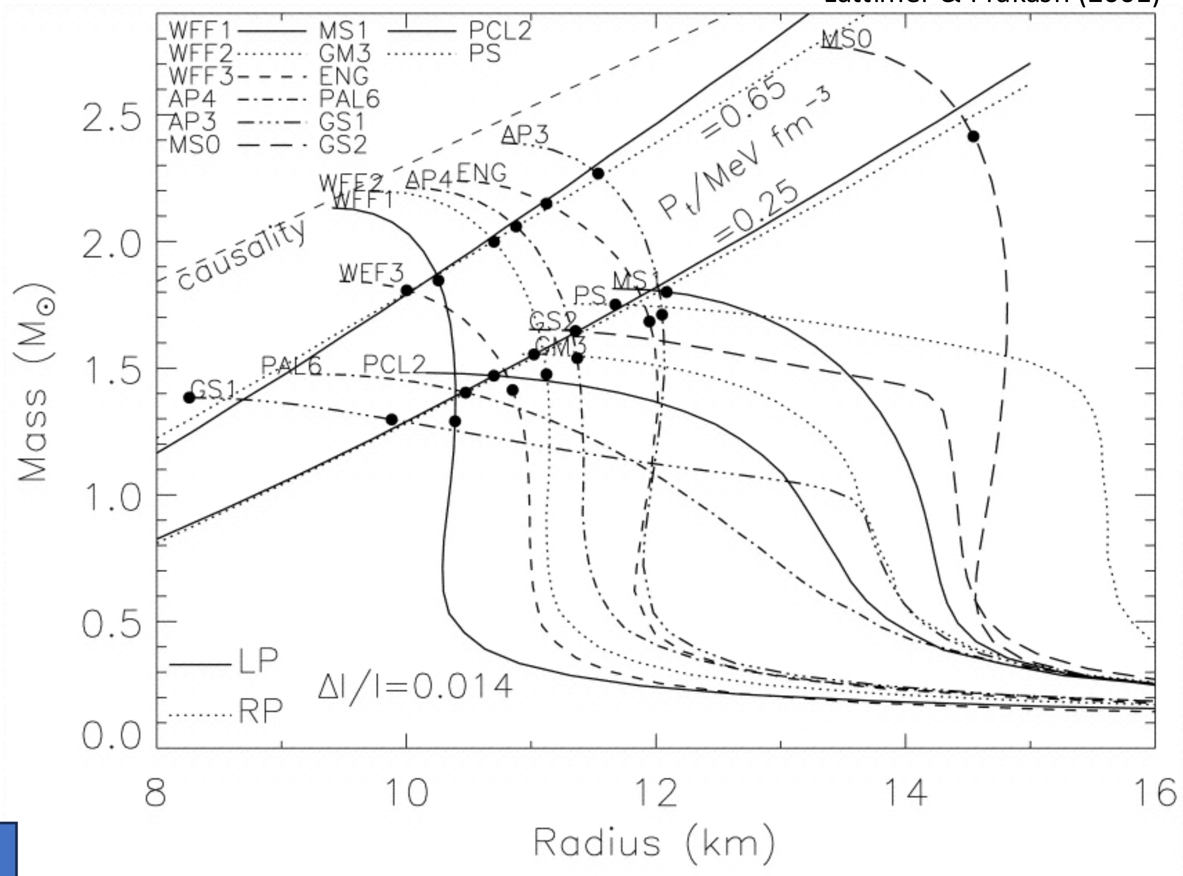
Interesting Astrophysical Questions can be Addressed by Improving Magnetic Field Models

- White Dwarfs:
  - What are the masses of magnetic white dwarfs?
  - Do they take a different evolutionary path?

- Neutron Stars:
  - What is the equation of state of the interior?

Accurate mass and radius determinations can help constrain the equation of state

Lattimer & Prakash (2001)



Masses and Radii of Neutron Stars

Gravitational redshift

$$1 + z = \frac{1}{\sqrt{1 - 2GM/Rc^2}}$$

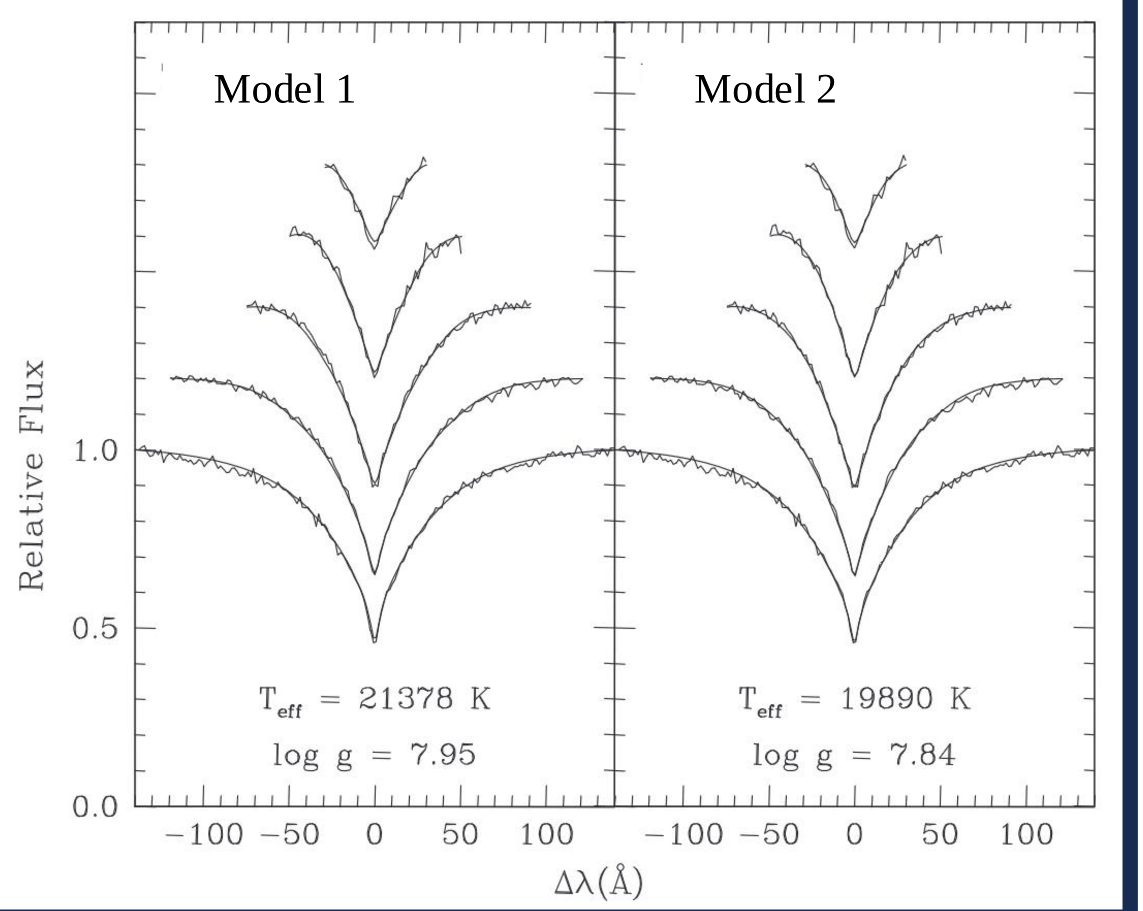
Gravitational acceleration from line shapes

