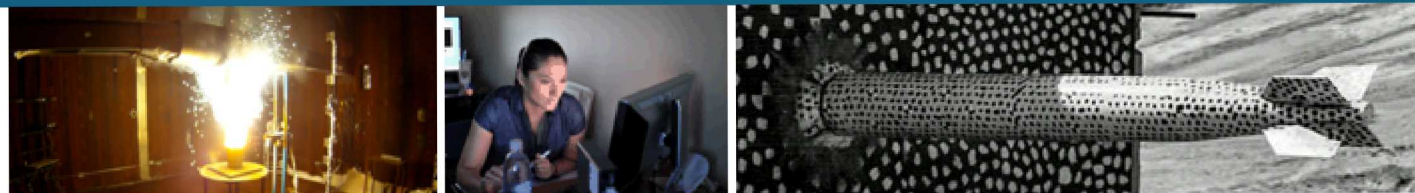


# Challenges and Progress Toward Modeling Carbon/Oxygen White Dwarf Spectra



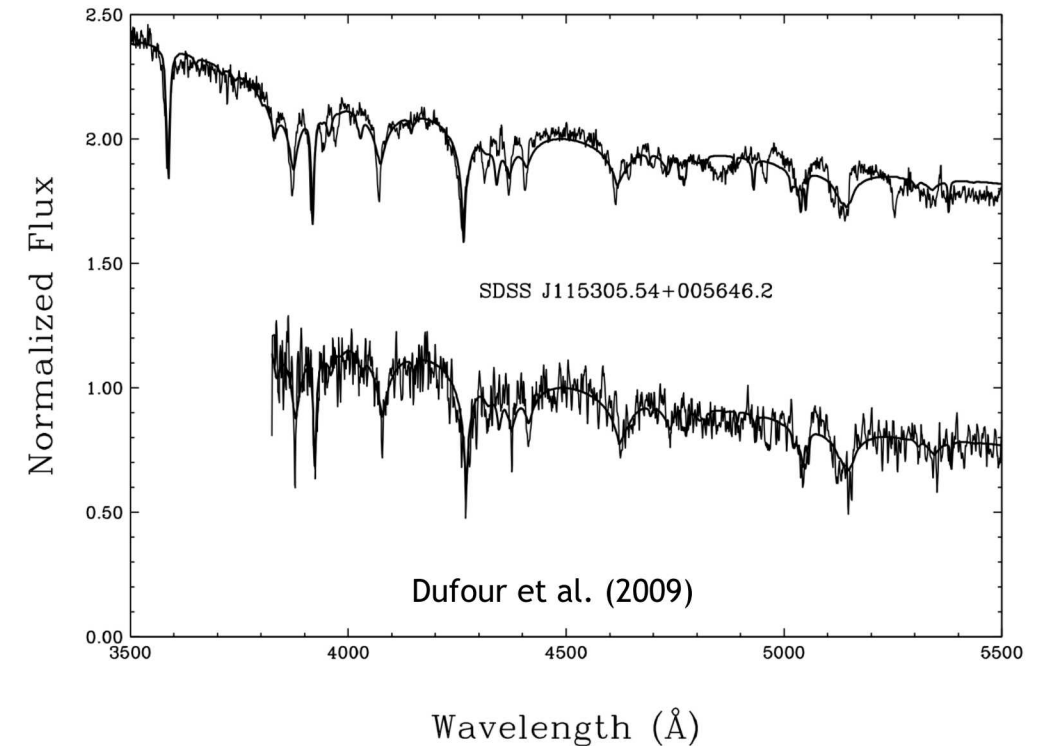
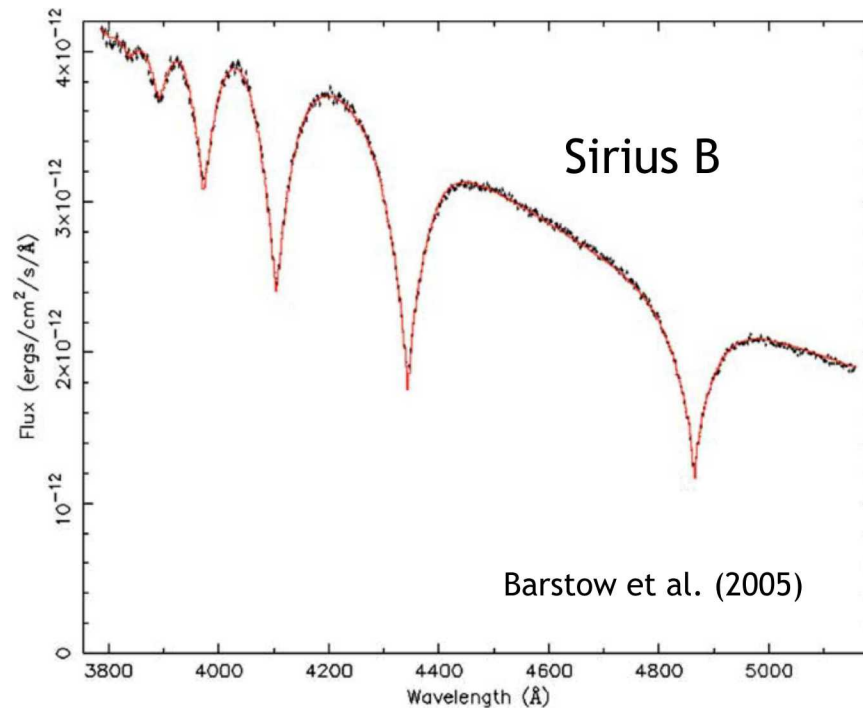
Thomas Gomez, T. Nagayama, C. Fontes, D. Kilcrease, M. Montgomery, D. Winget



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

# 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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This has never been measured, we have faith that our atmosphere models are correct (or close enough)

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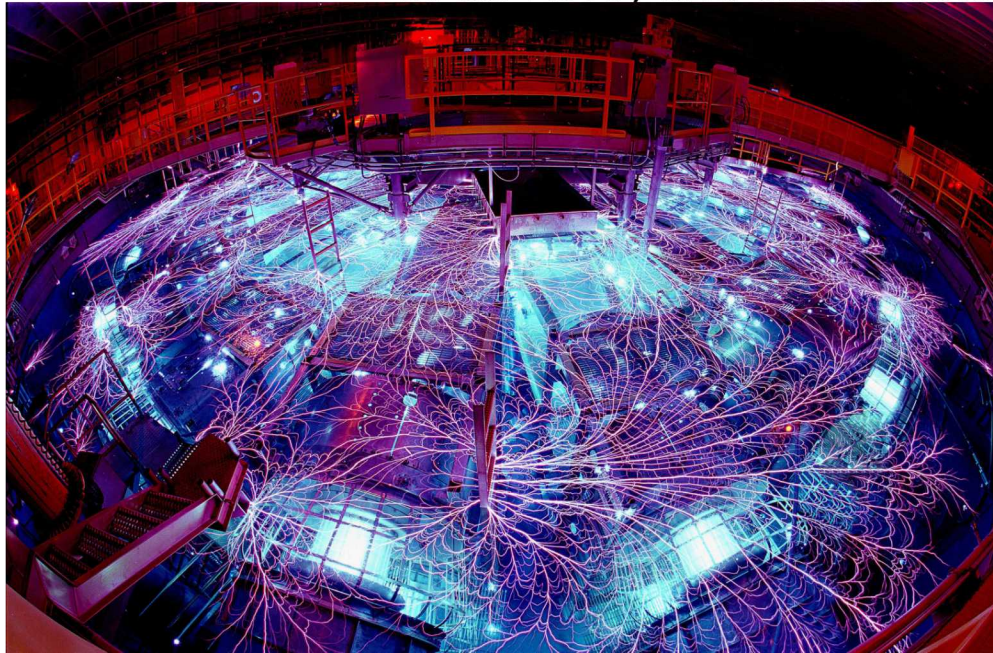
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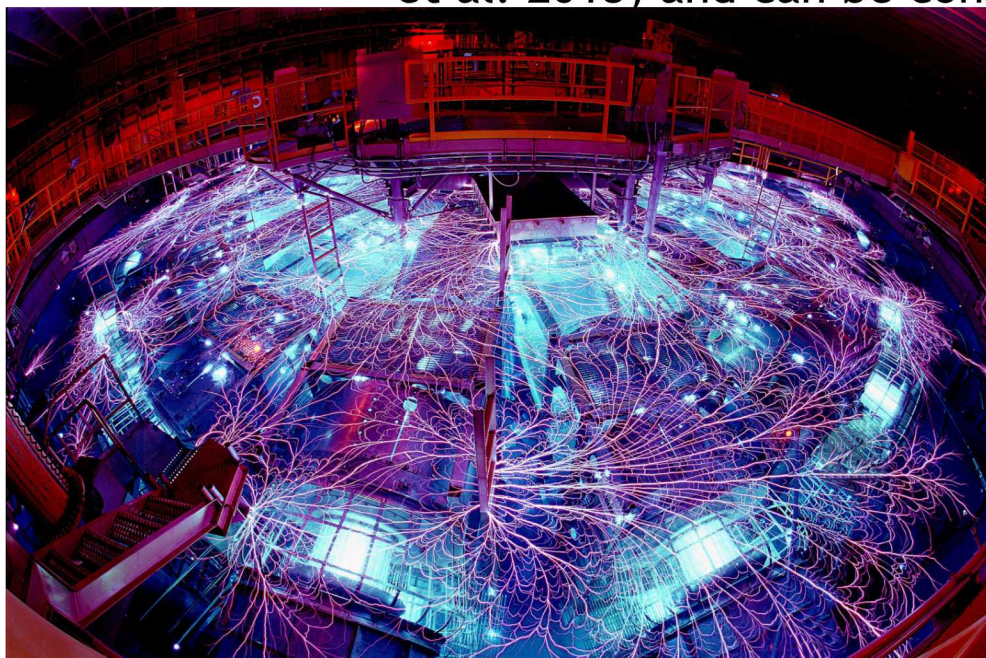
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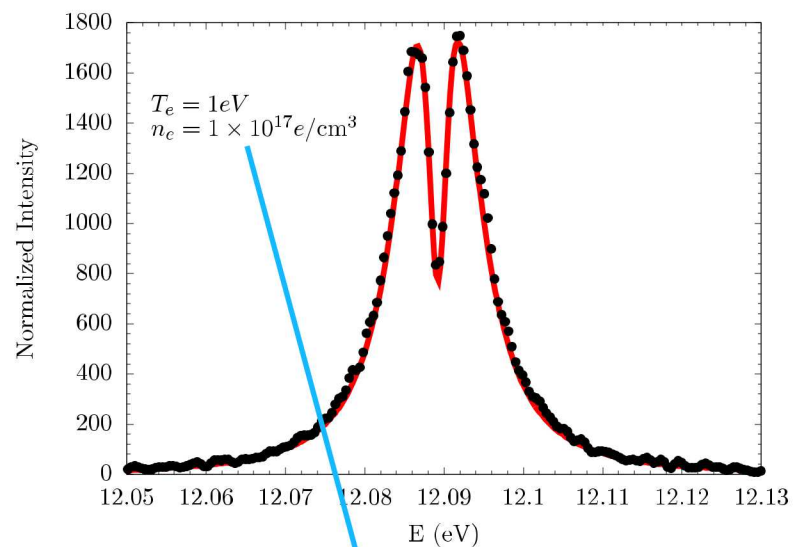
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# Line Broadening Models are used to Calculate Synthetic Spectra of White Dwarfs



