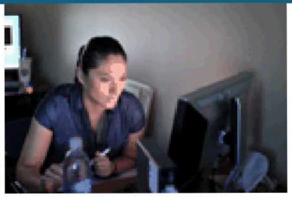
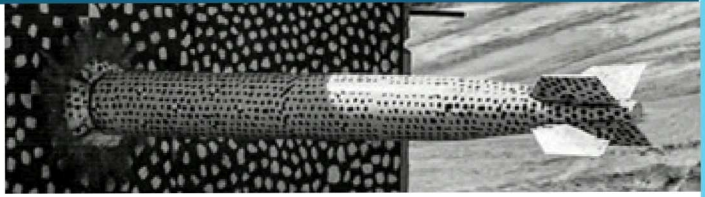
SAND2018-8248C

Challenges and Progress Toward Modeling Carbon/Oxygen White Dwarf Spectra





Thomas Gomez, T. Nagayama, C. Fontes, D. Kilcrease, M. Montgomery, D. Winget

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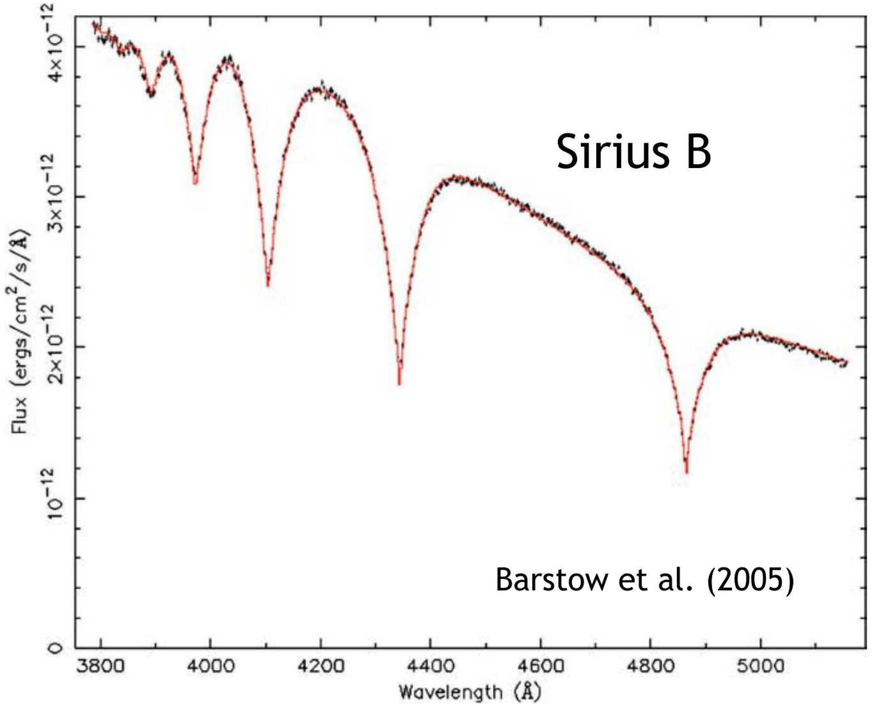
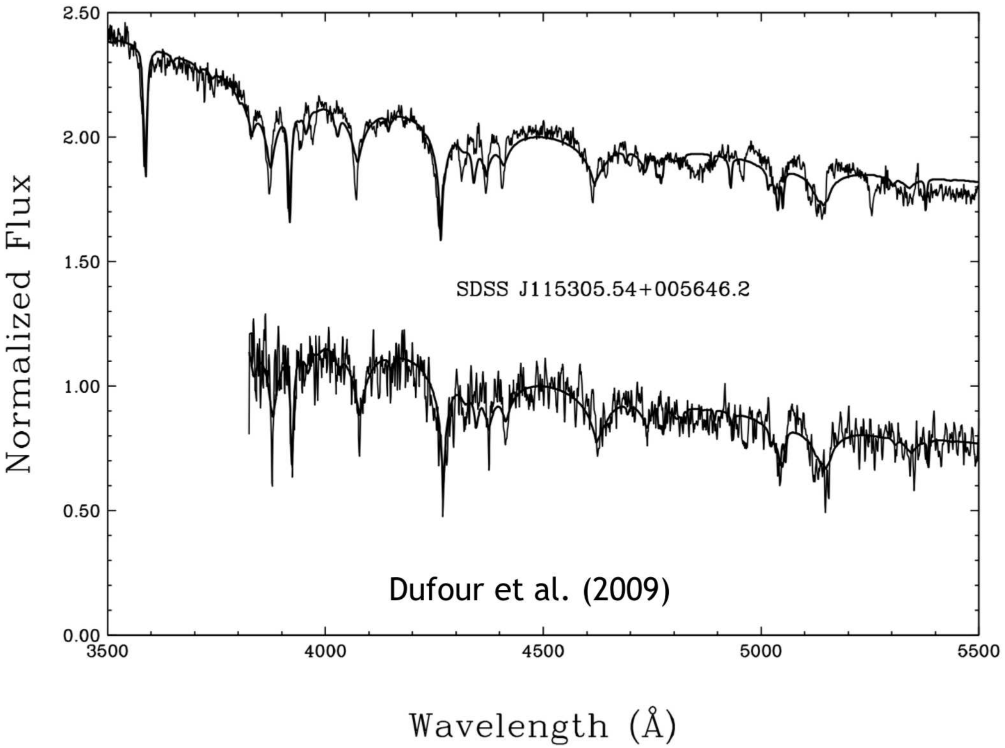
Synthetic Spectra are used to Determine White Dwarf Surface Conditions

Fitting measured spectra with a model can be used to determine surface conditions, such as gravity and temperature…





…Assuming that we know all of the relevant physics

Structure of the atmosphere

- Temperature
- Density

And at every level in the atmosphere we need necessary atomic data

- Atomic energy levels
- Atomic oscillator strengths
- Atomic populations
- The line broadening

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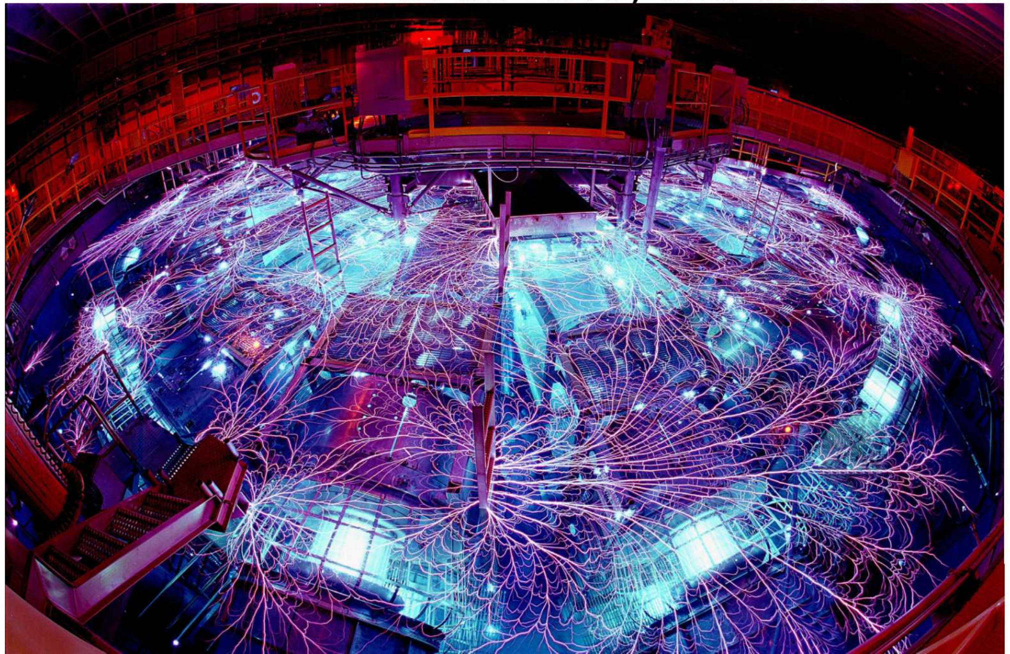
These parameters can be measured in the laboratory (e.g. Wiese et al. 1972; Falcon et al. 2015) and can be constrained



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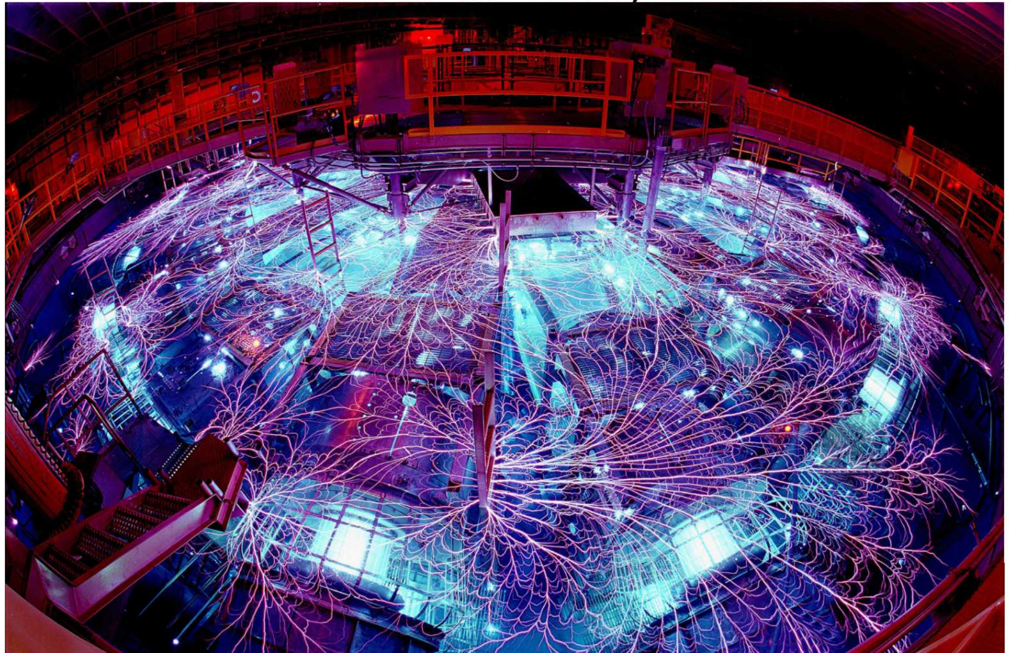
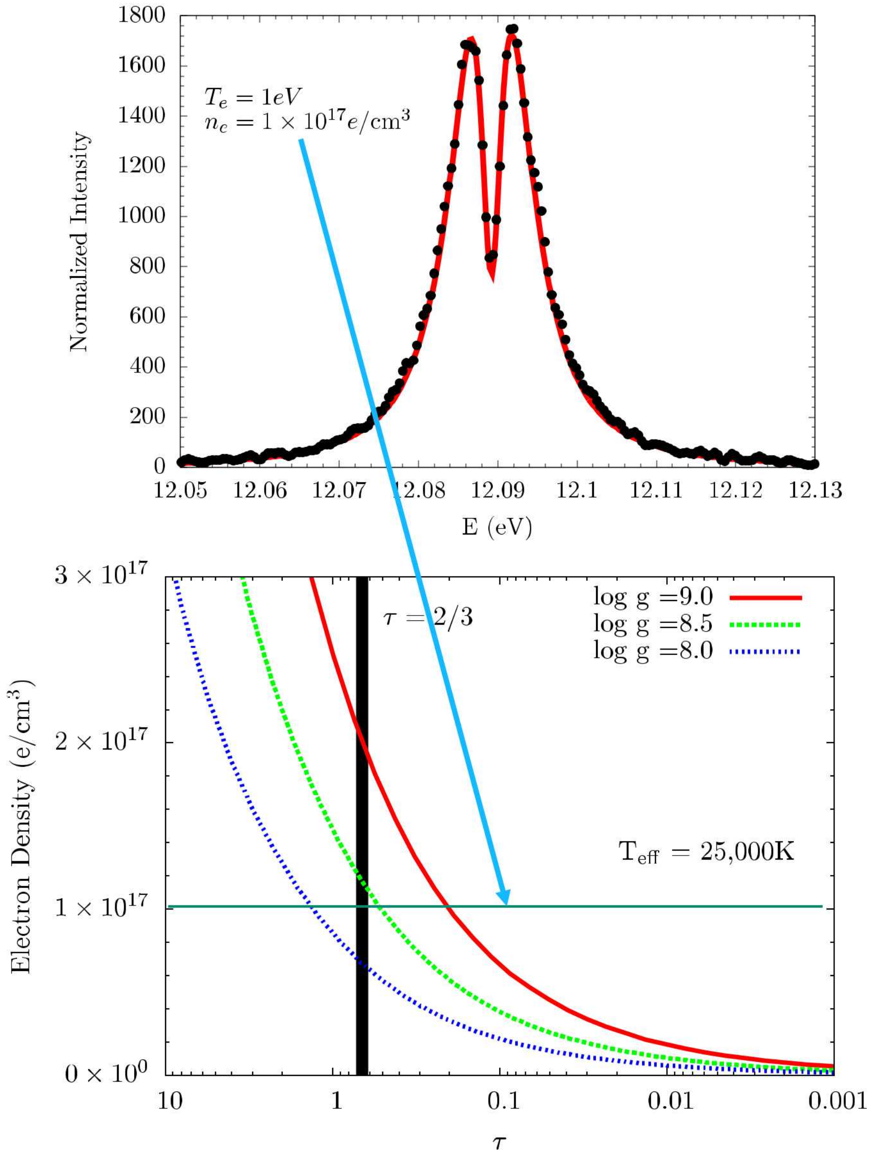