$$g = G\frac{M}{R^2}$$

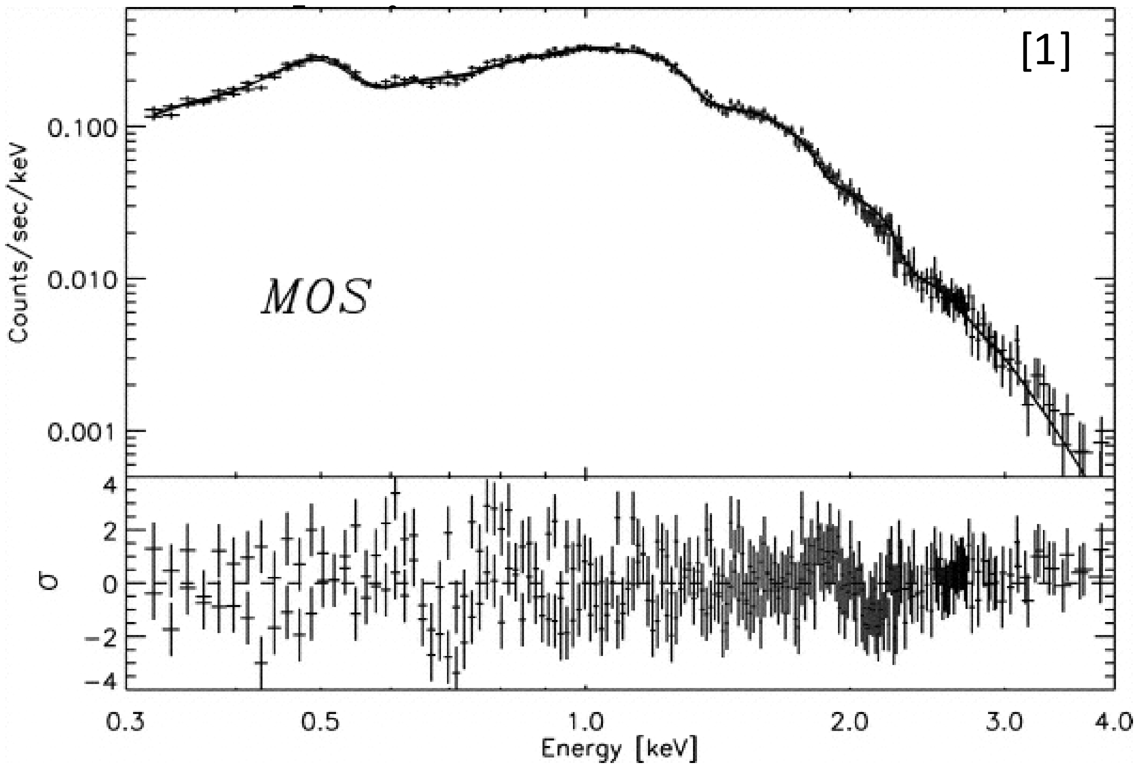
Gravitational redshift and gravitational acceleration will allow us to simultaneously obtain M and R

Information from Spectral Line Fitting

- The primary quantity we determine from line fitting is the gravity
  - Bergeron [1] Came up with the technique in 1992
- Without this information, it would be extremely difficult to determine mass and evolution of white dwarfs
  - Still some refinements to be made…
- We want to apply this technique to other systems, including carbon white dwarfs



NS Spectra are Possible, But…Higher Resolution are Needed



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Gravitational redshift and gravitational acceleration will allow us to simultaneously obtain M and R