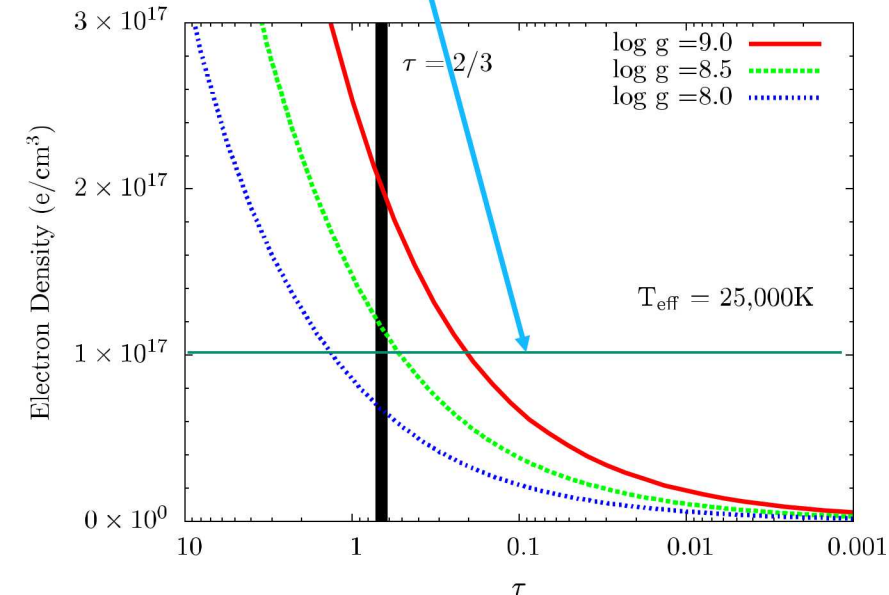
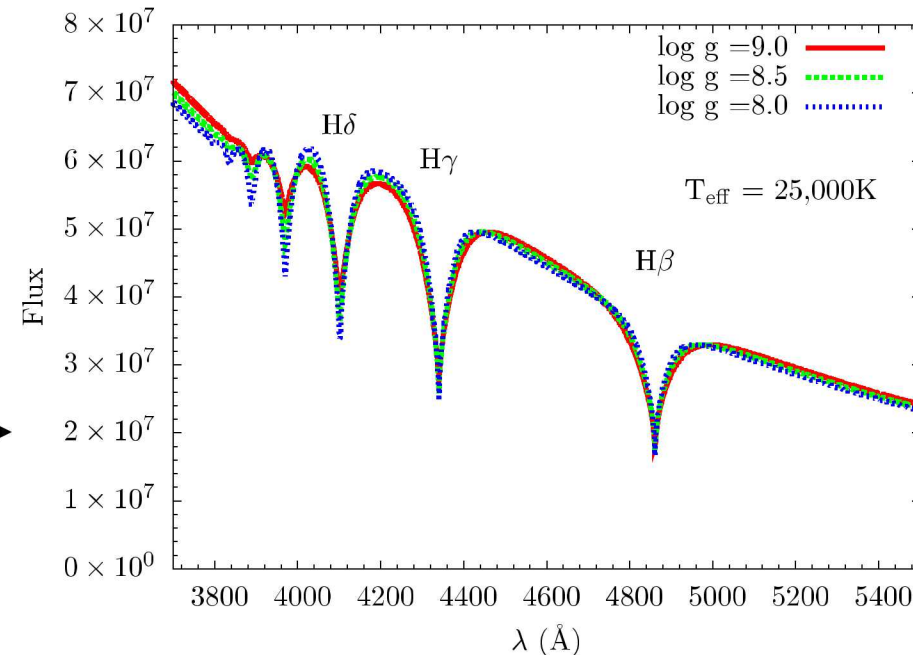
Spectral Line  
Shape at Different  
Plasma Conditions

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

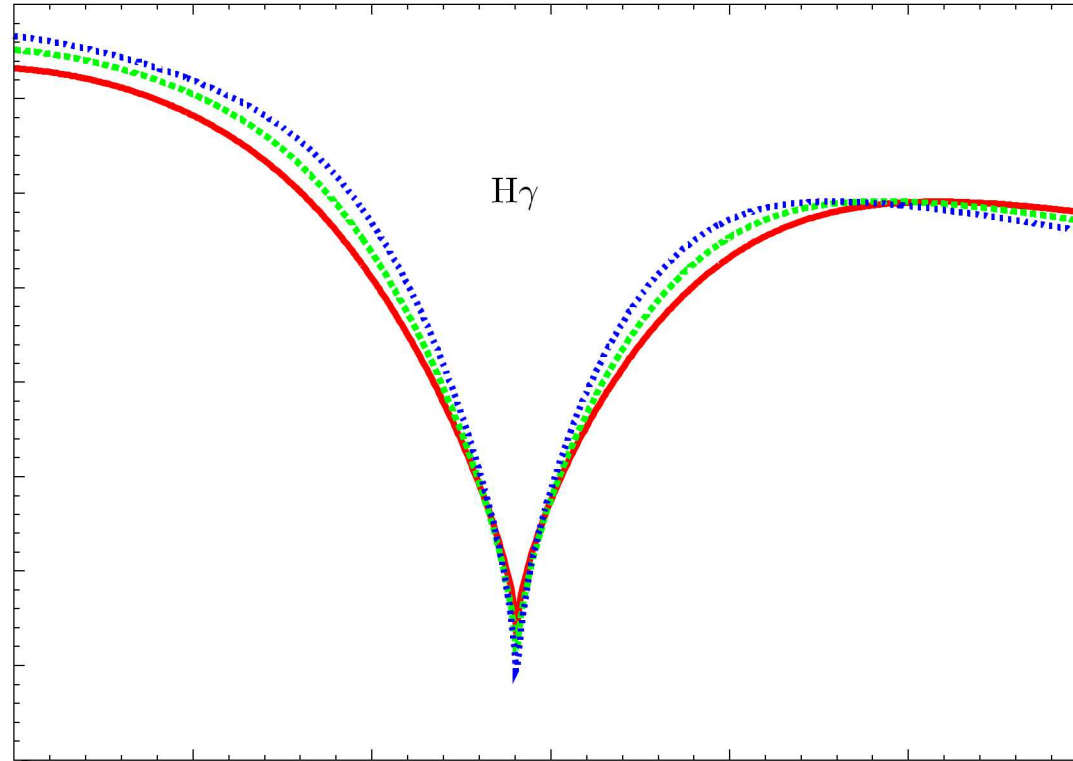
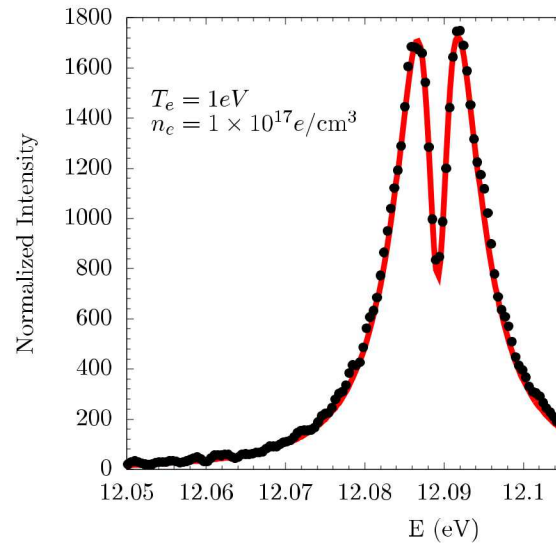
The reason for this is that