Line Broadening Models are used to Calculate Synthetic Spectra of White Dwarfs



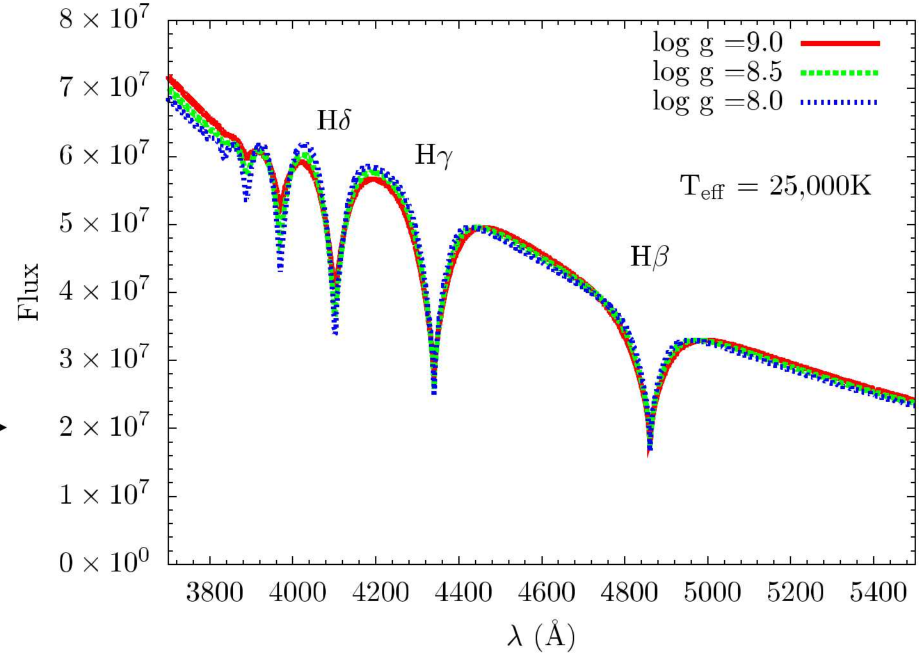
Spectral Line Shape at Different Plasma Conditions

Then Integrated over the different plasma conditions in the atmospheres Give the emergent Spectra

Probably the most direct application of line broadening by astronomers is to determine log g and T_{eff}

The reason for this is that

- line broadening is sensitive to the density
- Density is sensitive to gravity



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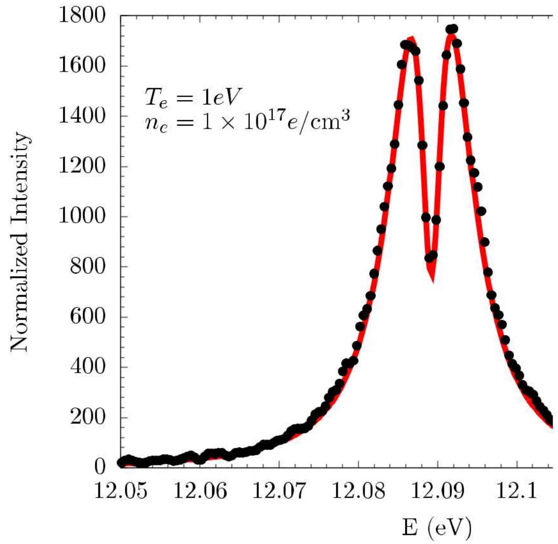

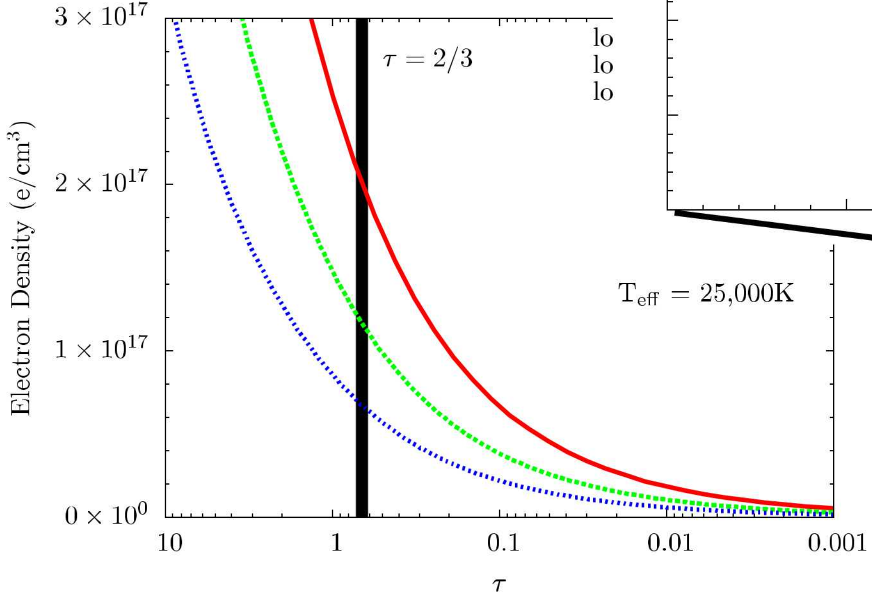

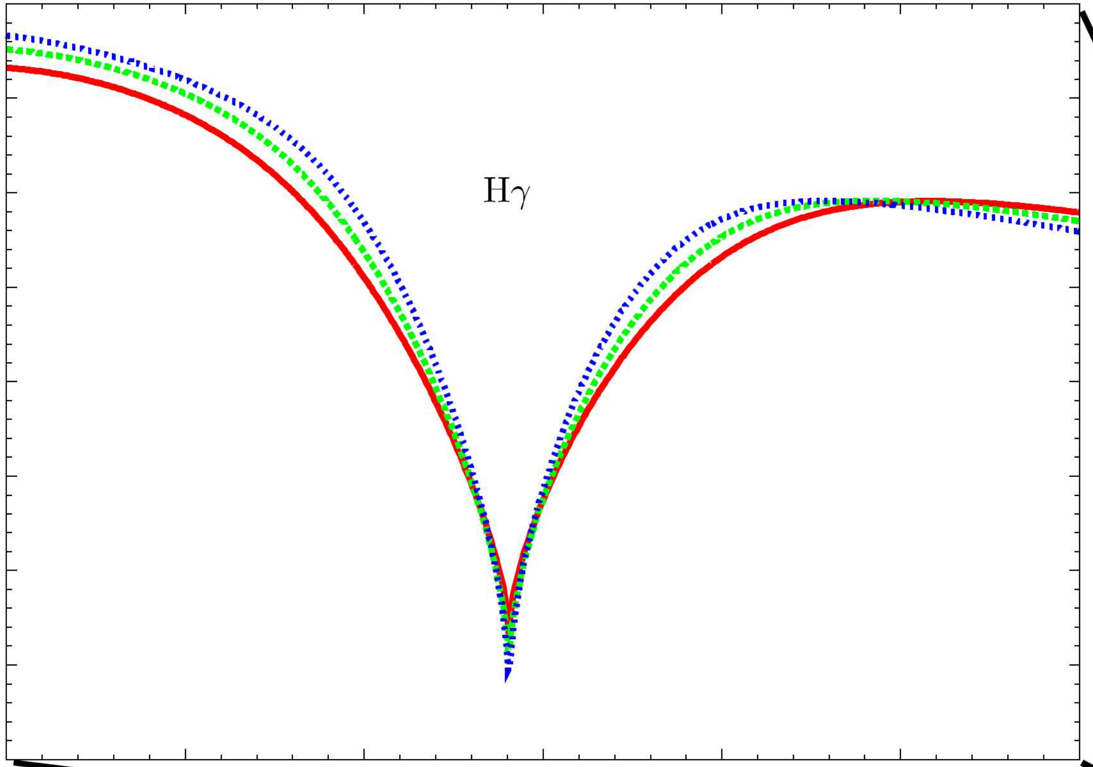

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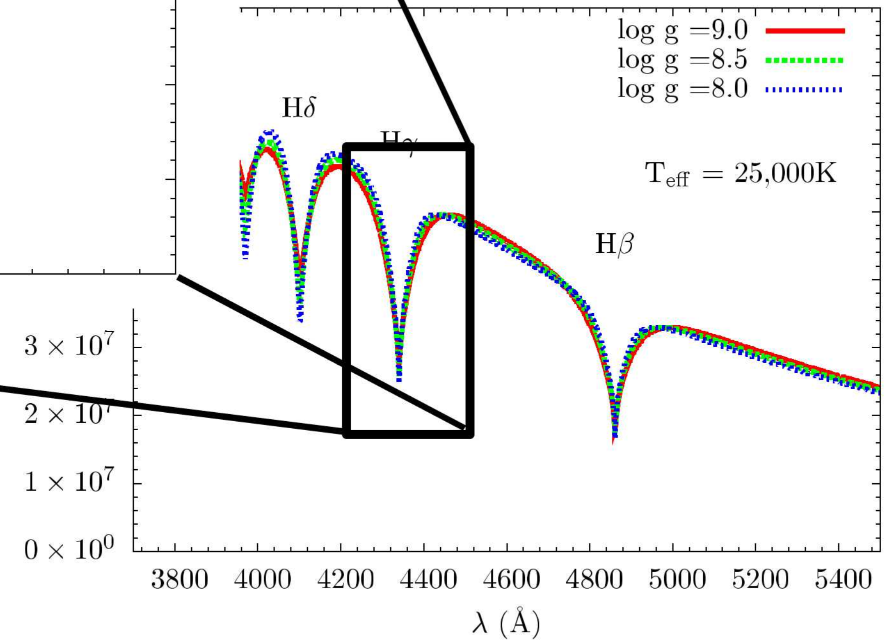
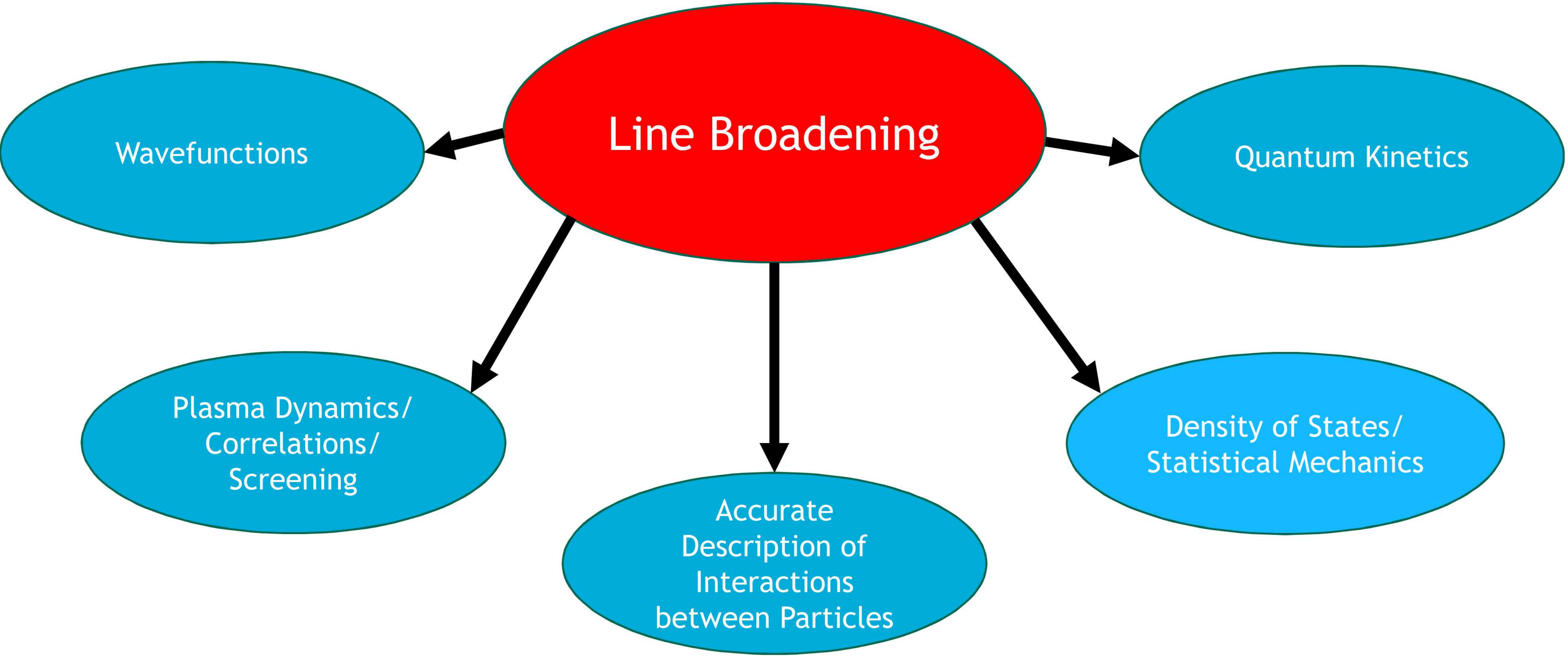