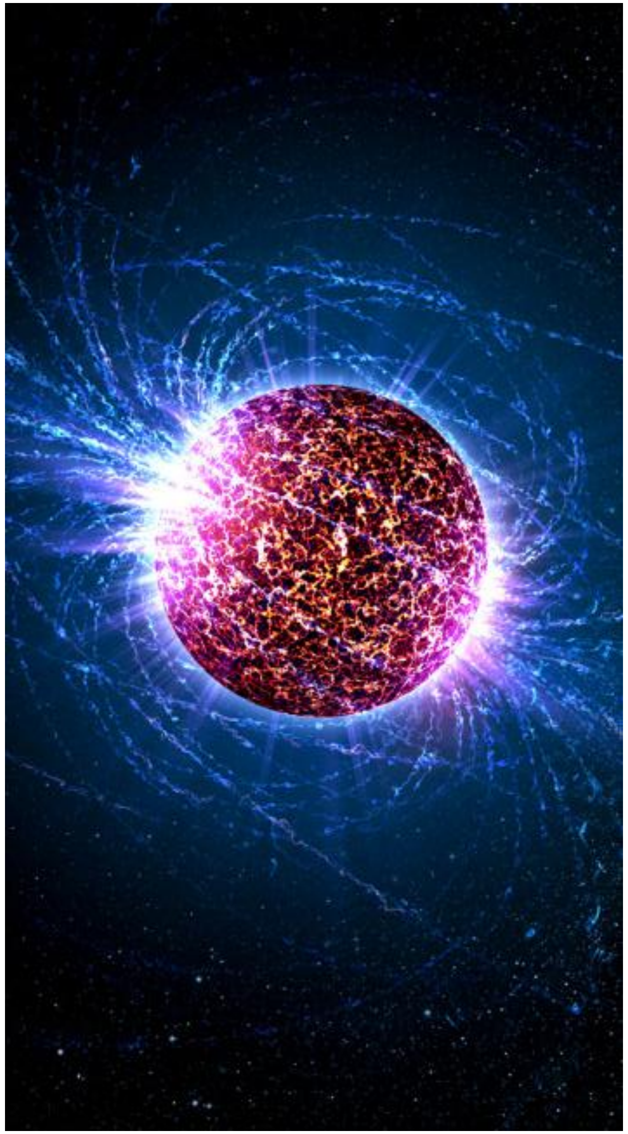
Higher-Resolution Spectroscopy is Needed

[1] Mori & Hailey (2006)

Models for Atom-Electron Collisions in a B field *do not Exist*

- There were some brief efforts to model scattering in the 1970s [1]
  - Only scattering off bare nuclei

- What are collisions needed for?
  - Spectral Line Shapes
  - Material/Transport Properties
    - Thermal/heat Conductivities
    - Electrical Conductivities



[1] Ventura (1973)

A Particle in a Magnetic Field is Confined in the x-y direction

- The kinetic energy term is modified to include a vector potential
- How the solution progresses will depend on the choice of gauge for *A(r)*
- Choose a symmetric gauge