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

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

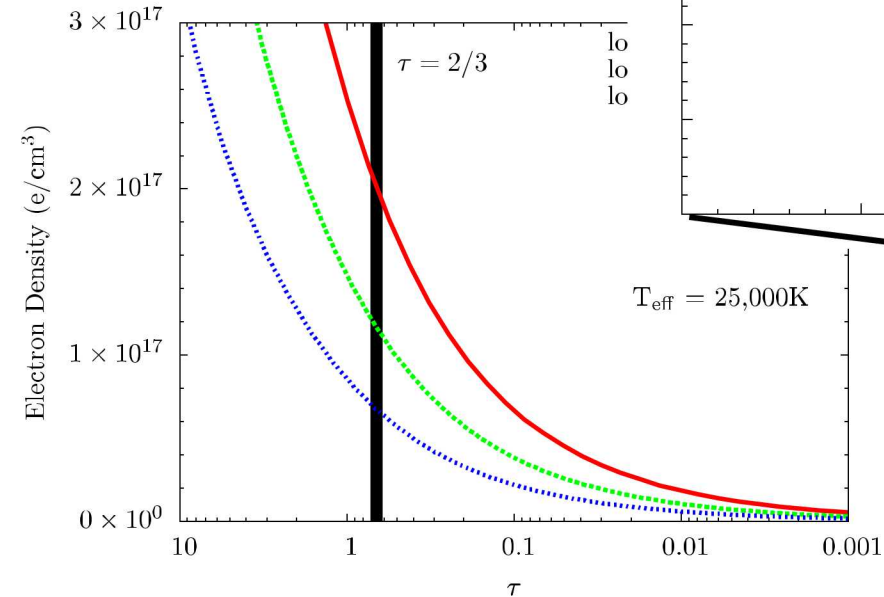


# Line Broadening Models are used to Calculate Synthetic Spectra of White Dwarfs

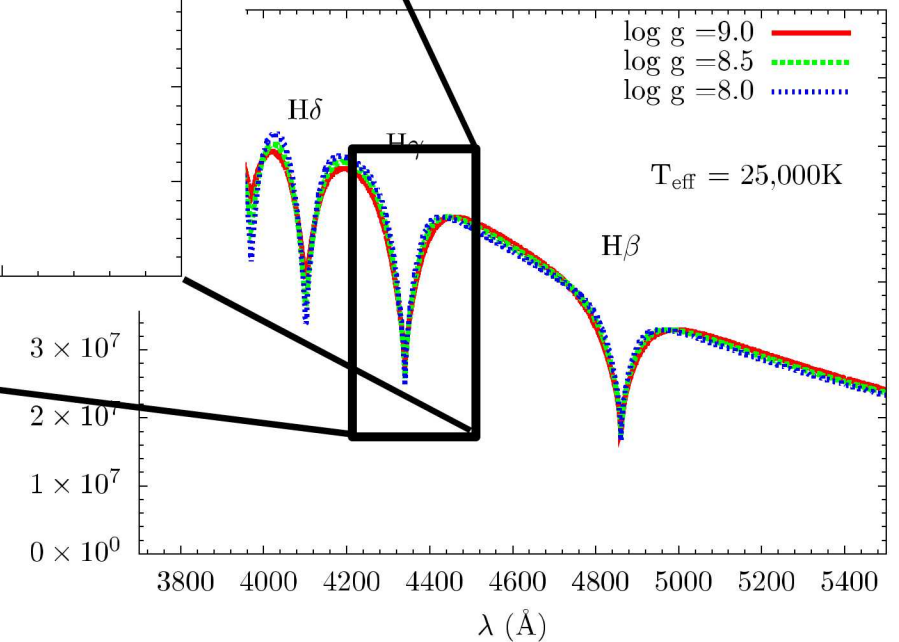


rect application of line  
omers is to determine log g

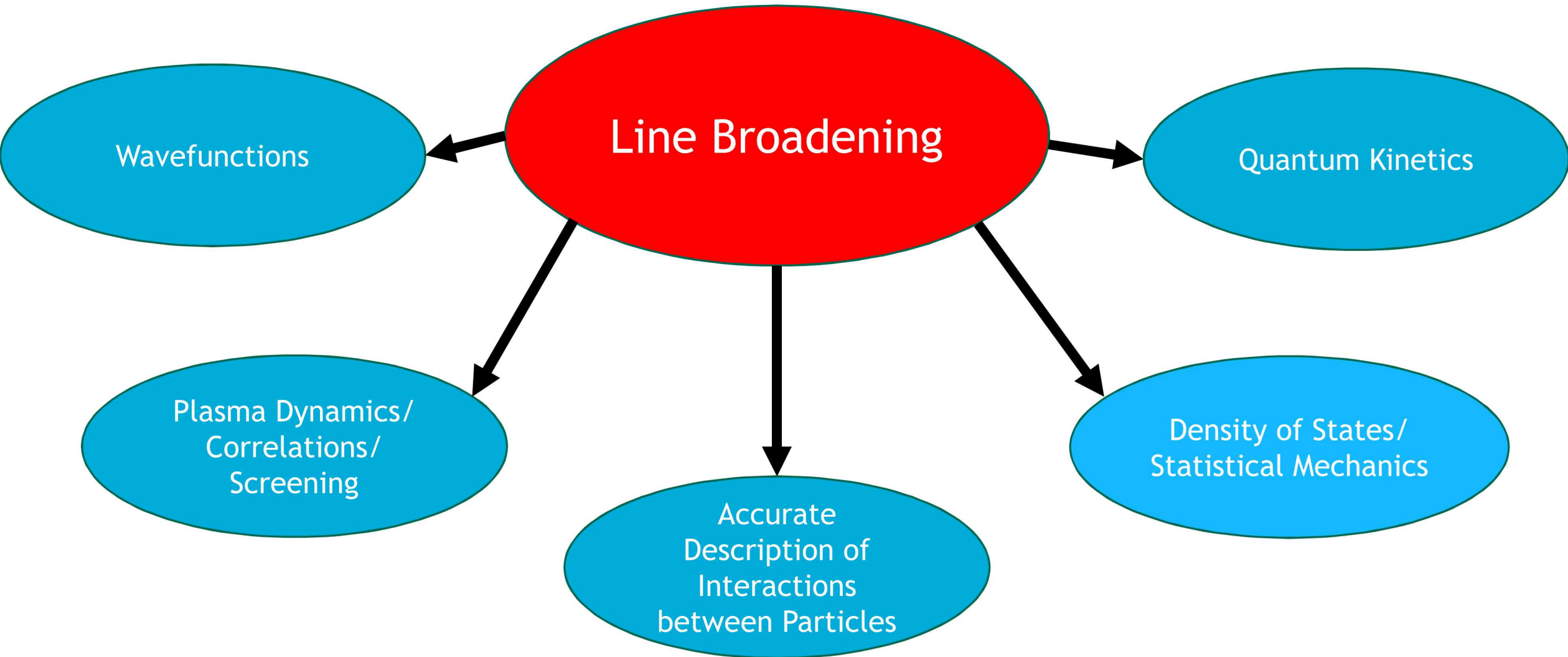
that  
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o gravity