Line-Broadening Requires Multi-Disciplinary knowledge



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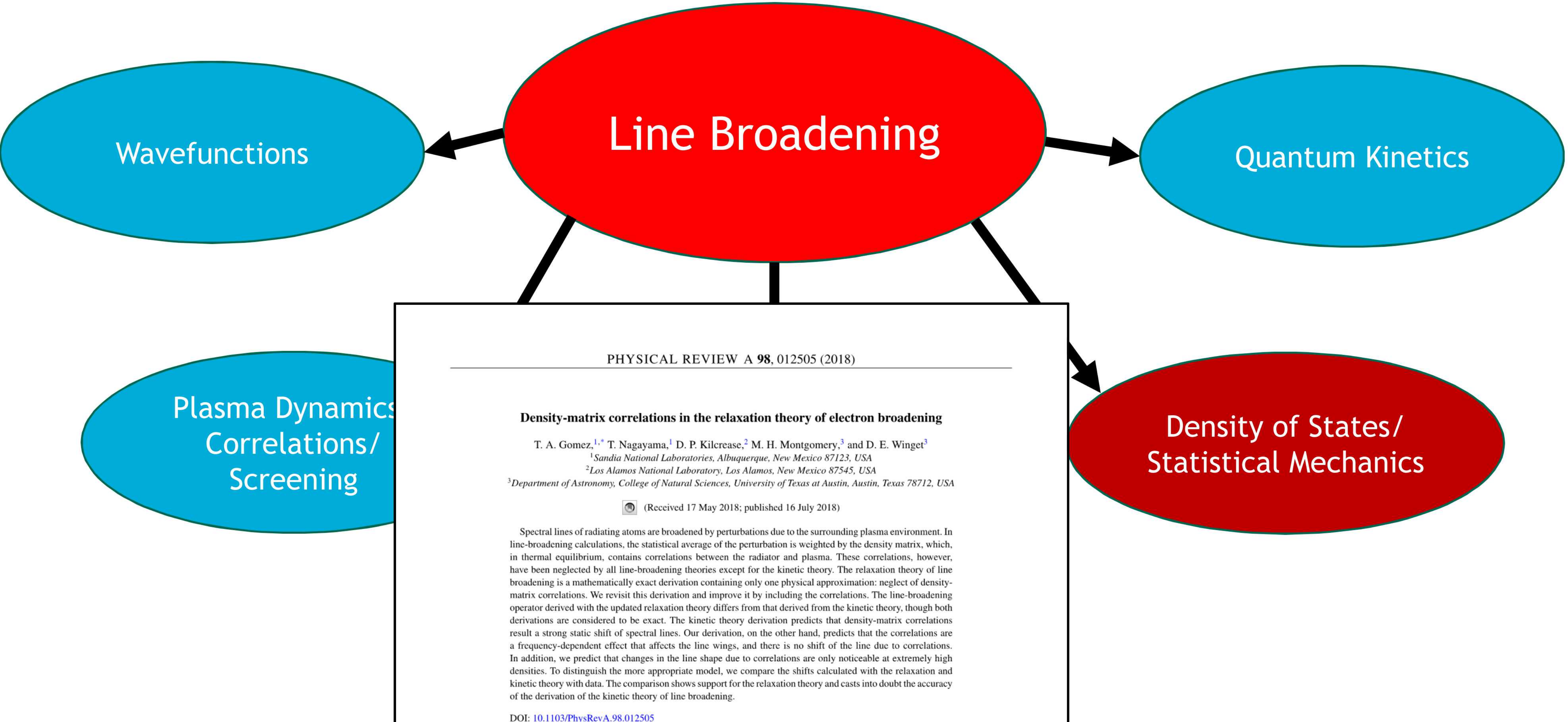

PHYSICAL REVIEW A **98**, 012505 (2018)

Density-matrix correlations in the relaxation theory of electron broadening

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(Received 17 May 2018; published 16 July 2018)

Spectral lines of radiating atoms are broadened by perturbations due to the surrounding plasma environment. In line-broadening calculations, the statistical average of the perturbation is weighted by the density matrix, which, in thermal equilibrium, contains correlations between the radiator and plasma. These correlations, however, have been neglected by all line-broadening theories except for the kinetic theory. The relaxation theory of line broadening is a mathematically exact derivation containing only one physical approximation: neglect of density-matrix correlations. We revisit this derivation and improve it by including the correlations. The line-broadening operator derived with the updated relaxation theory differs from that derived from the kinetic theory, though both derivations are considered to be exact. The kinetic theory derivation predicts that density-matrix correlations result a strong static shift of spectral lines. Our derivation, on the other hand, predicts that the correlations are a frequency-dependent effect that affects the line wings, and there is no shift of the line due to correlations. In addition, we predict that changes in the line shape due to correlations are only noticeable at extremely high densities. To distinguish the more appropriate model, we compare the shifts calculated with the relaxation and kinetic theory with data. The comparison shows support for the relaxation theory and casts into doubt the accuracy of the derivation of the kinetic theory of line broadening.

DOI: 10.1103/PhysRevA.98.012505

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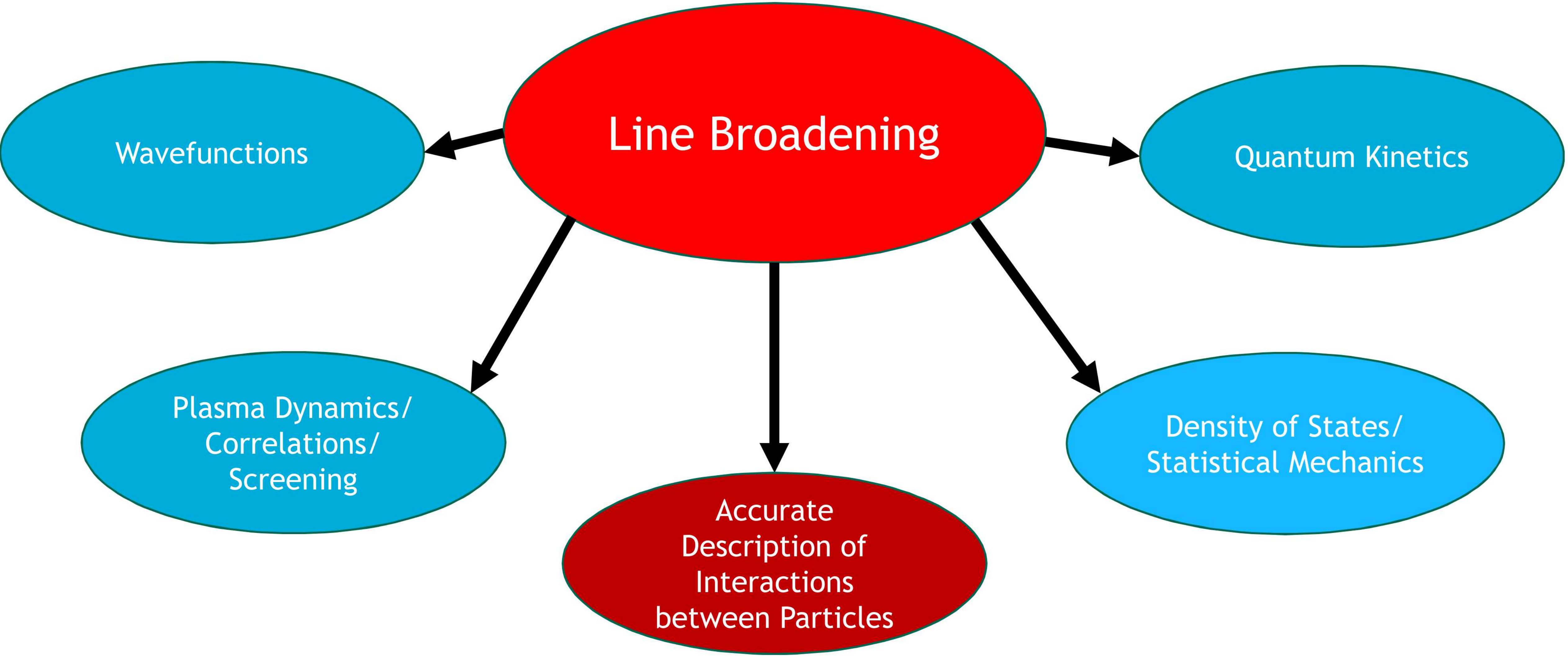
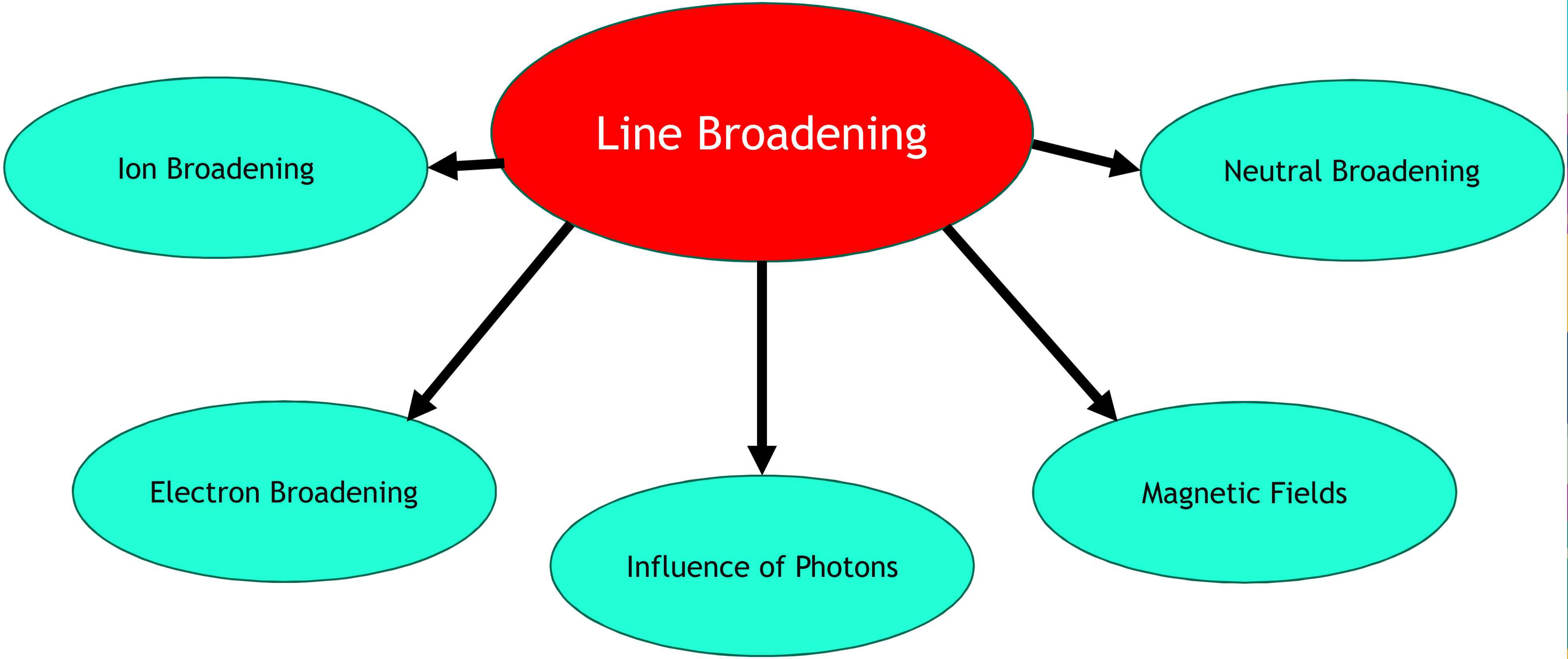