$$A(r) = \frac{1}{2}\vec{B} \times \vec{r}$$

- We have the additional potential

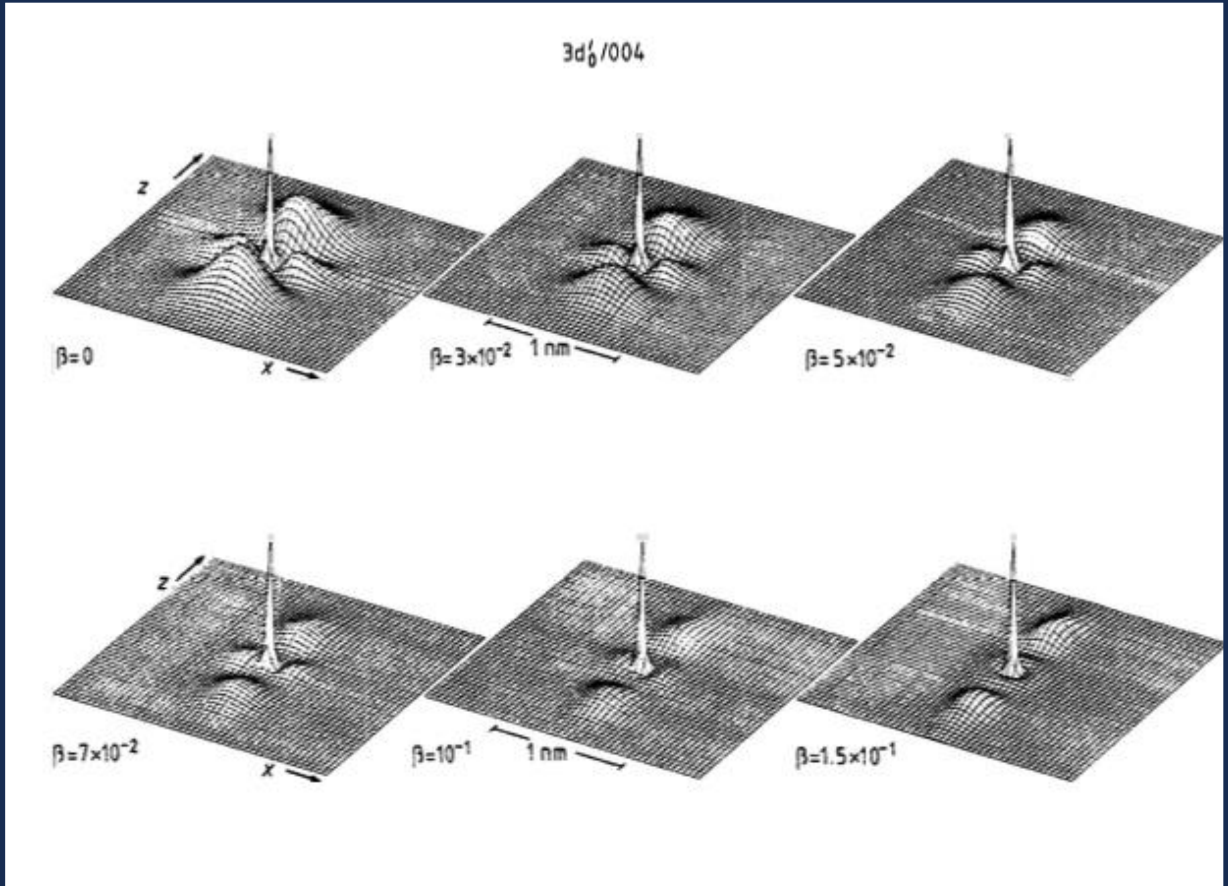
$$H = \frac{1}{2m}p^2 + V(r)$$

$$\Rightarrow \frac{1}{2m}[\vec{p} - eA(\vec{r})]^2 + V(r)$$

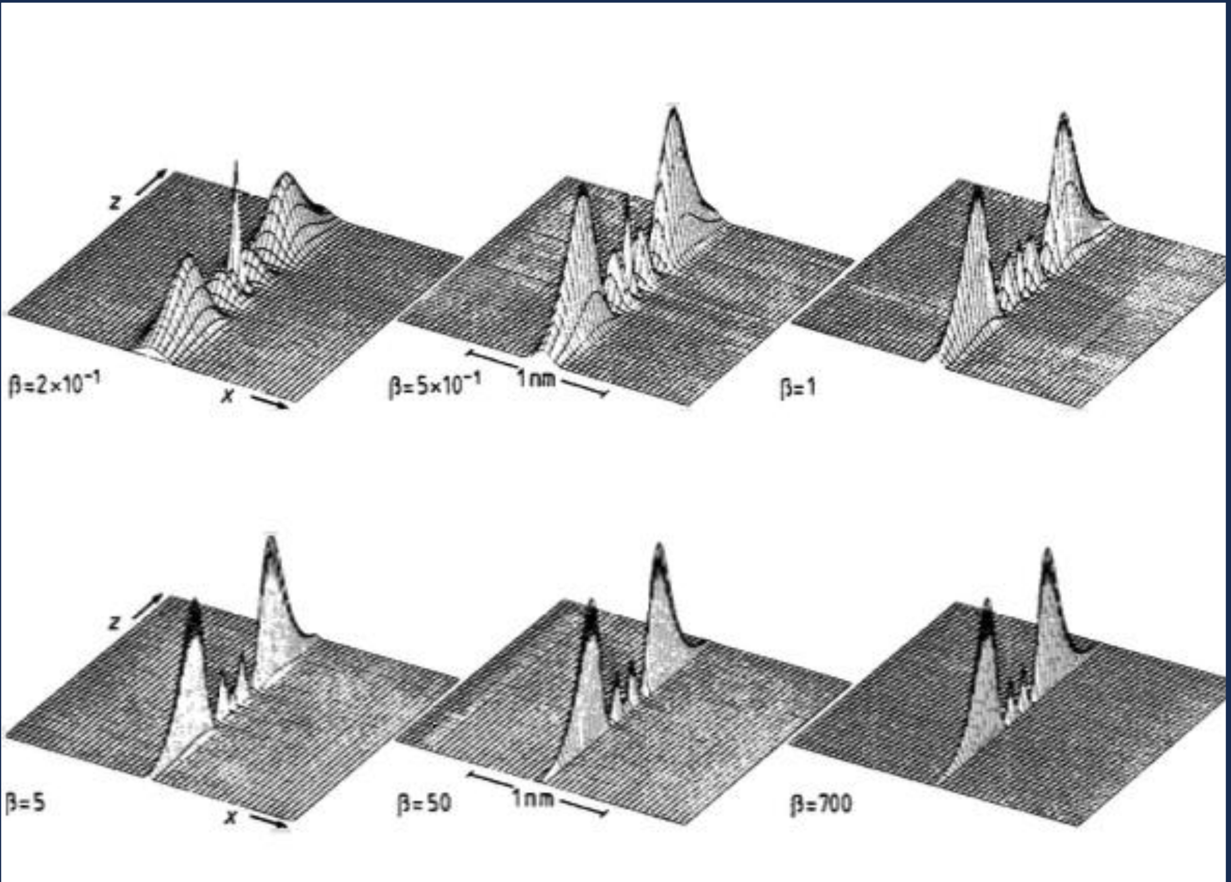
$$(\vec{p} - \frac{1}{2}e\vec{B} \times \vec{r})^2$$