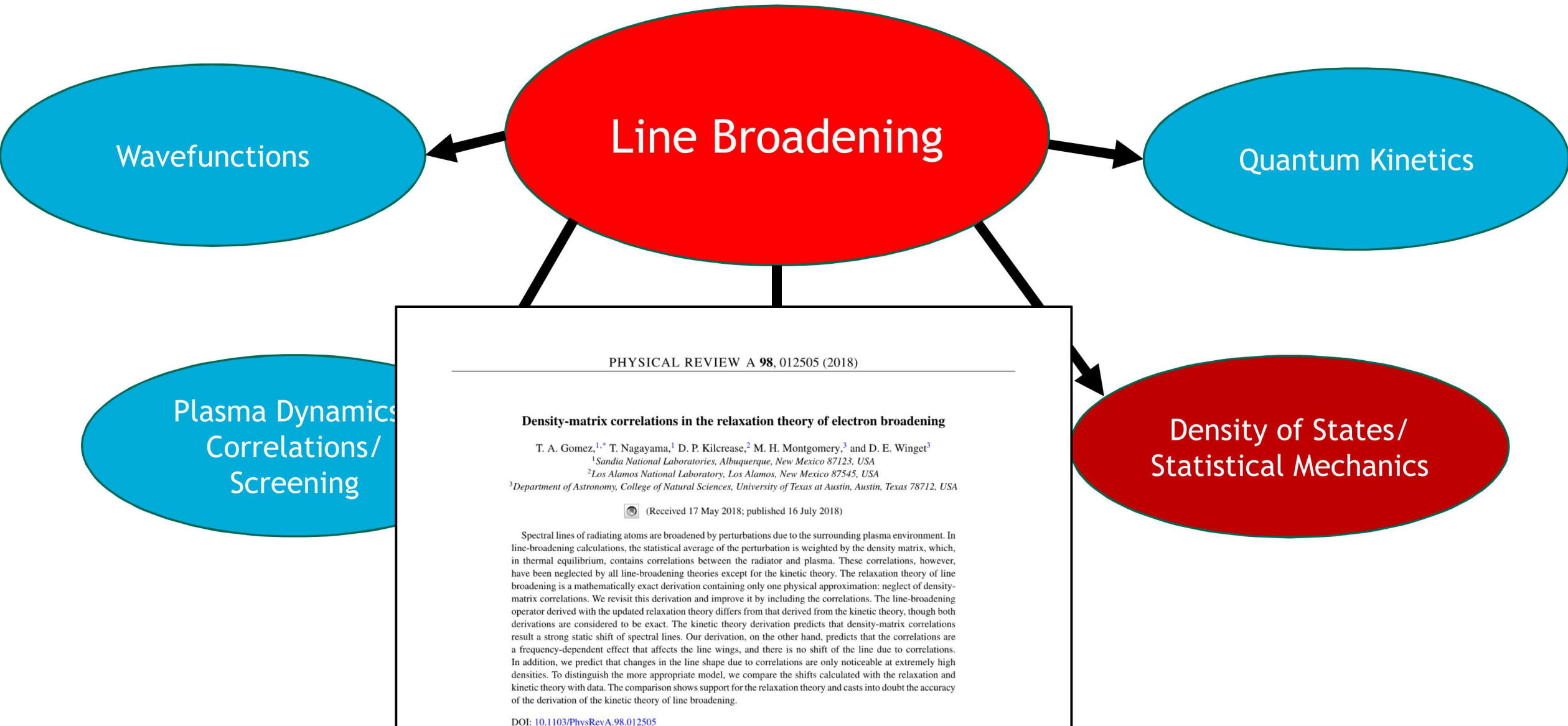
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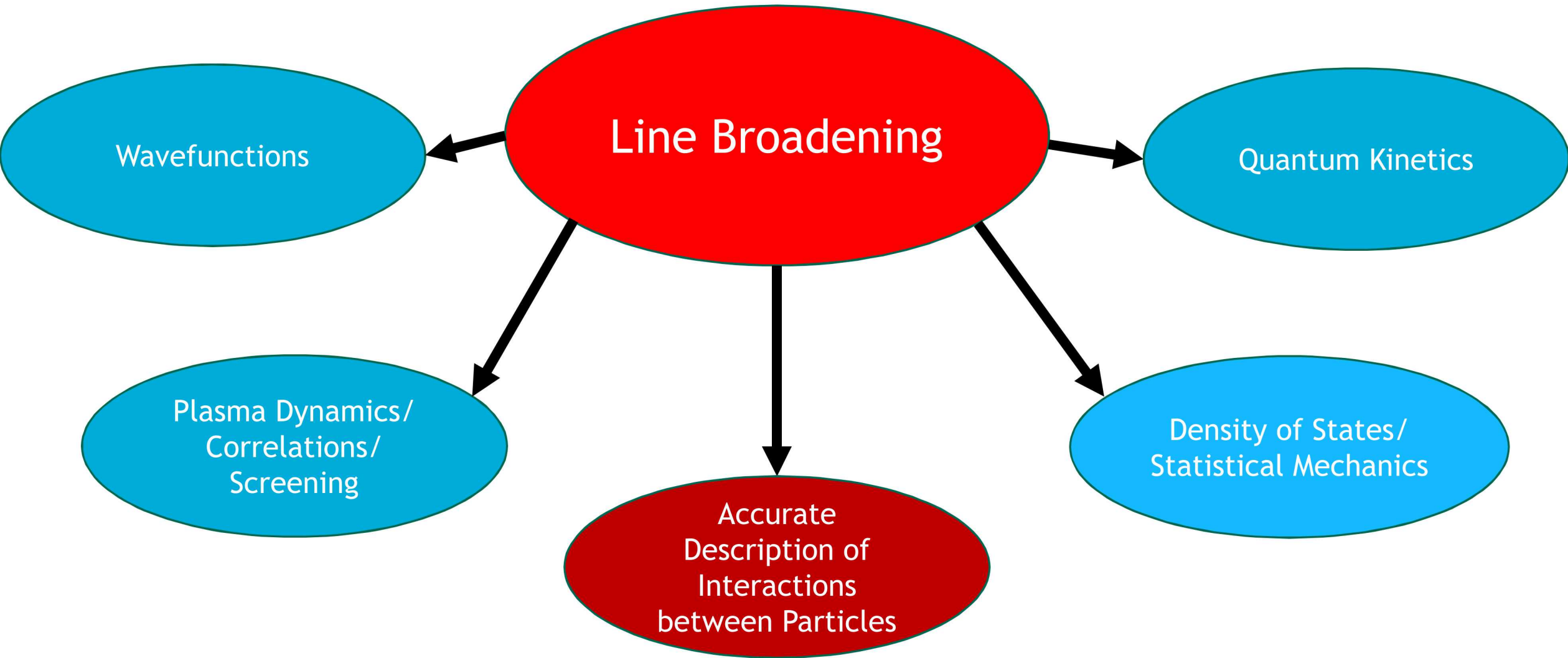