There are many Different Mechanisms that can Broaden Spectral Lines



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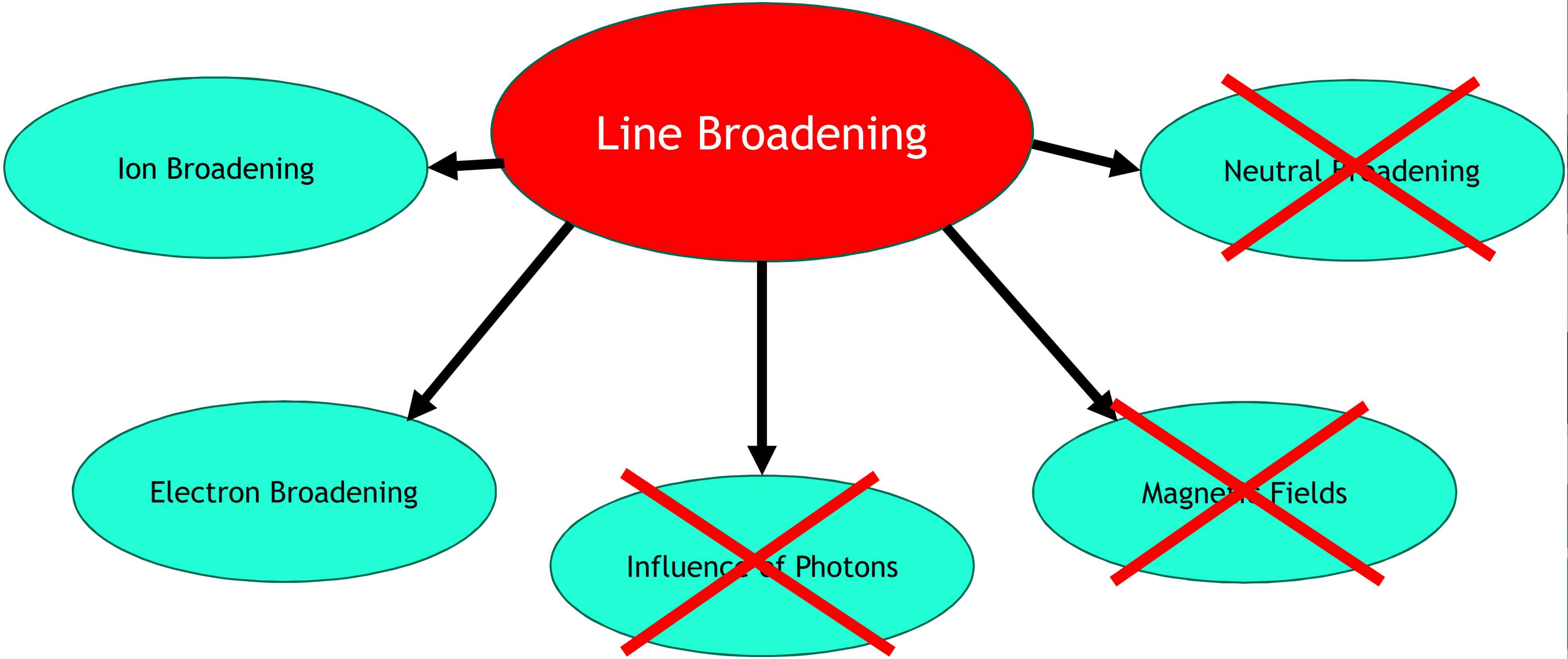

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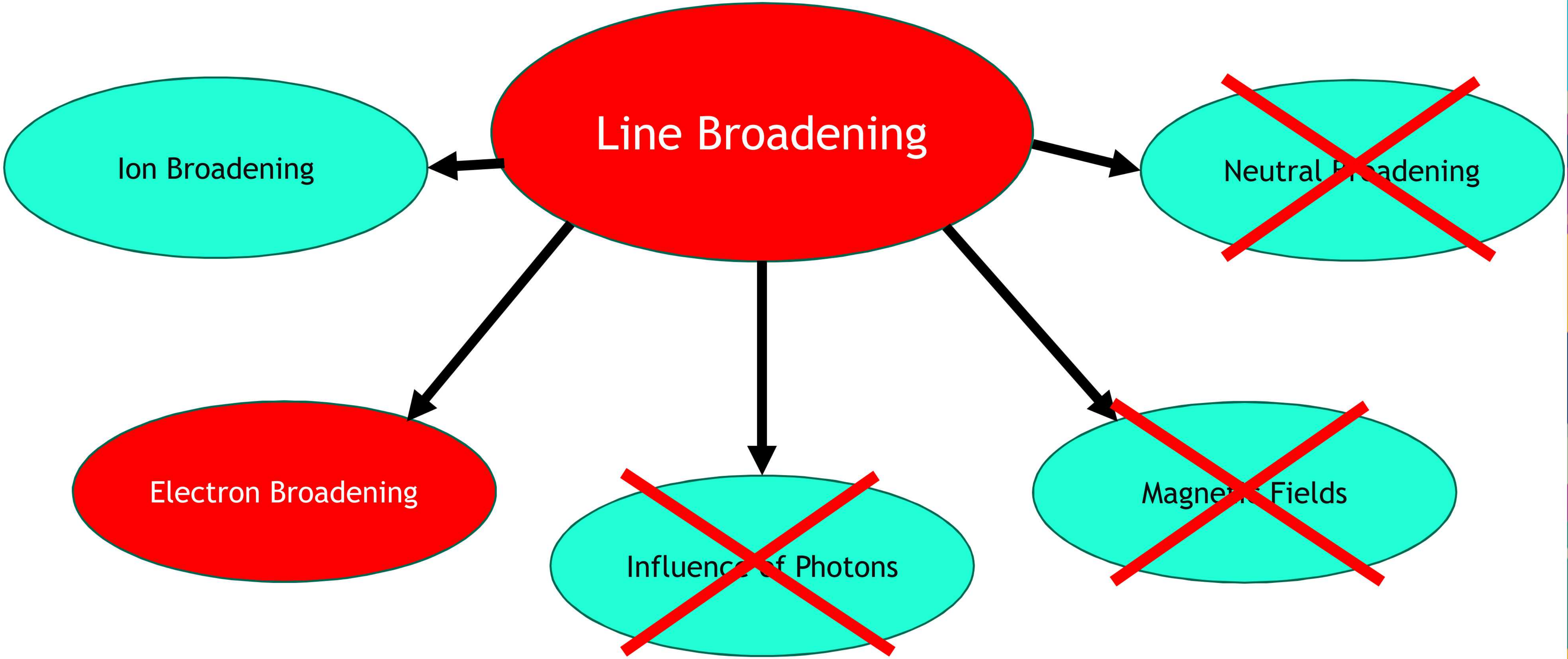

Broadening of Multi-Electron atoms is incomplete

Multi-Electron Atoms

Any atom that has more than one bound electron is considered a multi-electron atom

The simplest are those with one valence electron: Li-like, Na-like, K-like, etc.

The next simplest are those with closed *l* shells and one electron in an open shell: B-like, Al-like

The most complex are with more than one electron in open shells

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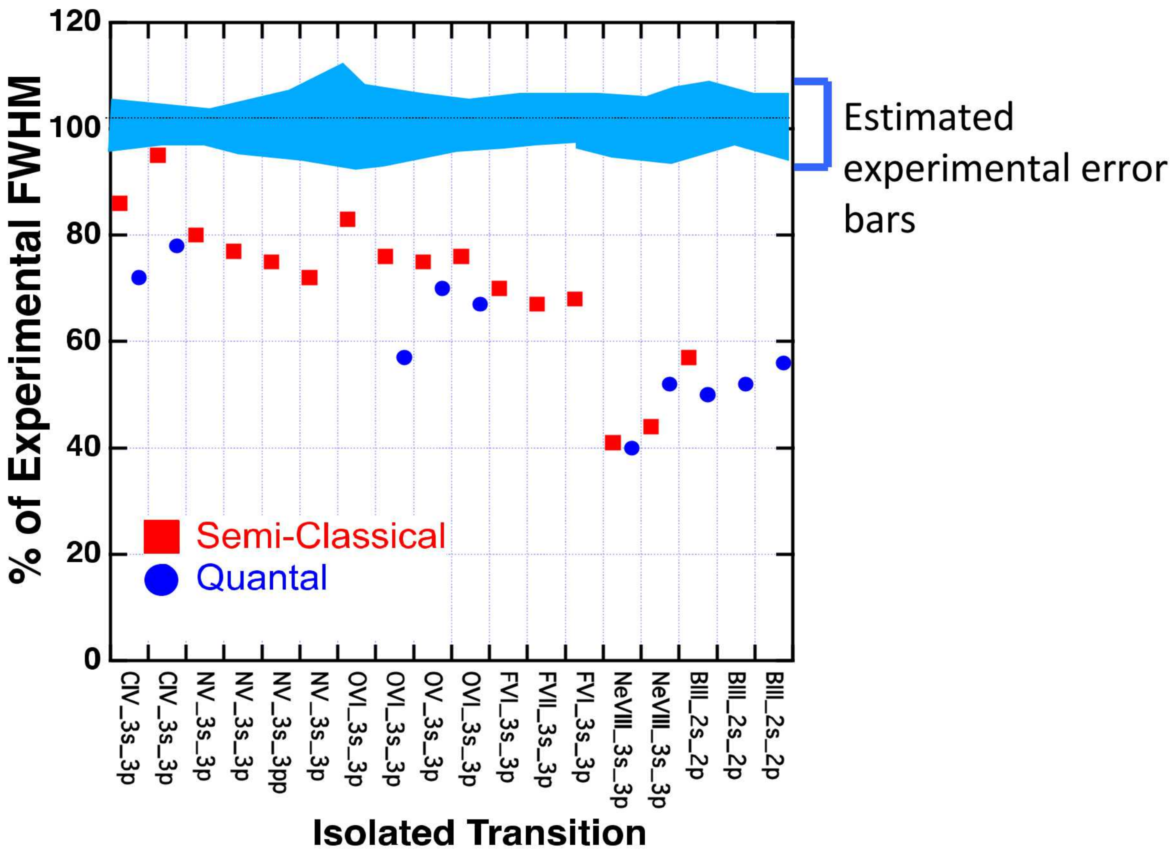
We ***DO NOT*** Understand the Broadening of the Simplest Multi-Electron Atoms

Calculations Cannot Match Line-Width Measurements for 3-Electron Atoms



Lee, Private Communication

There are measurements of 3-electron atoms with independent plasma diagnostics

Current *ab-initio* calculations of line broadening of simple 3-electron atoms currently cannot match measured widths

- Factor of two in some cases

Current *semi-empirical* calculations fare better

- uncertain within 20-30% for these lines.

Discrepancy is worse with large energy separation between states

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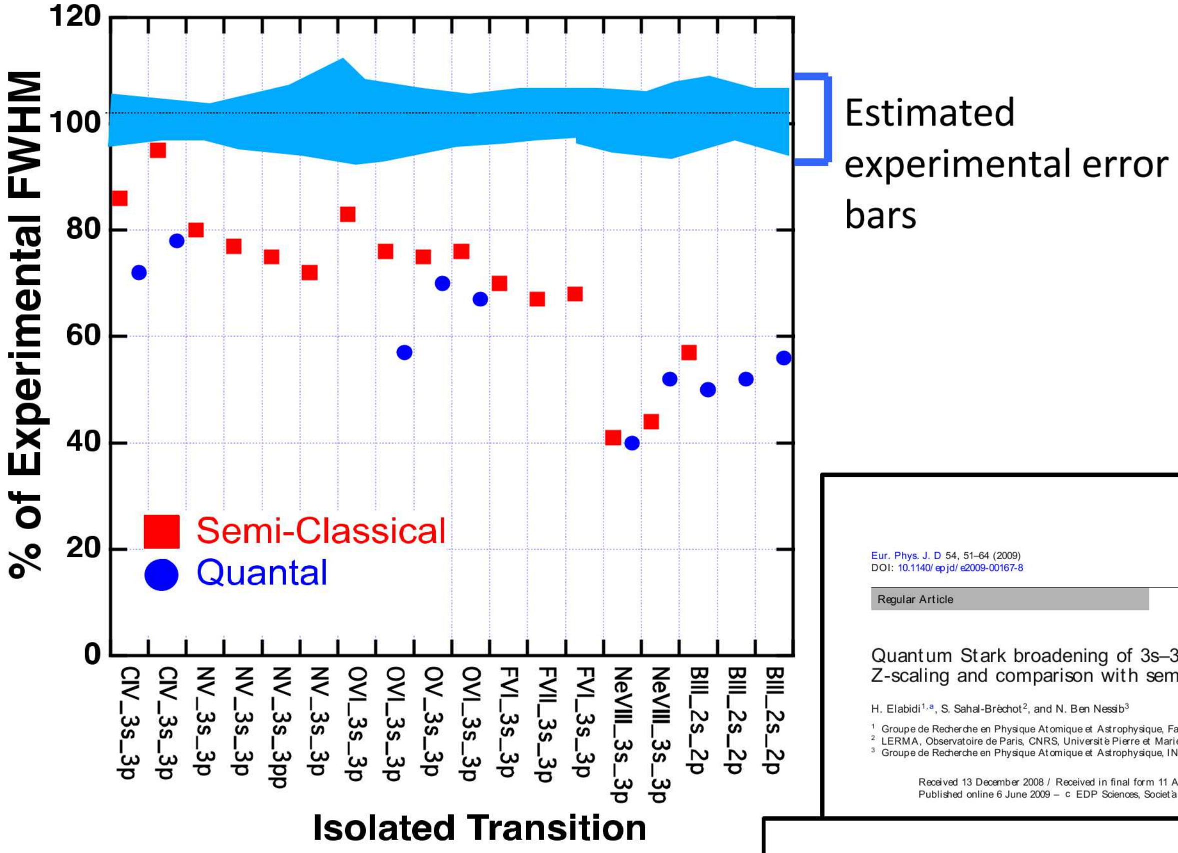