$$\Rightarrow p^2 - eB \cdot (\vec{r} \times \vec{p}) + \frac{e}{4}B^2\rho^2$$

B fields Cause Atomic Wavefunctions to Become Squished



Weak Fields

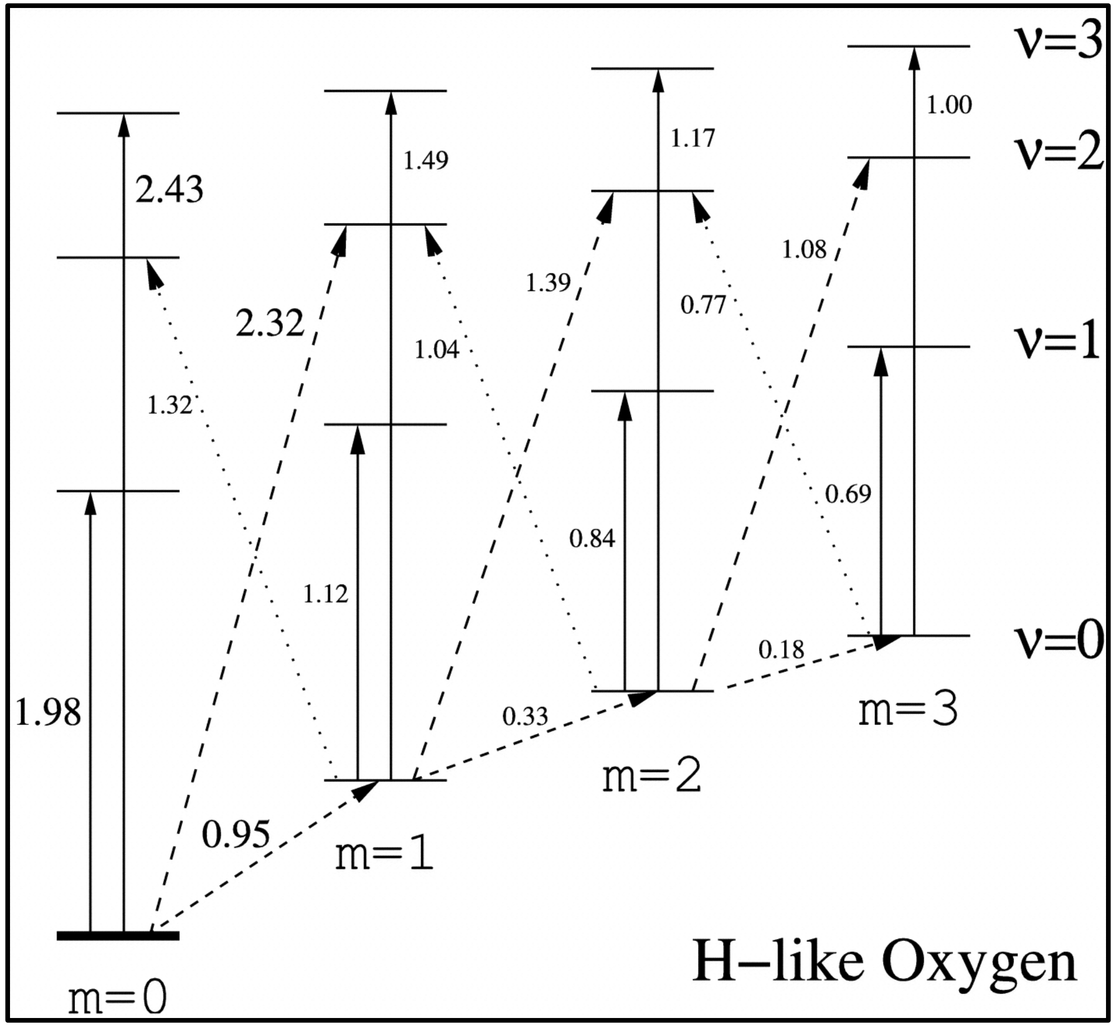


Strong Fields

[1] Rosner (1984)

There are many different regimes for Magnetic Fields

- Weak Field
  - Splitting by *M*
- Intermediate Regime
  - Field competes with FS
- Strong Regime (Paschen Back)
  - Field overpowers FS
  - Classic triplet pattern
- Extra Strong Regime (Landau)
  - Atoms are no longer spherically symmetric
  - Cylindrical
  - Energy levels no longer resemble the field-free values



…It’s not that simple though

- Need to include the finite mass of the nucleus*
  - Alters energy level structure
  - Motion of the nucleus through the magnetic field creates an additional field

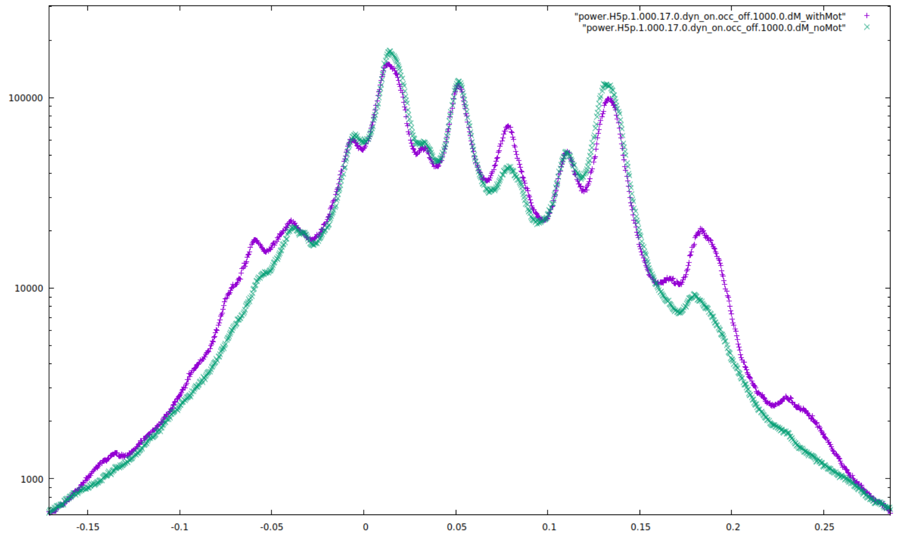
$$E'_{\parallel} = E_{\parallel}$$

$$B'_{\parallel} = B_{\parallel}$$

$$E'_{\perp} = \gamma(E_{\perp} + v \times B)$$

$$B'_{\perp} = \gamma\left(B_{\perp} - \frac{1}{c^2} v \times E\right)$$

- Motional Stark Effect
  - Additional electric field due to atom’s motion in plasma
  - Changes ratio of components
  - Forbidden components



Criteria for Quantum Mechanical Collisions

- There has been much effort exploring collisions and perturbations from a classical perspective
- But at some point, classical treatment will break down
- The usual criteria is that the relevant length scales has to be of order or less than the thermal de Broglie wavelength

- If we equate the Larmor radius to the thermal de Broglie wavelength, we have a criteria for a quantum mechanical treatment of plasma electrons

$$r_L = mv_\perp/|q|B$$

$$B_{QM} \gtrsim \; 4.8\frac{m}{m_e}\frac{1}{|q|}T_{\mathrm{eV}} \;\; \mathrm{kT},$$

- The true threshold may be lower than this…

Collisions in a Magnetic Field

- The general formulae haven't changed
- The physical quantity of interest that we want is from the collision "transition" or T-matrix
  - From this, we can derive a collision amplitude and a cross section
  - This is used to calculate electron broadening widths
- The scattered wave is written in terms of T-matrices
- The only difference is that now, the Hamiltonians have a magnetic field

$$T(E) = V + V\frac{1}{E - H_0}T(E)$$

$$|\Psi\rangle = |\phi\rangle + \frac{1}{E - H_0}V|\Psi\rangle$$

$$= |\phi\rangle + \frac{1}{E - H_0}T(E)|\phi\rangle$$

Free Electron in a Magnetic Field is Confined in the ρ direction

$$H_0^p = -\frac{1}{2}\nabla^2 + \frac{1}{2}L_z\beta + \frac{1}{2}\left(\frac{\beta}{2}\right)^2\rho^2 + S_z\beta + V_{\text{nuc}}(z,\rho)$$