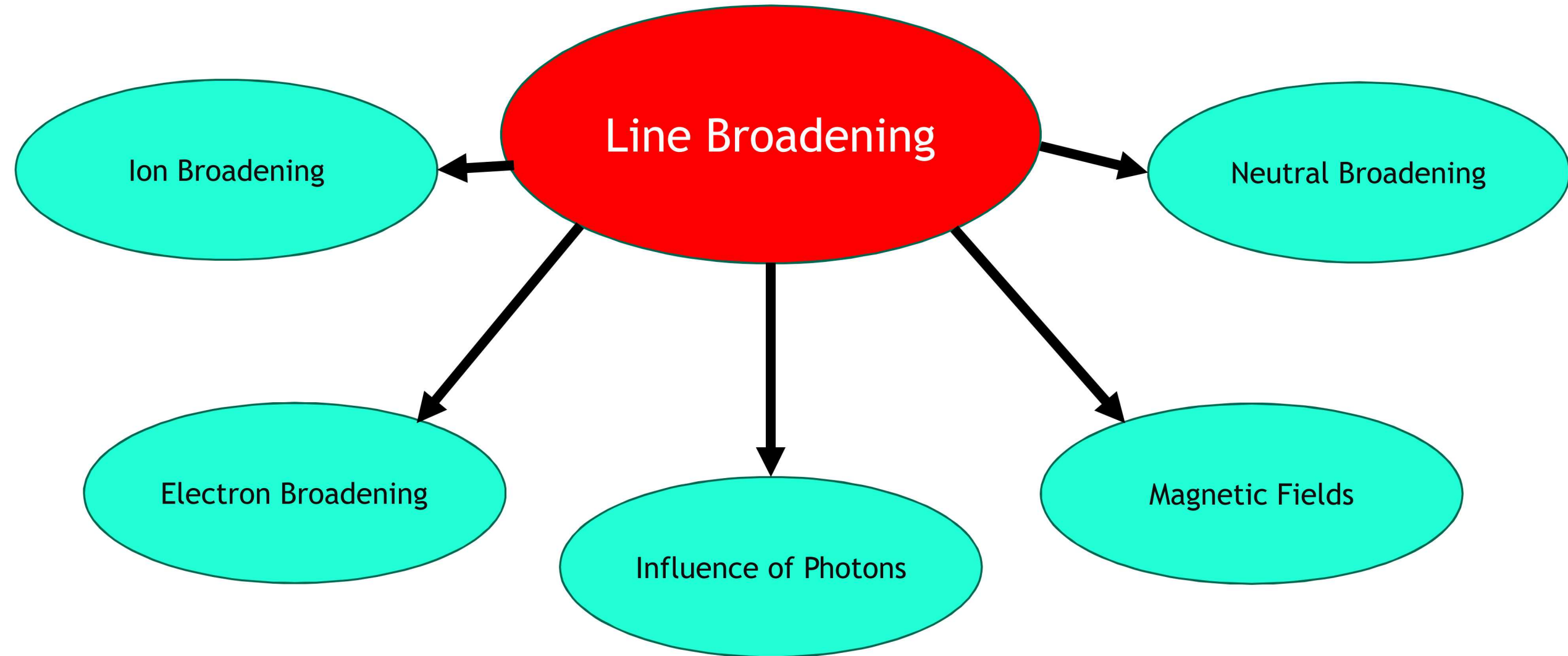




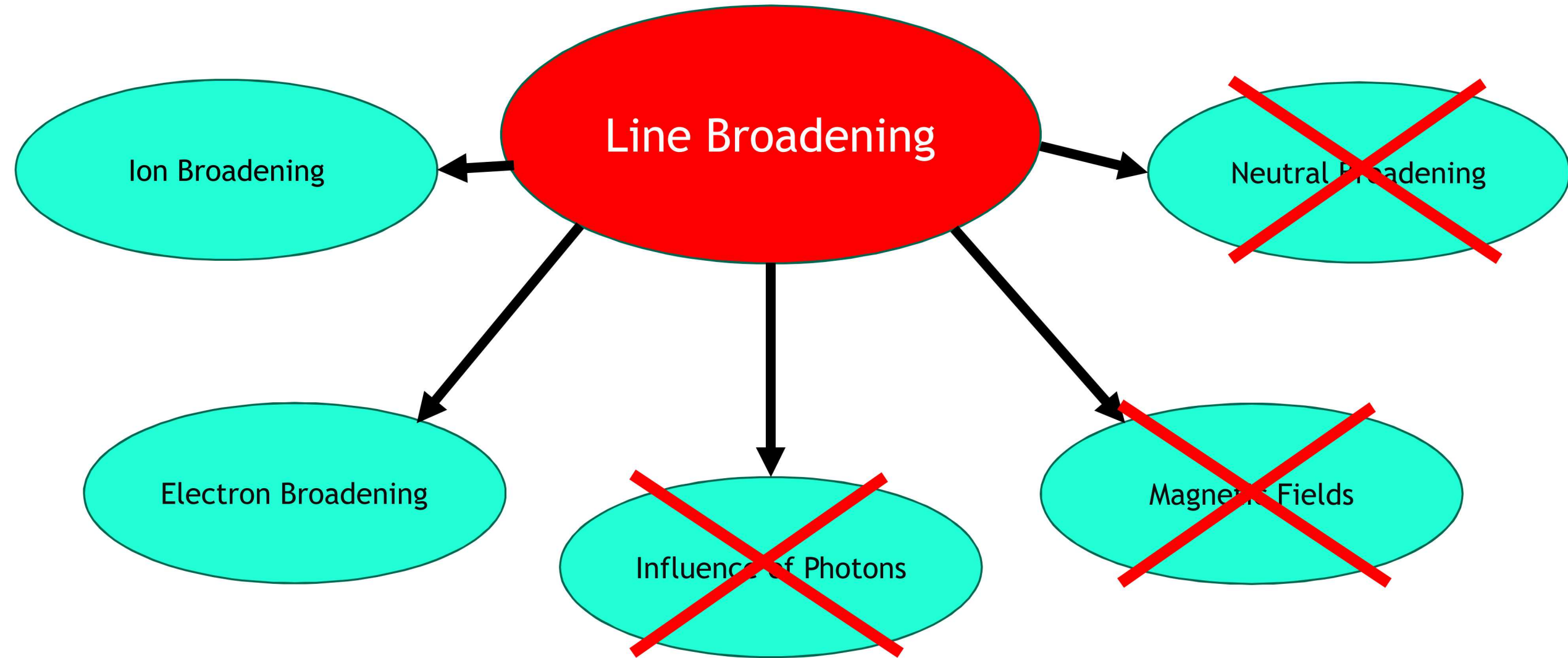
# Line-Broadening Requires Multi-Disciplinary knowledge

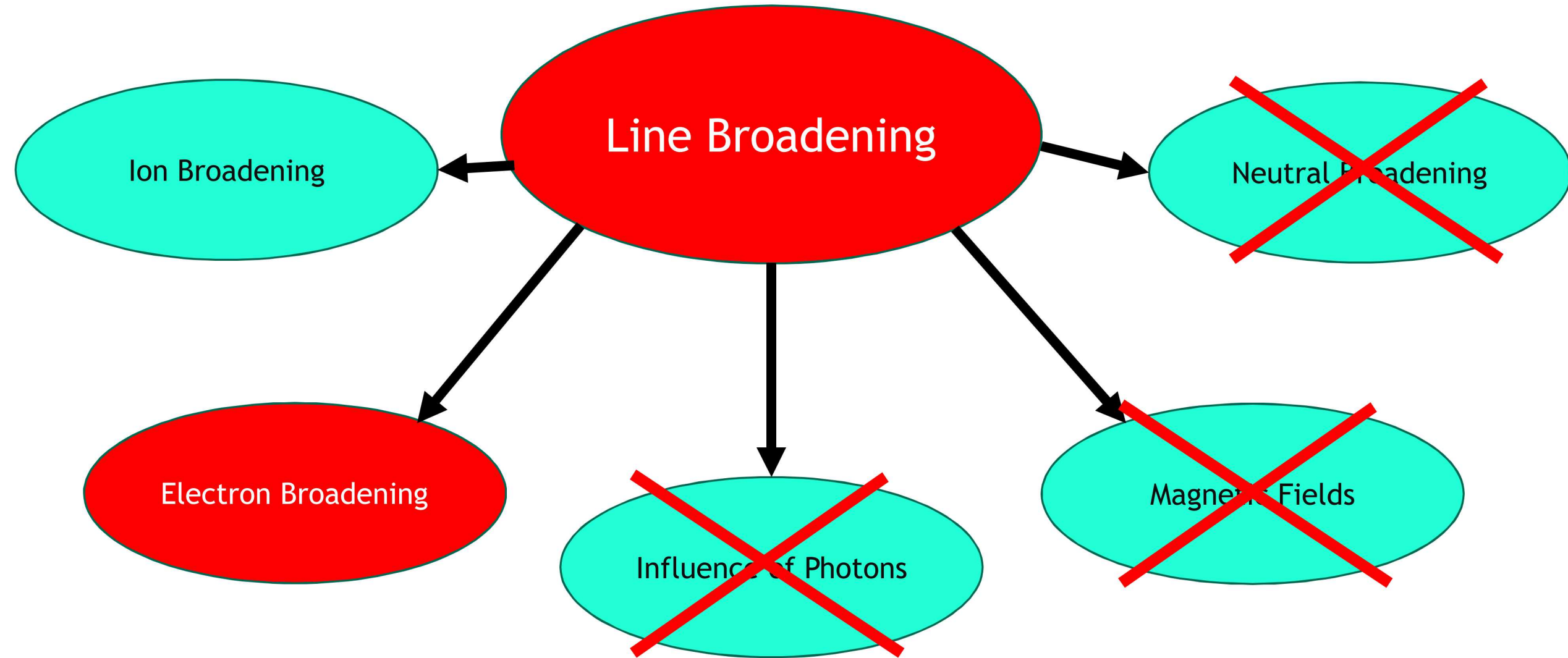












Broadening of Multi-Electron atoms is incomplete

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 / shells and one electron in an open shell: B-like, Al-like

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



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

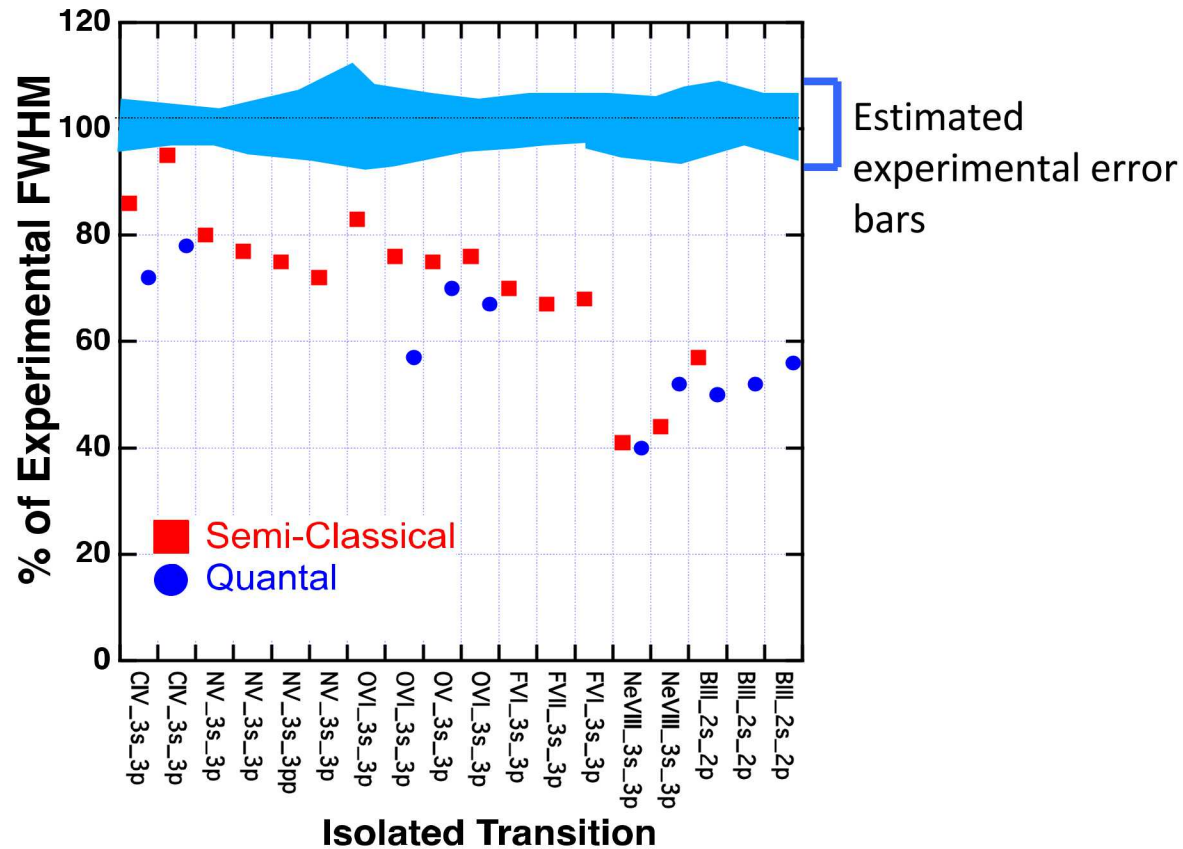
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The most complex are with more than one electron in open shells