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Current *ab-initio* calculations of line broadening of simple 3-electron atoms currently cannot match measured widths

This is known as the isolated-line problem and has led to a decades-long investigation

Things to Consider for Electron Broadening

Size of Atomic Basis set

Accuracy of Atomic Wavefunctions

Density of States/Populations

Description of Plasma Electrons
- Classical
- Quantum
  - Exchange

Interaction between Atom and Plasma
- Dipole Approximation
- Coulomb Interaction

Collision Treatment
- Coulomb-Born
- Distorted-Wave
- CCC

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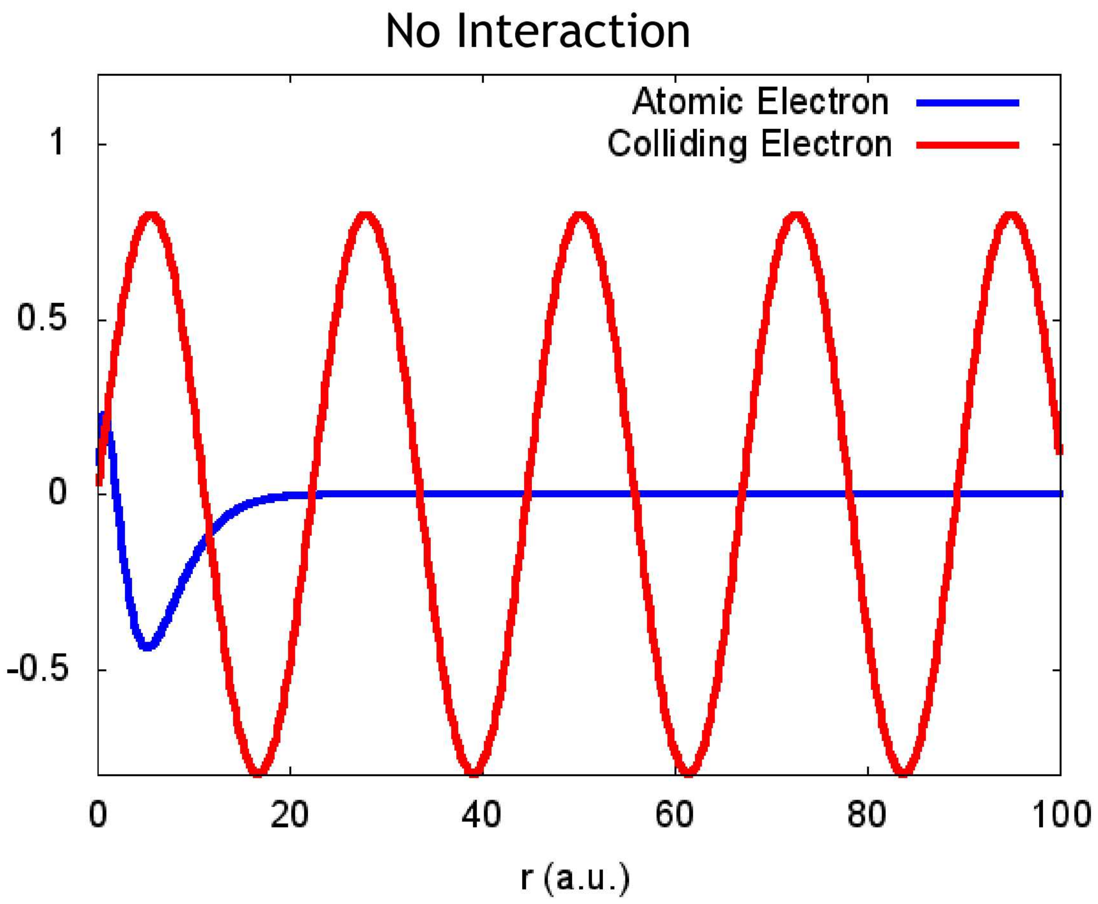
Wavefunction Time Evolution

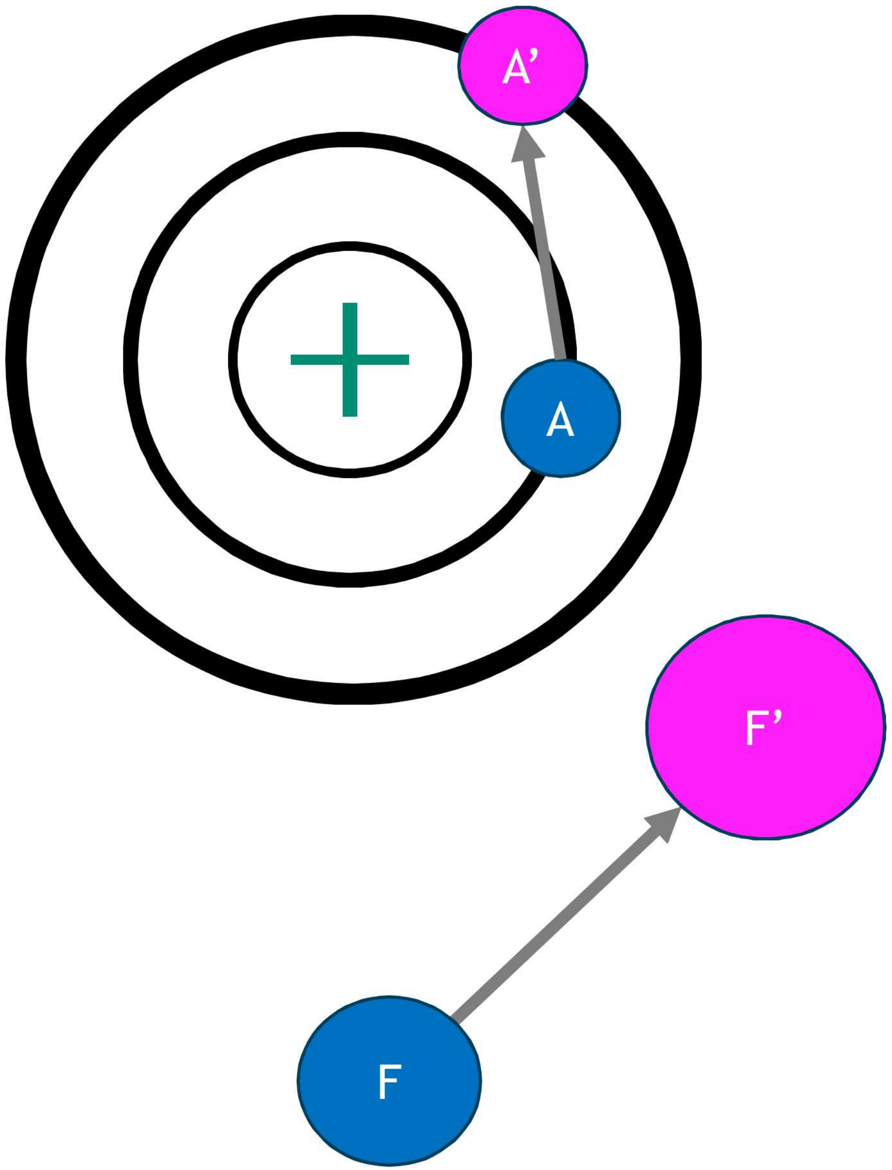


Direct Interactions are Straightforward

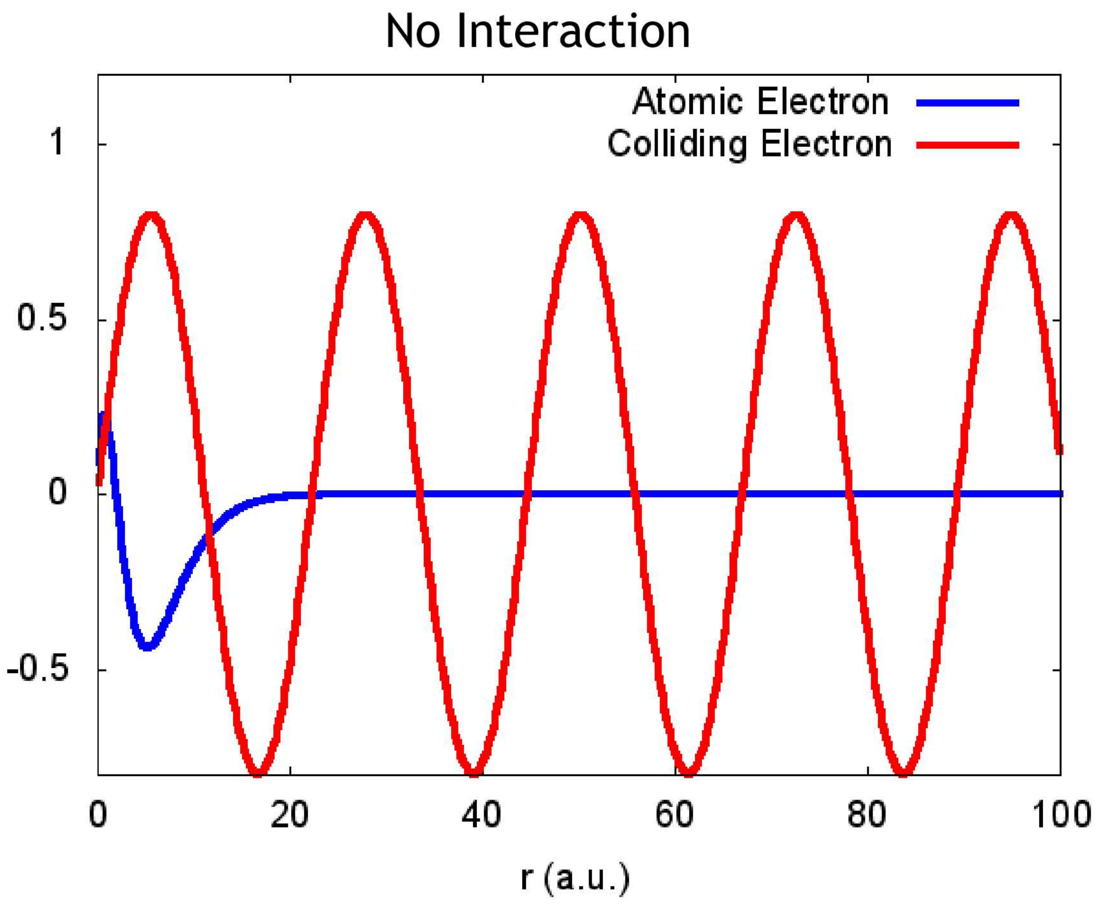
This type of interaction is where the atom and electrons change states

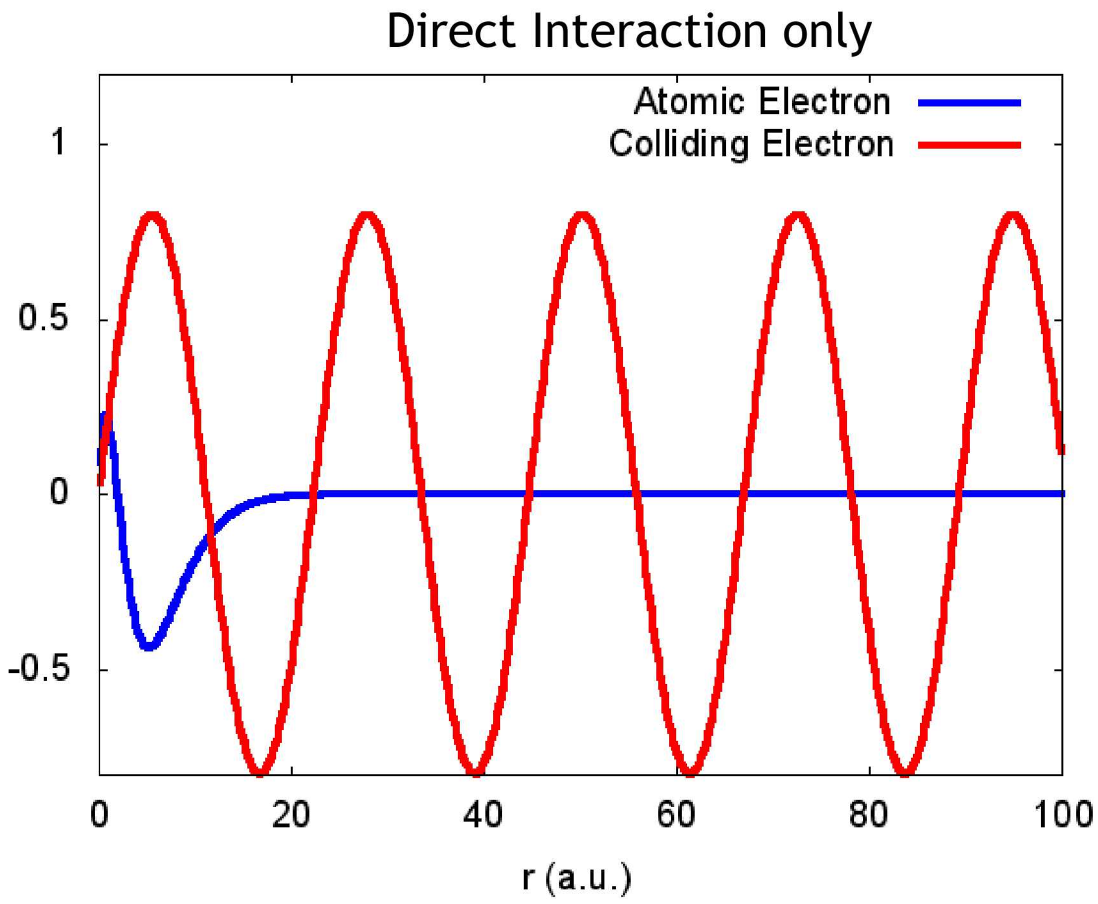
But the atomic electron remains the atomic electron and the free electron remains the free electron