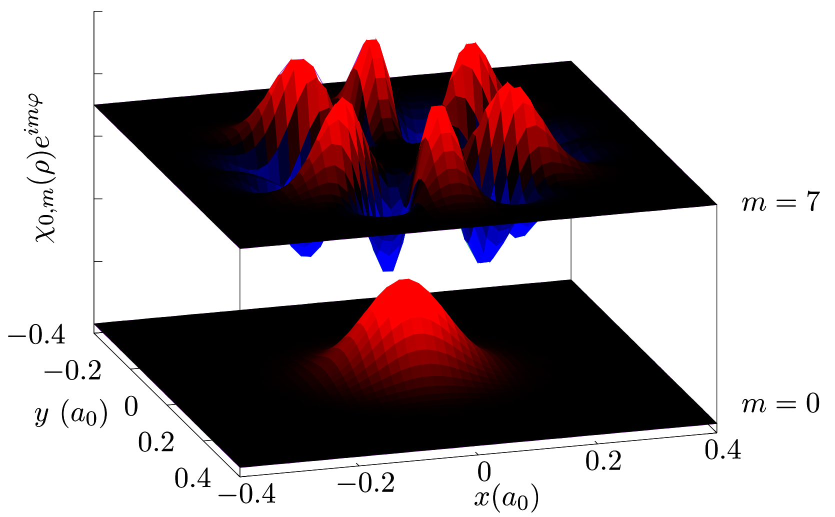
- In a large magnetic field, the electron motion is best described in cylindrical coordinates
- The wavefunctions propagate freely in z, but is a harmonic oscillator in ρ

$$\langle\vec{r}|knm\rangle = Ne^{ikz}e^{-\beta\rho^2/4}\left(\frac{\beta}{2}\rho\right)^{|m|/2} L_n^{|m|}(\beta\rho^2/2)e^{im\phi}$$

- The corresponding energies are

$$\varepsilon_{knm} = \frac{1}{2}k^2 + \frac{\beta}{2}(2n + |m| + m + 1) + m_s\beta$$

  - k is z-momentum, n is landau number, and m is azimuthal quantum number



*classically, this corresponds with helical motion

Requirements for Scattering

- The scattering S-matrix must be unitary
  - This is accomplished by solving the T-matrix to all-order using a linear solve technique [1]
- The wavefunctions must be anti-symmetric with exchange of coordinates
- With a magnetic field, however, the boundary conditions change

$$S^\dagger S = I$$

$$\Psi(\vec{r}_1, \vec{r}_2) = (-1)^S \Psi(\vec{r}_2, \vec{r}_1)$$

$$\langle \phi_k | f_{j,i} \rangle = (-1)^S \langle \phi_j | f_{k,i} \rangle$$

No Field

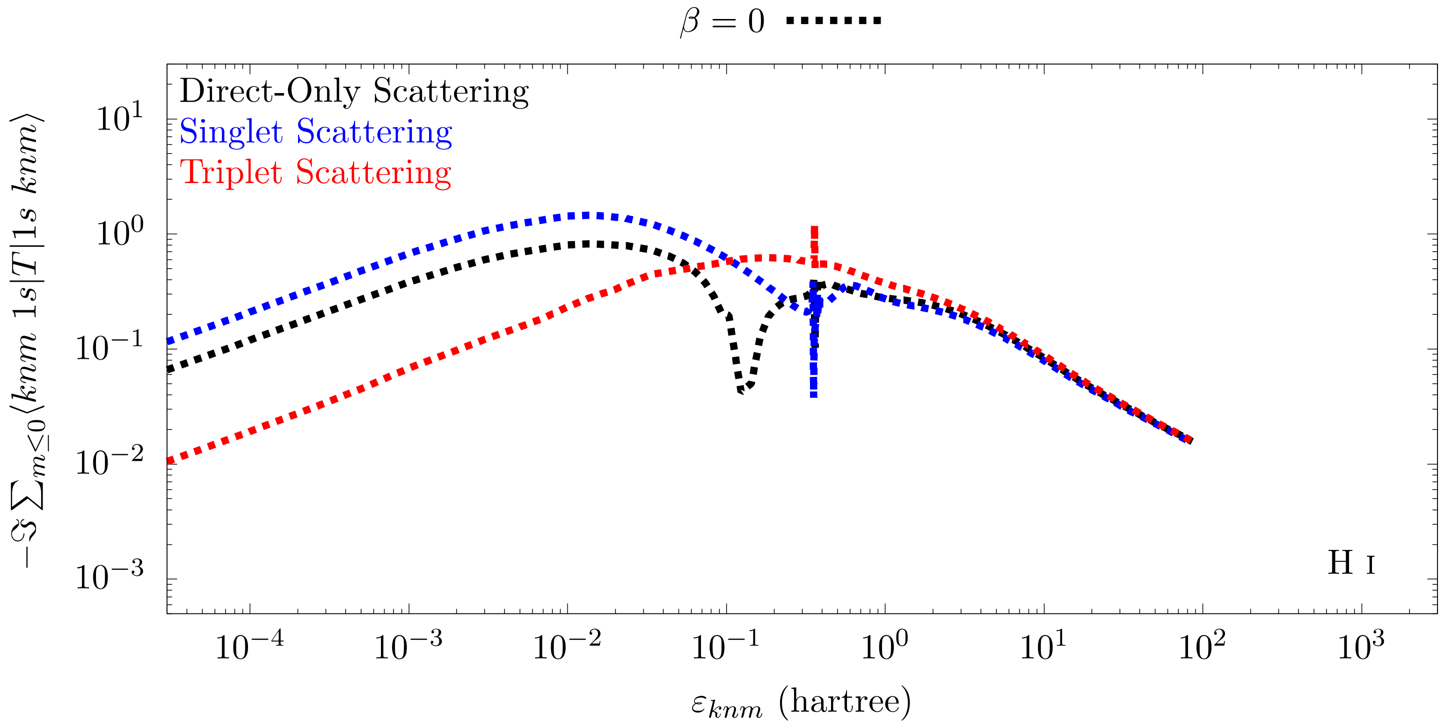
$$f_i(r) = e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}$$