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

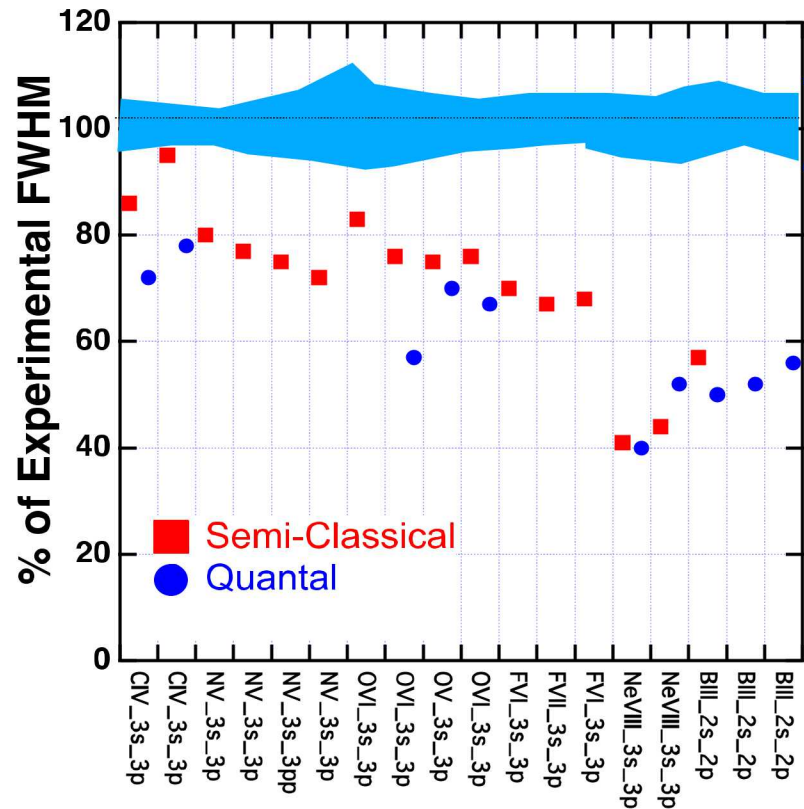
- Factor of two in some cases

Current *semi-empirical* calculations fare better

- uncertain within 20-30% for these lines.

Discrepancy is worse with large energy separation between states

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



Estimated experimental error bars

Isolated Transition

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

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

Eur. Phys. J. D 54, 51-64 (2009)  
DOI: 10.1140/epjdr/a2009-00167-8

THE EUROPEAN  
PHYSICAL JOURNAL

Regular Article

Quantum Stark broadening of 3s-3p spectral lines in Li-like Z-scaling and comparison with semi-classical perturbation

H. Elabidi<sup>1,\*</sup>, S. Sahal-Brechot<sup>2</sup>, and N. Ben Nessib<sup>3</sup>

<sup>1</sup> Groupe de Recherche en Physique Atomique et Astrophysique, Faculté des Sciences de Bizerte, Zarzouna 702  
<sup>2</sup> LERMA, Observatoire de Paris, CNRS, Université Pierre et Marie Curie, Place Jules Janssen, 92190 Meudon  
<sup>3</sup> Groupe de Recherche en Physique Atomique et Astrophysique, INSAT, Centre Urbain Nord B.P. 676, 1080 T

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Journal of Quantitative Spectroscopy &  
Radiative Transfer 99 (2006) 10–20

www.elsevier.com/locate/jqsrt

Semiclassical calculations of line broadening in plasmas  
Comparison with quantal results

S. Alexiou, R.W. Lee\*

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7000 East Avenue, Livermore, CA 94550, USA

Atoms 2014, 2, 157–177; doi:10.3390/atoms2020157

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ISSN 2218

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Article

The Second Workshop on Lineshape Code Comparison:  
Isolated Lines

Spiros Alexiou<sup>1,\*</sup>, Milan S. Dimitrijević<sup>2</sup>, Sylvie Sahal-Brechot<sup>3</sup>, Evgeny Stambulchik<sup>4</sup>,  
Bin Duan<sup>5</sup>, Diego González-Herrero<sup>6</sup> and Marco A. Gigusos<sup>6</sup>

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<sup>3</sup> LERMA-UMR CNRS 8112 and UPMC, Observatoire Paris Meudon, 5 Pl Jules Janssen,  
Meudon 92195, France; E-Mail: sylvie.sahal@obspm.fr

PHYSICAL REVIEW A

VOLUME 45, NUMBER 12

15 JULY 1992

Stark broadening of spectral lines along the isoelectronic sequence of Li

S. Glenzer, N. I. Uzelac,\* and H.-J. Kunze  
Institut für Experimentalphysik V, Ruhr-Universität, 4630 Bochum, Federal Republic of Germany  
(Received 13 January 1992)

Experimental Stark widths of the  $3s^2S - 3p^2P$  transitions in the Li-like ions CIV, NV, OVI, and NeVIII are reported. The measurements were performed for a set of plasma parameters so that the density and temperature behavior of the Stark widths could be observed and compared with calculations. The experimental results did not show a scaling with  $Z^{-2}$ , where  $Z$  is the spectroscopic charge number, which is expected from theoretical calculations in the electron-impact approximation. Furthermore, deviations from linear scaling appear for  $Z = 8$ .

PACS number(s): 32.70.Kz, 32.70.Jz

1. INTRODUCTION

Investigations of Stark widths of highly charged non-hydrogenic ions along isoelectronic sequences are of great interest since cross sections for impact broadening scale

II. THEORETICAL STARK WIDTH

For the calculation of the Stark widths we used semiclassical impact theory of Ref. [5] and a semiempirical approach as given in Ref. [6].



PERGAMON

Journal of Quantitative Spectroscopy &  
Radiative Transfer 81 (2003) 371–384

www.elsevier.com/locate/jqsrt

Electron-impact broadening of the 3s-3p lines  
in low-Z Li-like ions

Yu.V. Ralchenko<sup>a,\*</sup>, H.R. Griem<sup>b</sup>, I. Bray<sup>c</sup>

<sup>a</sup>Faculty of Physics, Weizmann Institute of Science, Rehovot 76100, Israel

PHYSICAL REVIEW A

VOLUME 49, NUMBER 1

JANUARY 1994

Collision operator for isolated ion lines in the standard Stark-broadening theory with applications  
to the Z scaling in the Li isoelectronic series 3P-3S transition

Spiros Alexiou  
Department of Nuclear Physics, Weizmann Institute of Science, Rehovot 76100, Israel  
(Received 8 March 1993)

In this work we review some aspects of the semiclassical dipole impact approximation for isolated ion lines with a view to the questions on Z scaling raised by two recent experimental studies. Some theoretical and practical aspects of line-shape calculations are discussed. Detailed calculations are performed in the semiclassical (dipole) impact approximation for the Li isoelectronic 3P–3S line. Particular emphasis is given to inelasticity effects. In contrast to previous calculations, very good agreement is obtained for the lighter elements of the isoelectronic series. Ion dynamical corrections are also considered and are found to be negligible in the dipole approximation.