This interaction is usually well modeled because of the simple interactions involved



Wavefunction Time Evolution With Interactions

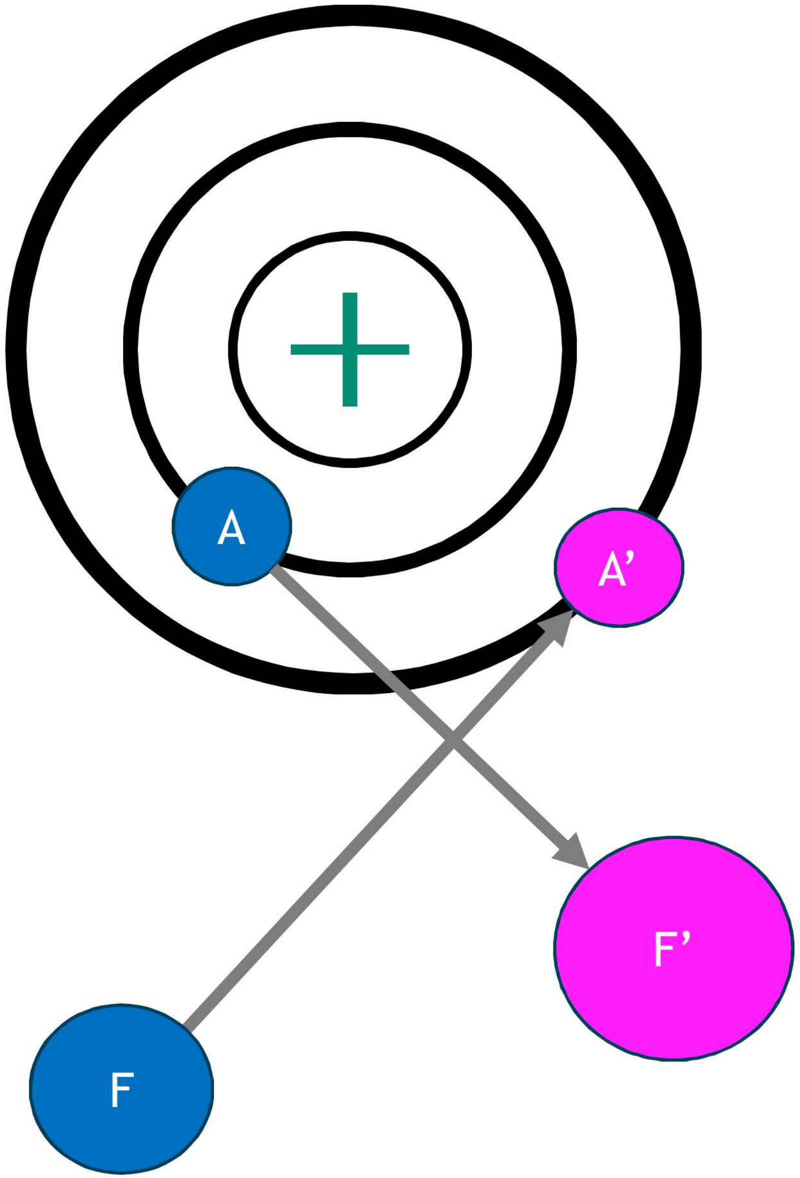




Exchange Interactions

The atomic electron can exchange places with the free electron and change states in this way

This adds some complexity to the calculation, but is manageable



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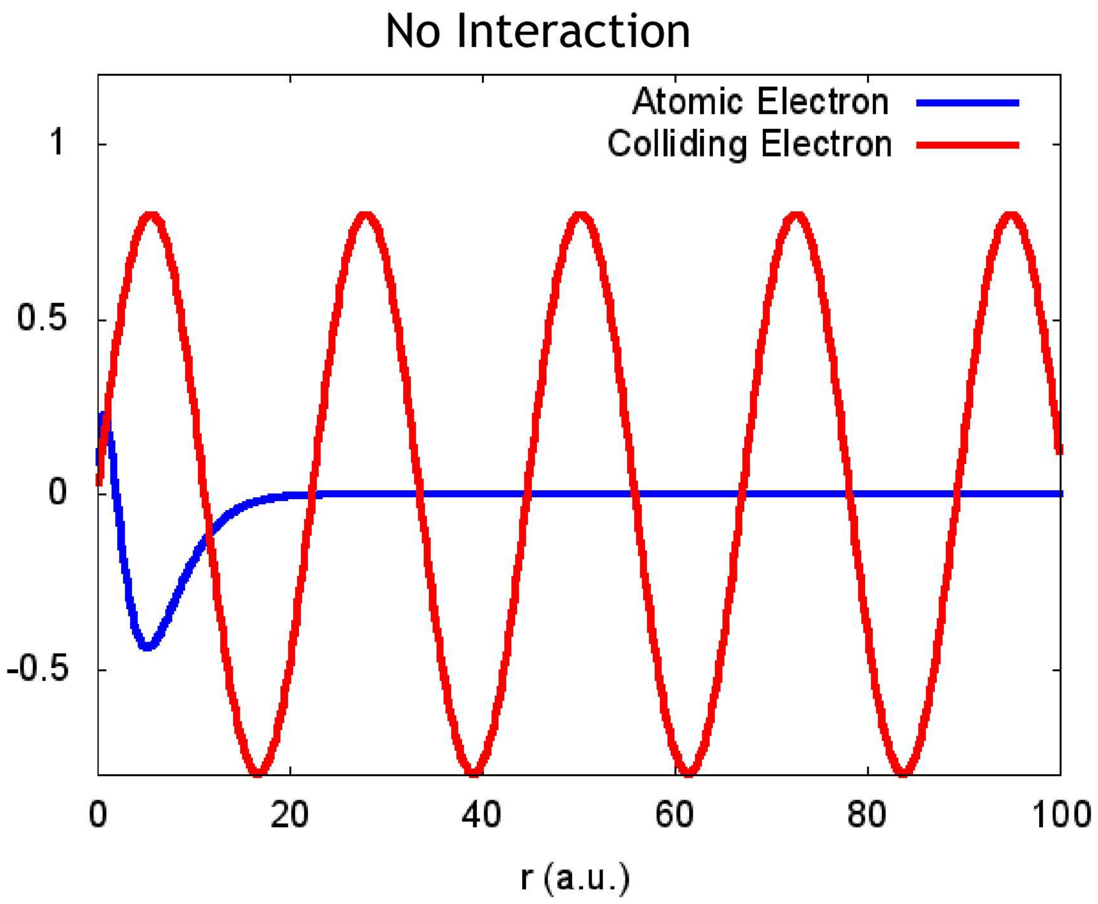
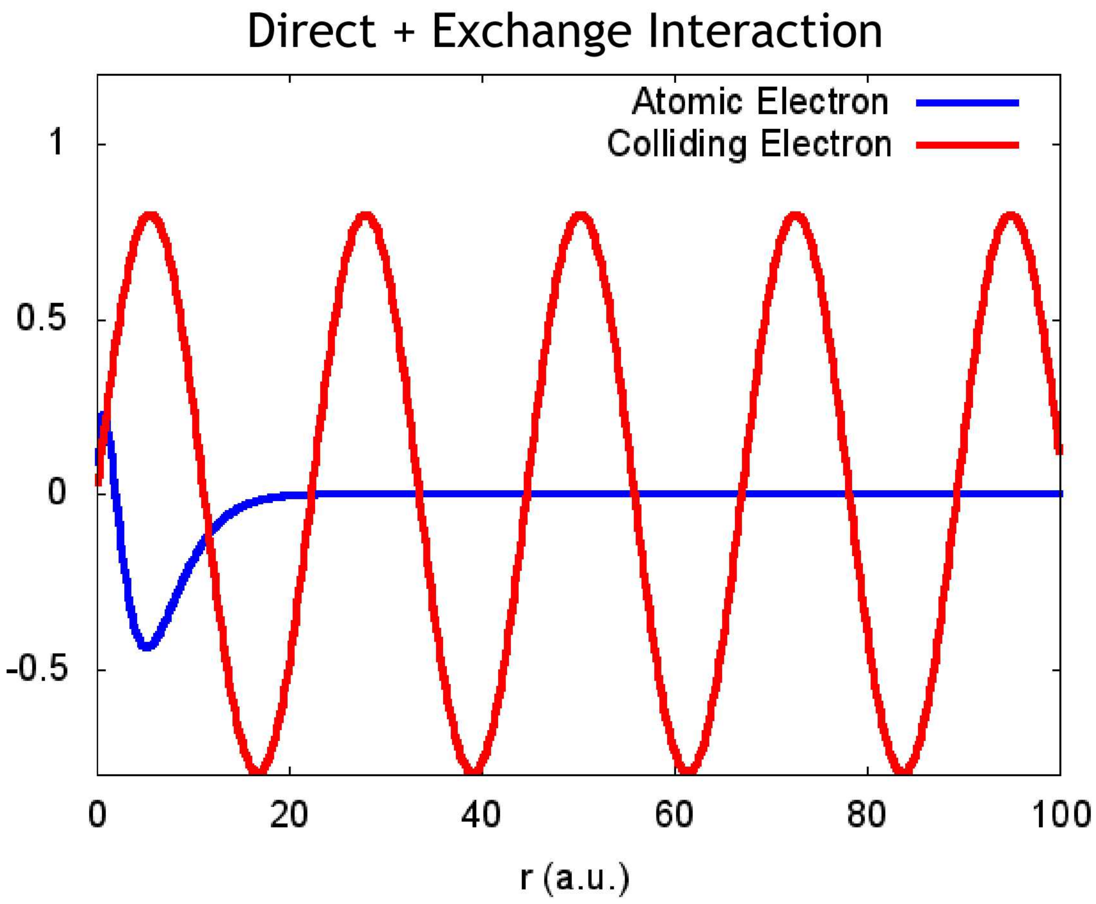