With a Field

$$f_i(r) = e^{ikz} \chi_{nm}(\rho, \phi) + i f \frac{e^{\pm ik' z}}{|k'|} \chi_{n'm'}(\rho, \phi)$$

The Effect of Exchange on Collision Cross Sections of Hydrogen

Field-free cross sections are not that different when including the effects of exchange



The Effect of Exchange on Collision Cross Sections of Hydrogen

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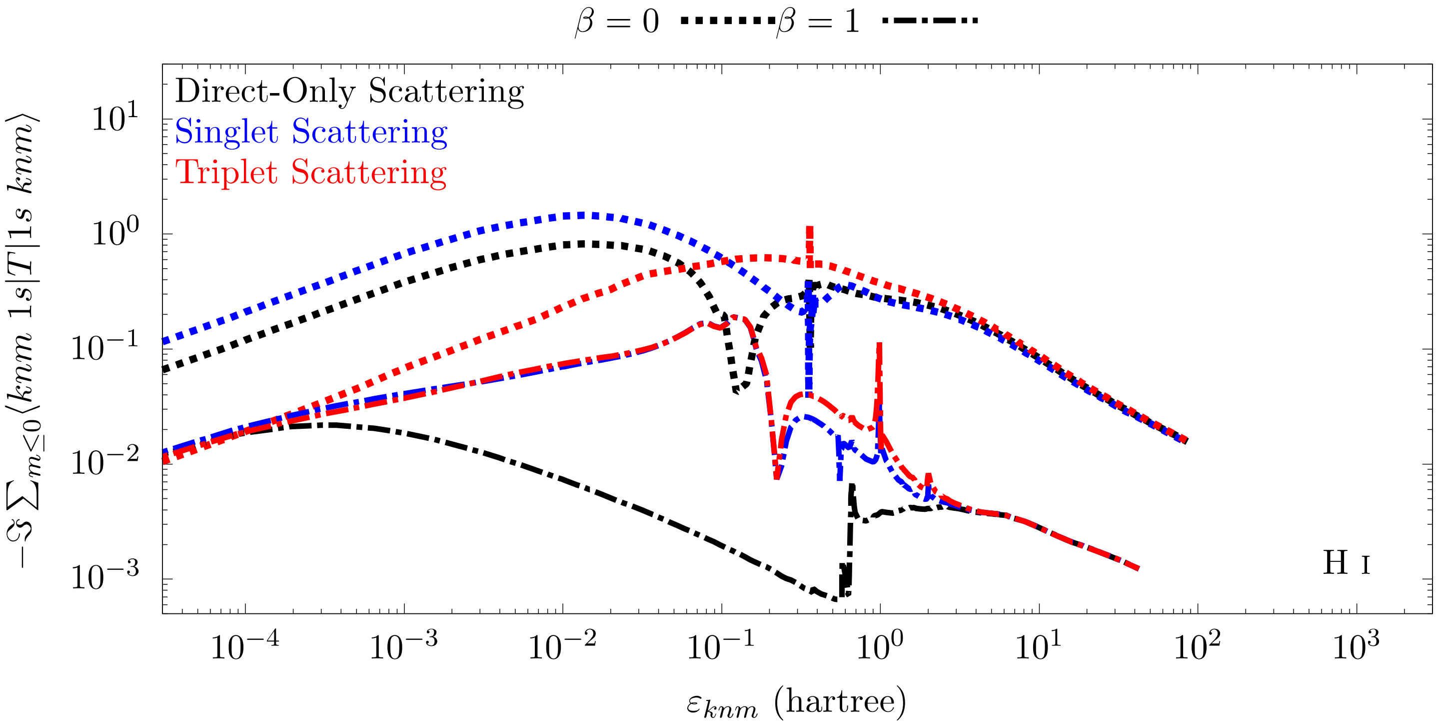
At moderate fields (B=2.35x10^{5}T), then exchange causes significant increases in the collision cross sections