PACS number(s): 32.70.Jz, 32.30.Jc, 32.60.+i

# 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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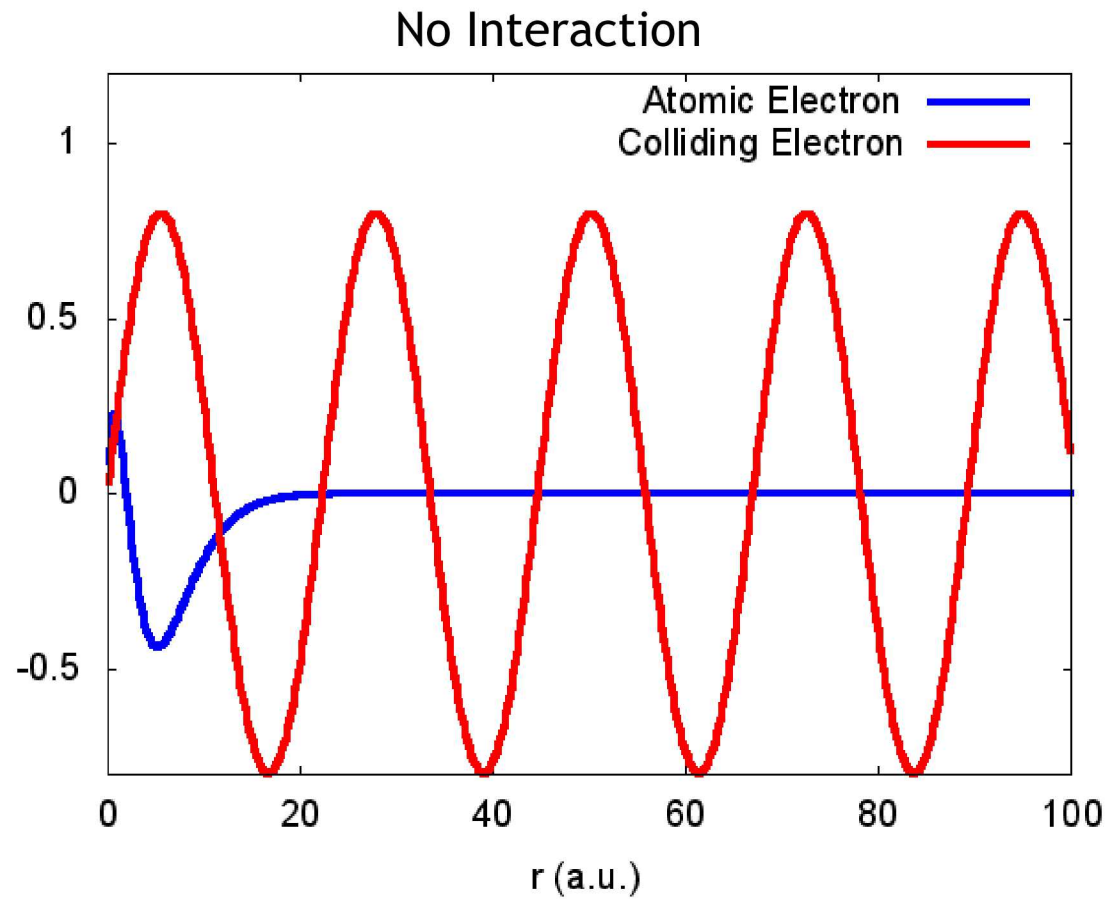
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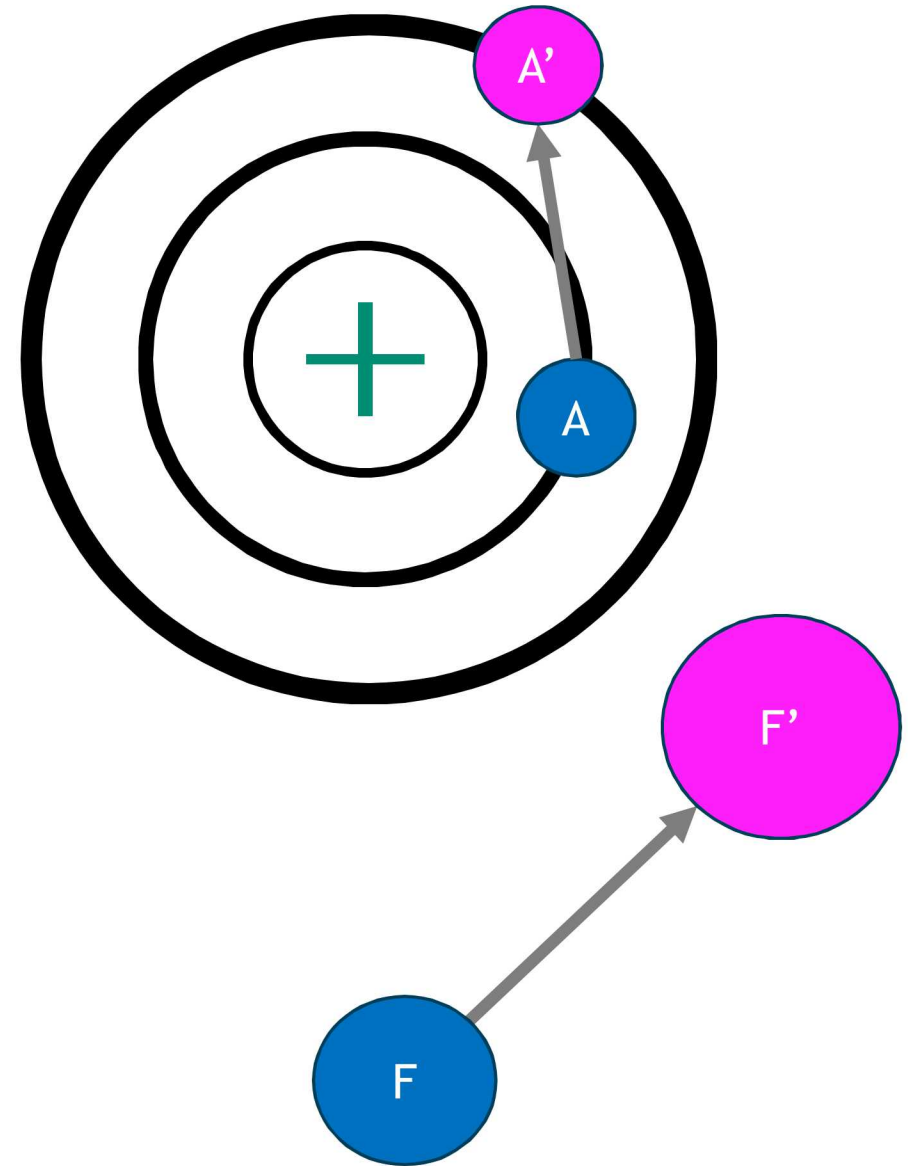


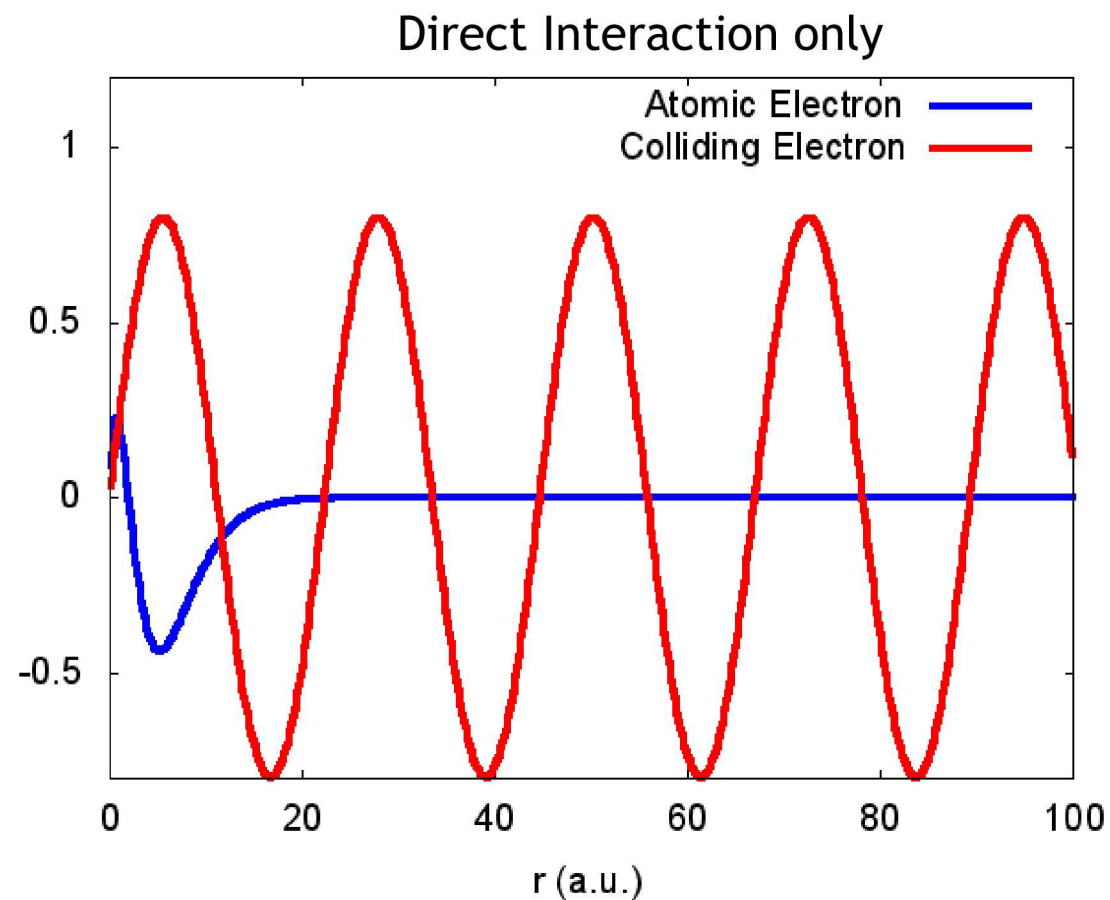
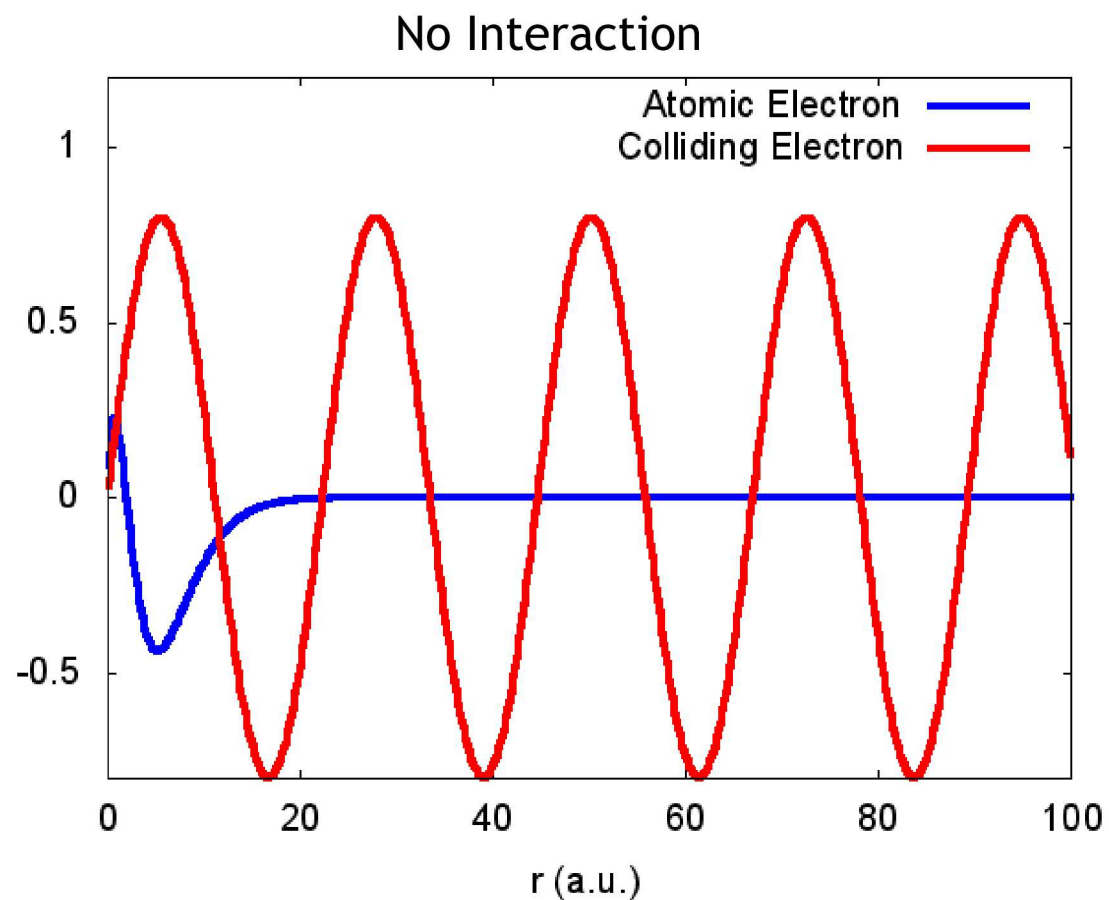
## Direct Interactions are Straightforward