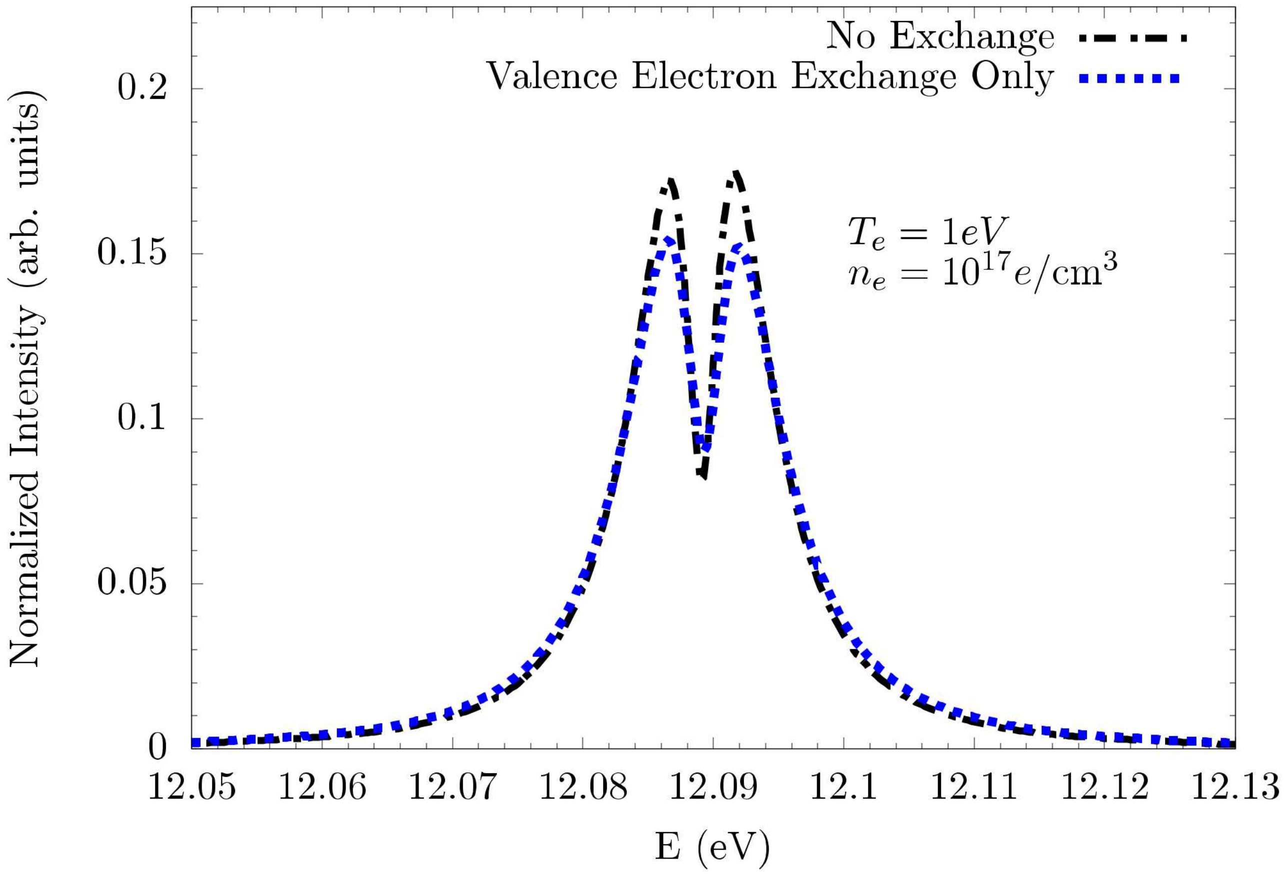


Exchange is Important Even for Hydrogen

One might be led to the conclusion that because hydrogen spectra is accurately modeled by semi-classical methods that exchange is unimportant

But this is not true in the slightest

Exchange can add substantial broadening for hydrogen



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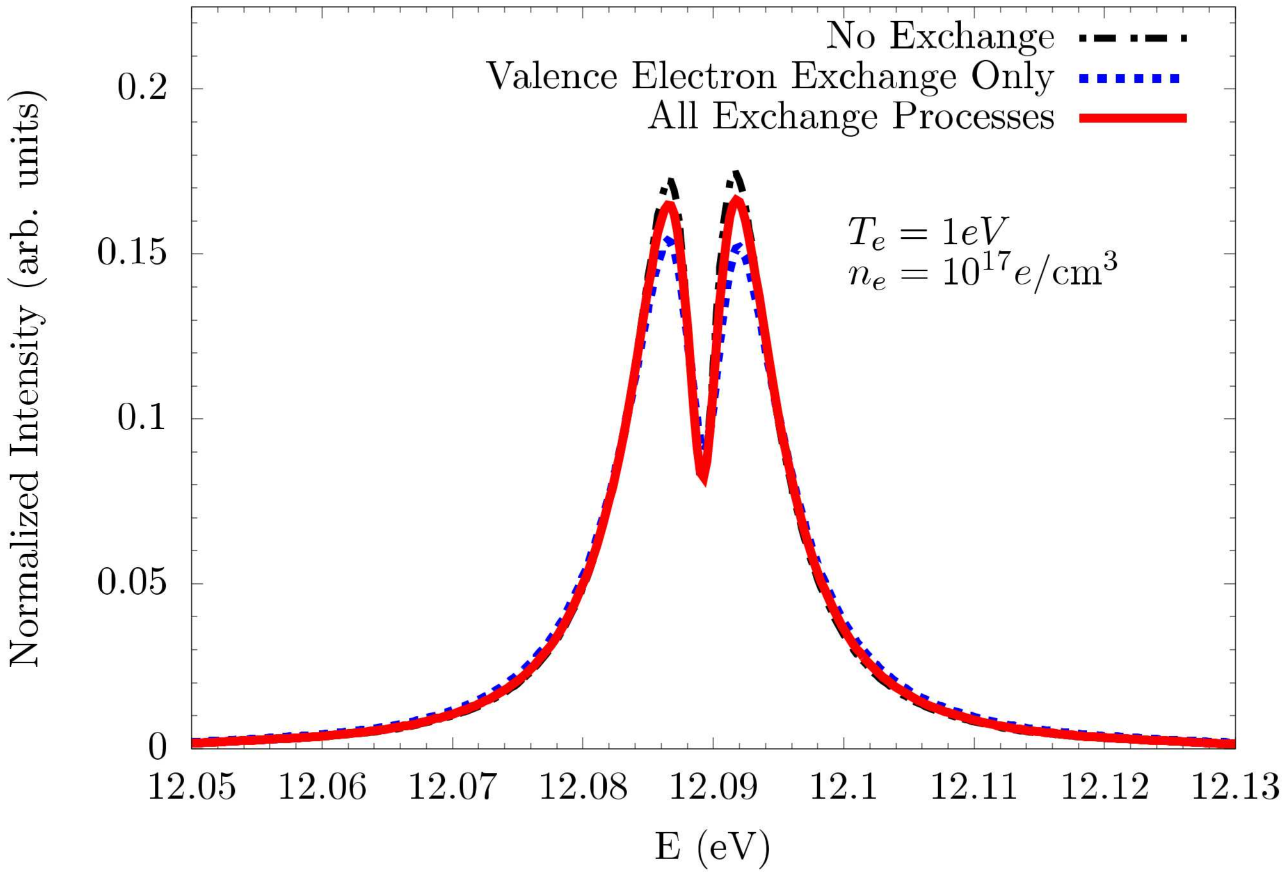
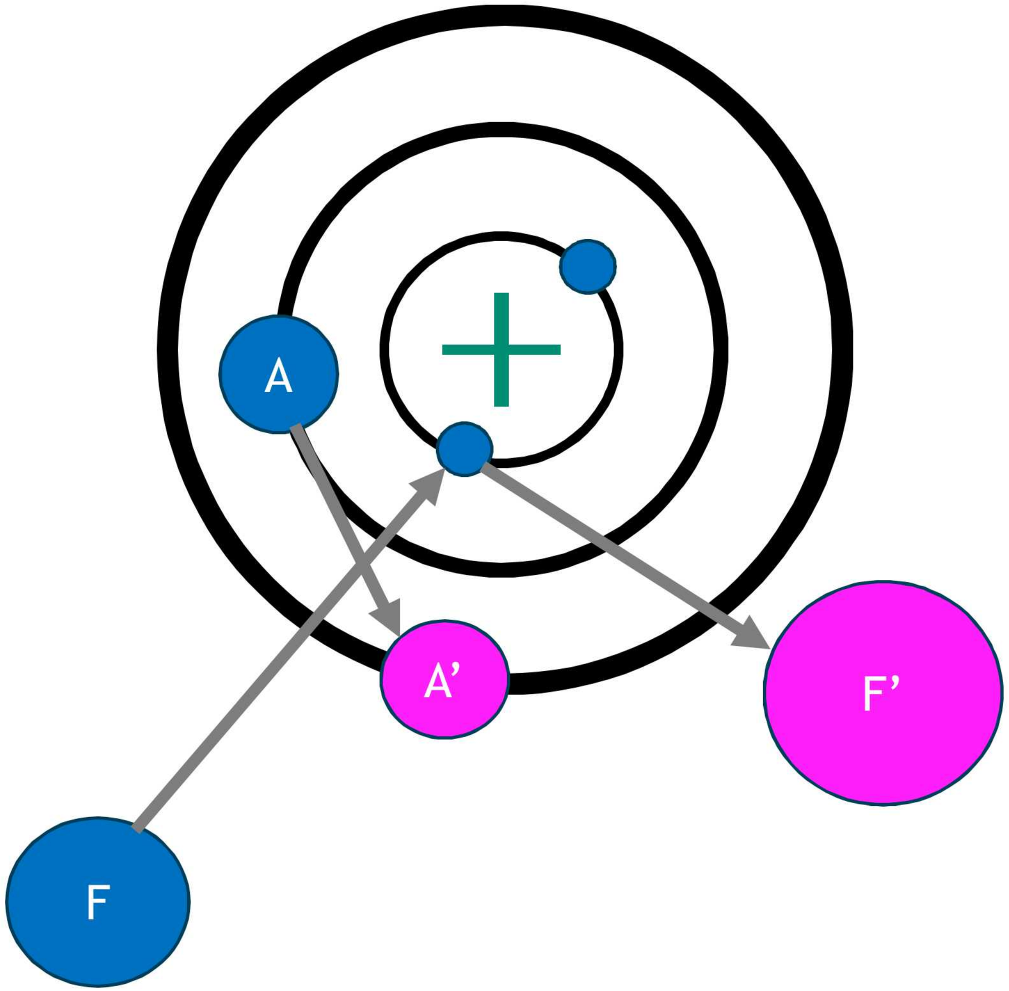
But because exchange can also occurs with nuclear interactions, the effect of exchange is largely cancelled for hydrogen



Exchange Interactions for Multi-Electron Atoms

Seaton (1953) laid out the relevant exchange processes in collisions

These include not only two-body exchange, but three-body exchange as well (assuming atomic wavefunctions are roughly orthogonal)



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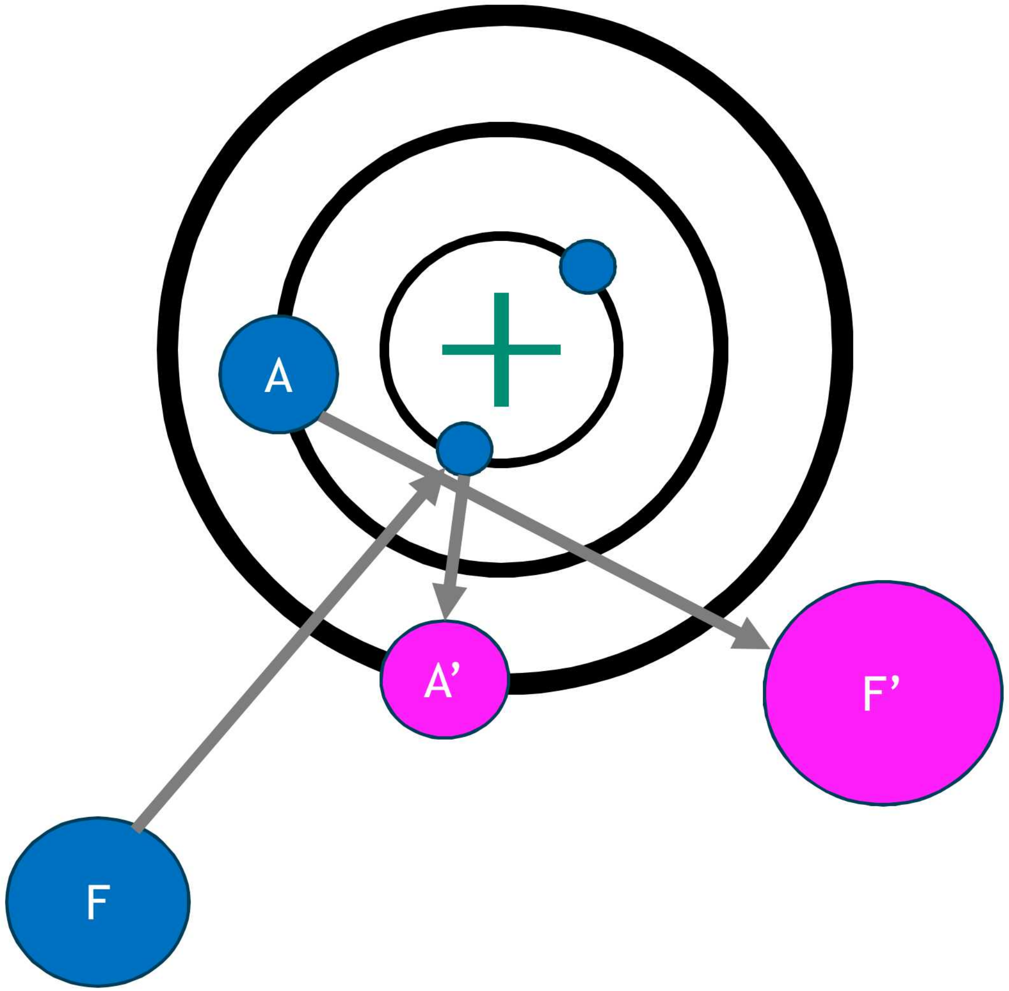