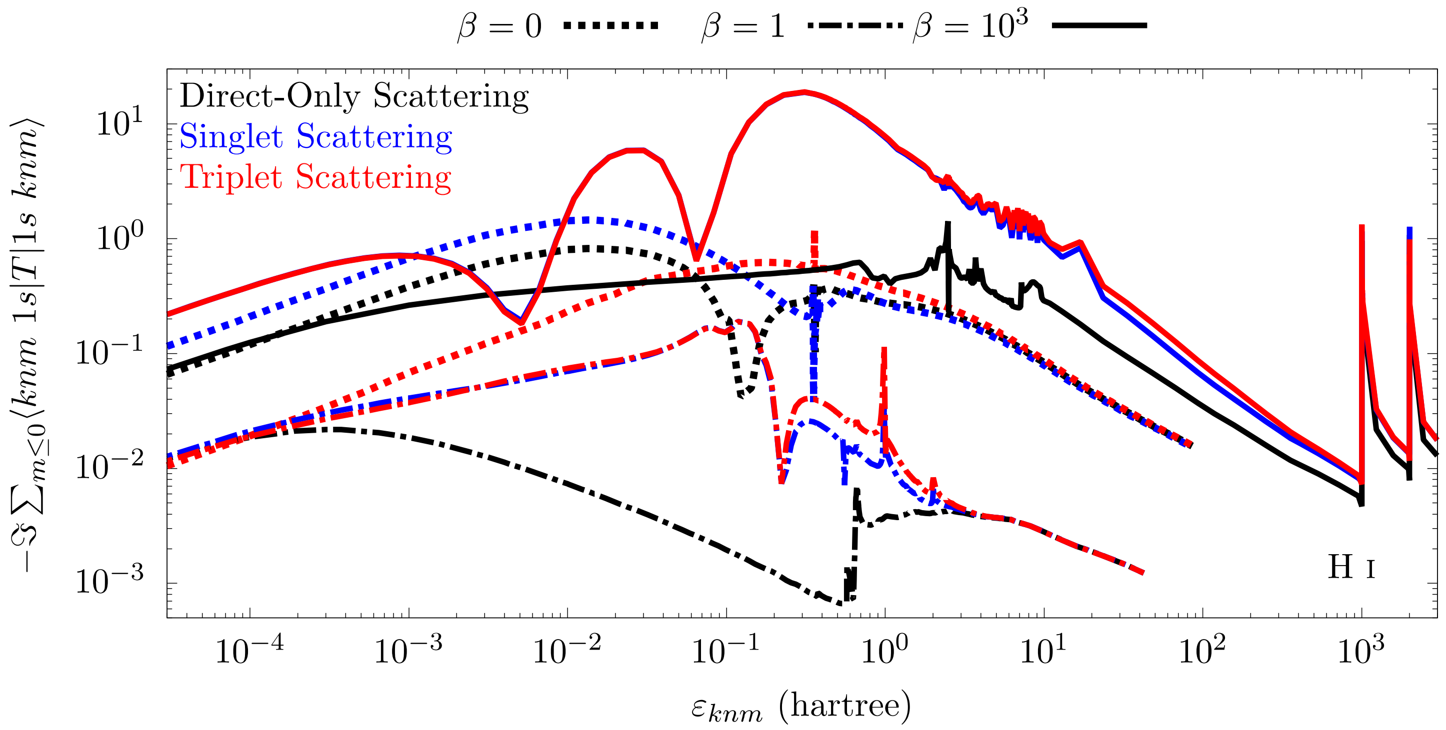


The Effect of Exchange on Collision Cross Sections of Hydrogen

Field-free cross sections are not that different when including the effects of exchange

At moderate fields ($B=2.35 \times 10^5$T), then exchange causes significant increases in the collision cross sections

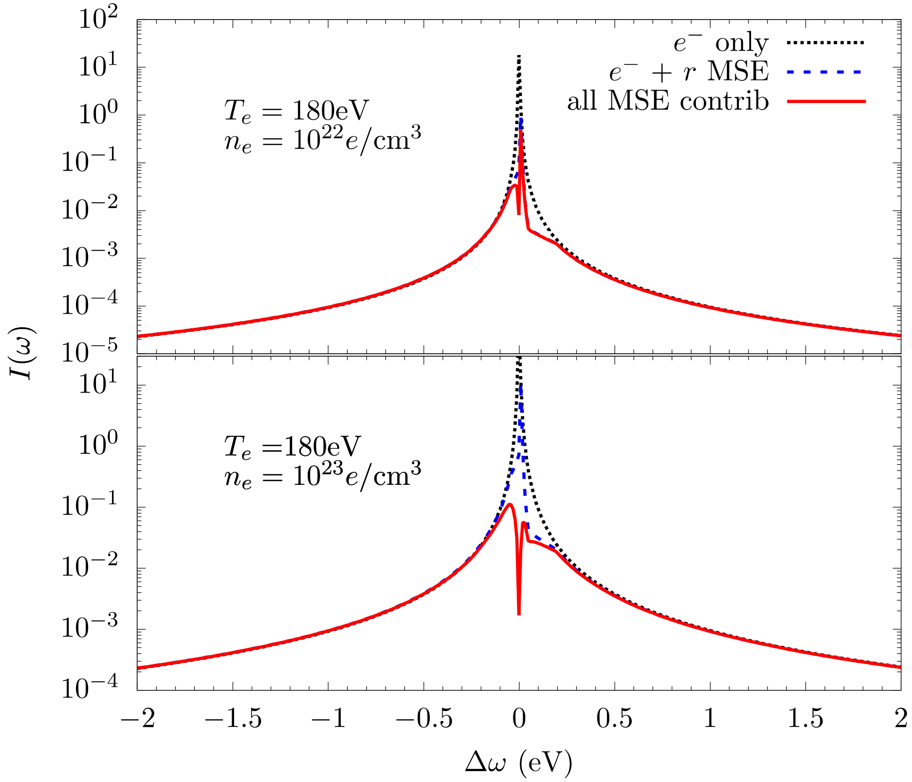
At typical NS fields ($B=2.35 \times 10^8$T), then exchange causes at least an order of magnitude increase of the cross section. The increase covers a larger range of projectile energies



Next Steps for Neutron Star Diagnostics

- Now that exchange is included, we need to now include the motional Stark effect properly [1]
- There are two contributions from the MSE, though only one has been so-far considered
  - The radiator will have an MSE contribution—this was assumed to be dominant broadening mechanism [2]—and is only source that is currently considered
  - The trajectory of the projectile will also be affected by the motion of the nucleus and the motional Stark effect [1].
- A more detailed treatment of the MSE is required

Crude MSE model by [1]

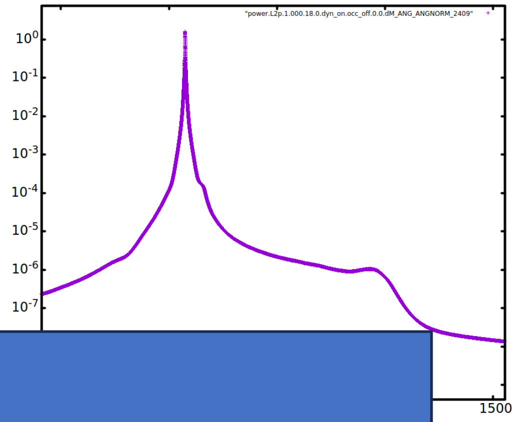


Prospects

- This work has been spurred on by high resolution spectra of Puppis A measured by Chandra
- With the launches of XRISM happening this month, and ARCUS in the planning stages, we can learn much more about neutron star spectra
- This is an exciting time to be starting to explore spectroscopy in magnetic fields

Outline

- Introduction of the WCAPP team
- Line shape primer
- Recent updates by students
  - Penetrating collisions of Ions
  - Carbon line shapes with Simulations
- Magnetic Collisions and Line Shapes
  - Neutron Stars



Thank you!

Questions?