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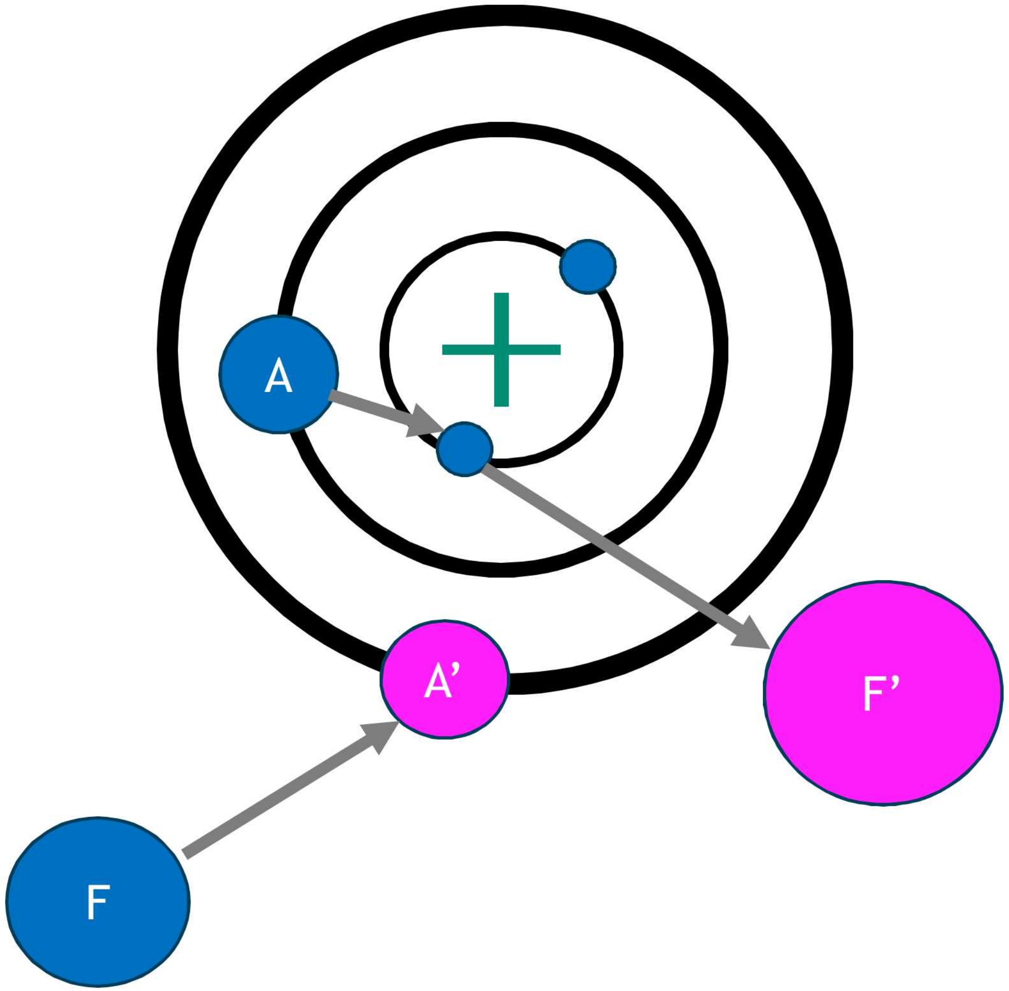

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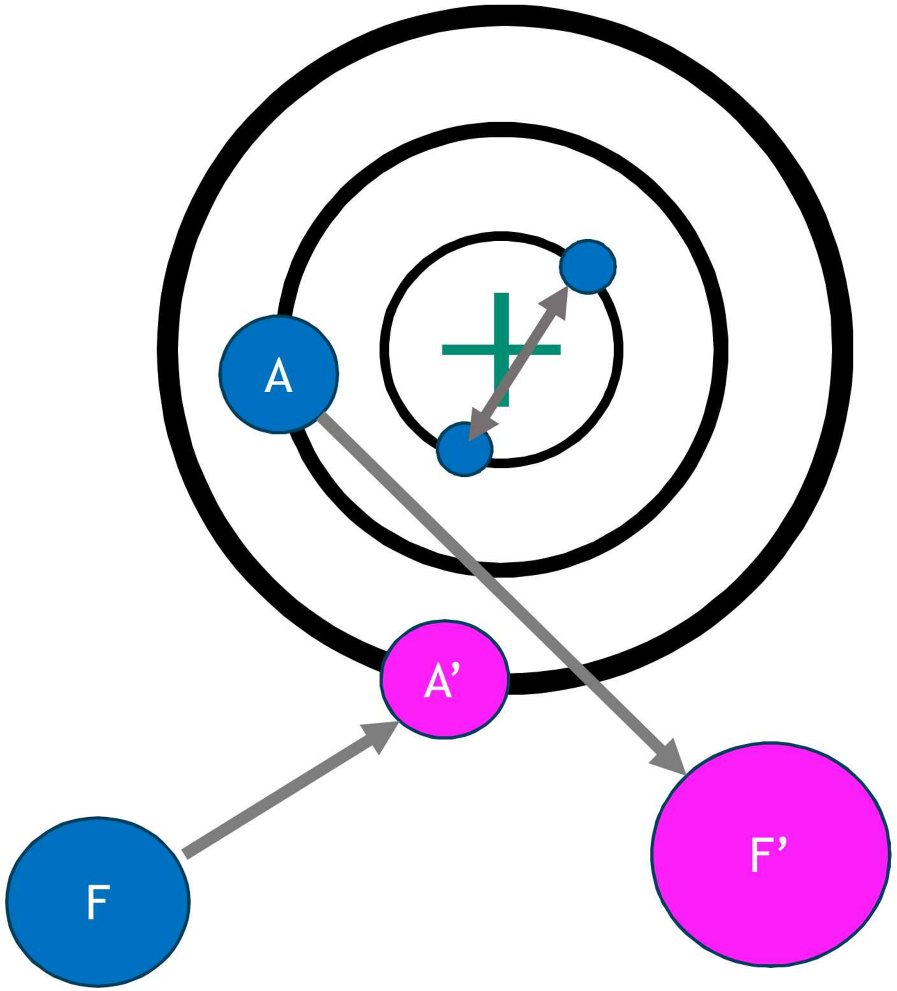
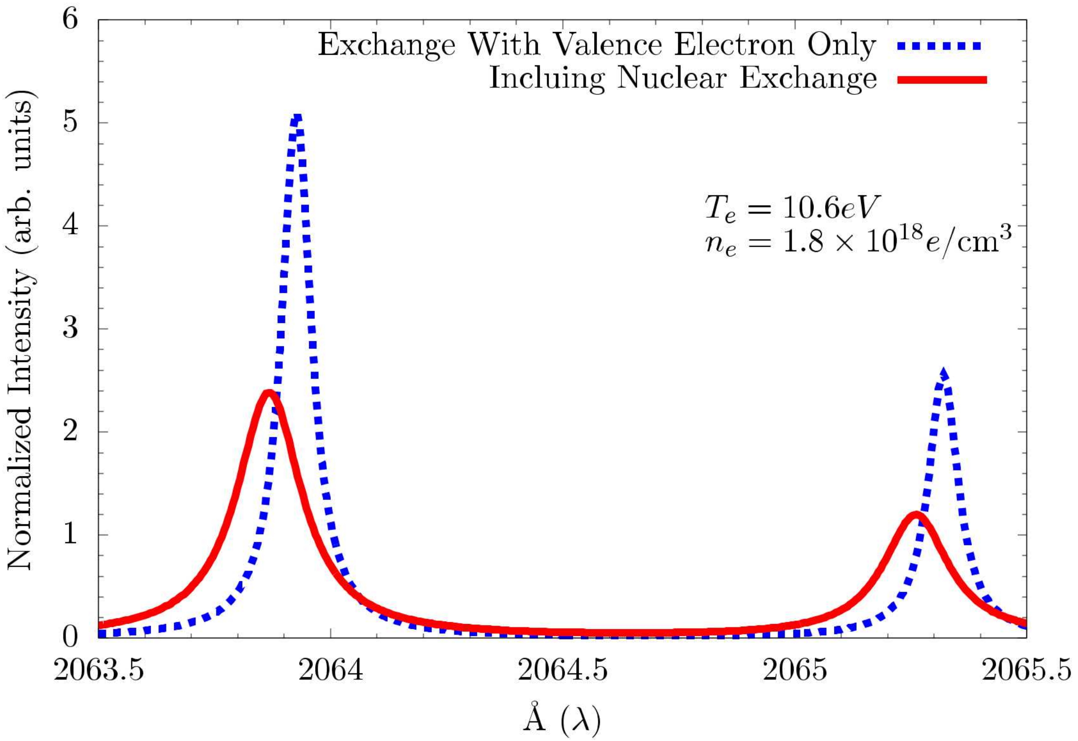


These Exchange Terms are Large

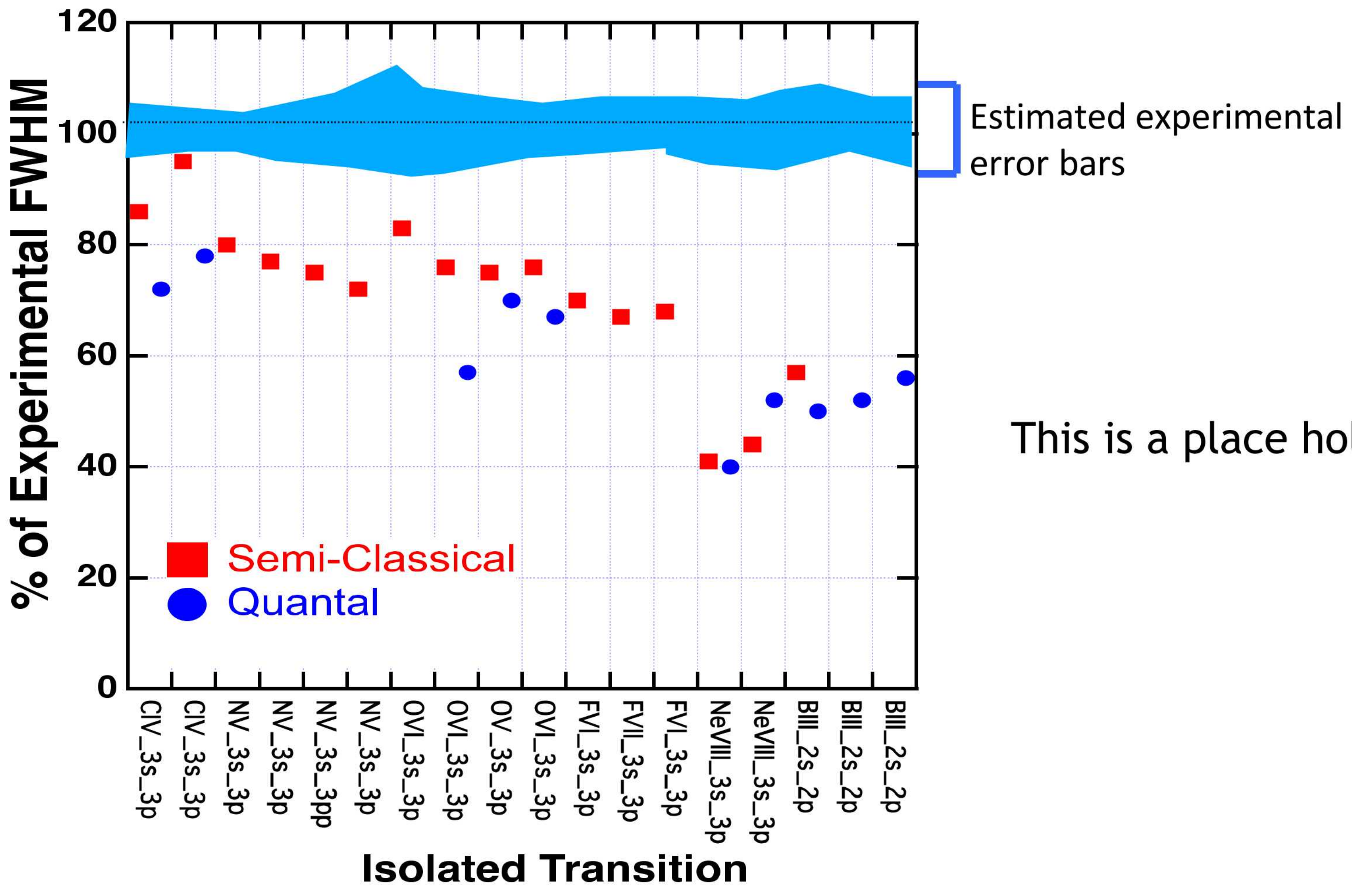
One exchange process—such as the nuclear contribution—can contribute a factor of two in the line shape

This shows that exchange processes are important

Exchange has no classical analog and semi-classical calculations cannot model these systems from an *ab-initio* calculation



Current Progress on Matching Experimental Data



This is a place holder

Conclusions

This is a work in progress to accurately model—from an *ab-initio* method—multi-electron systems

This work will be valuable for determining masses of white dwarfs with carbon-rich atmospheres

- thought to be some of the most massive white dwarfs

This will also be important for calculating line broadening and line shifts of helium lines that will aid in determining their masses as well (See Marc Scheauble's talk)