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

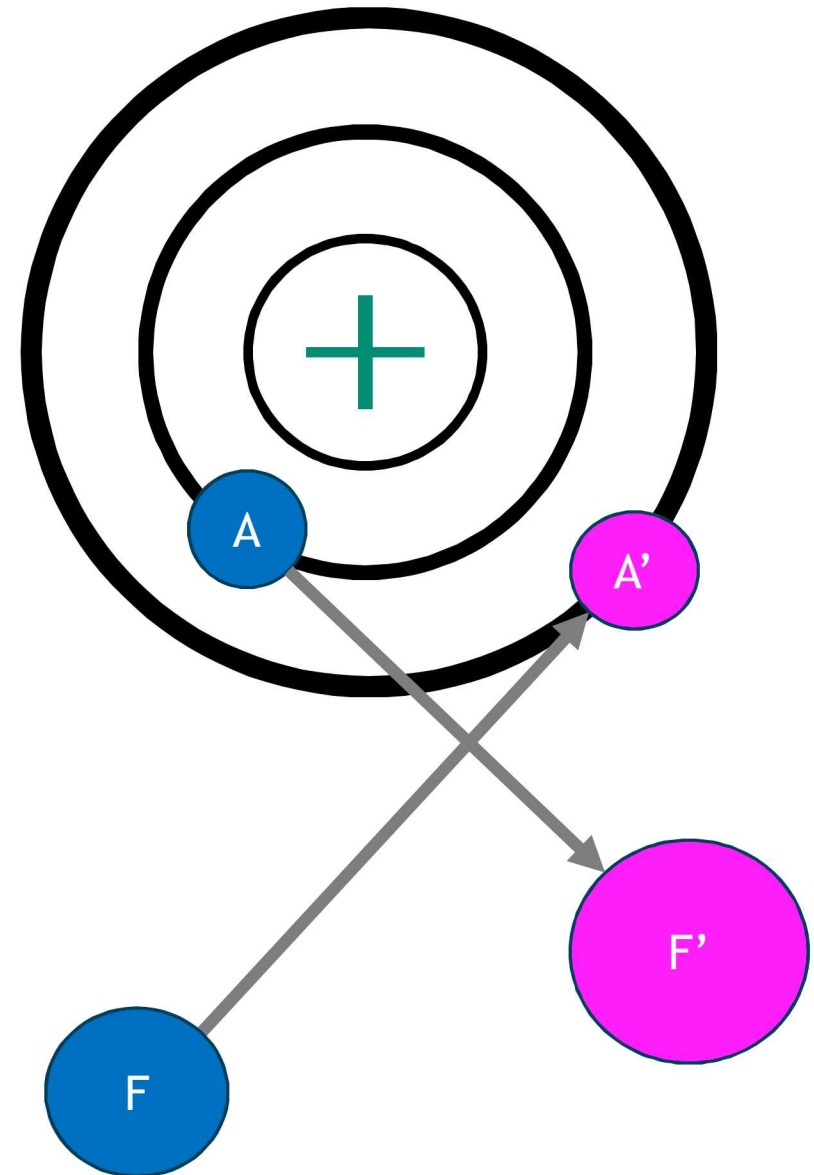


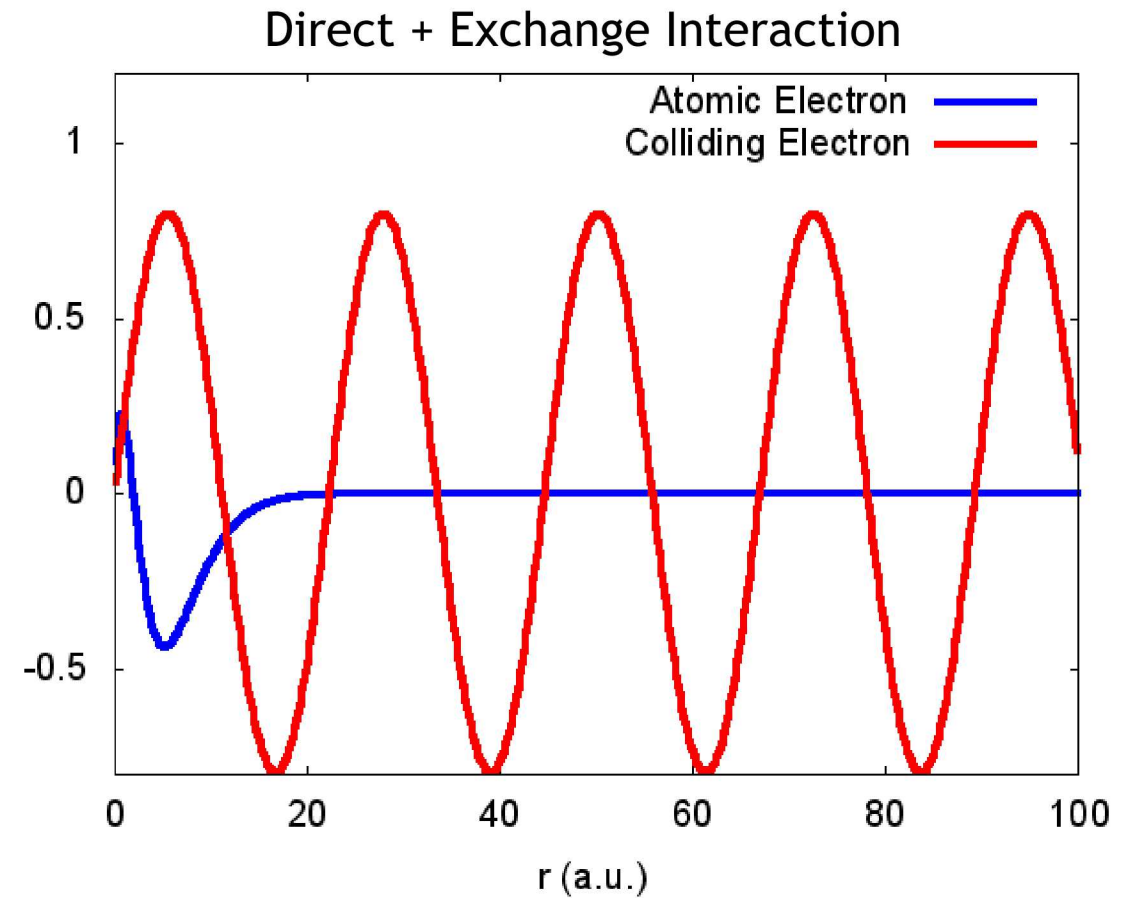
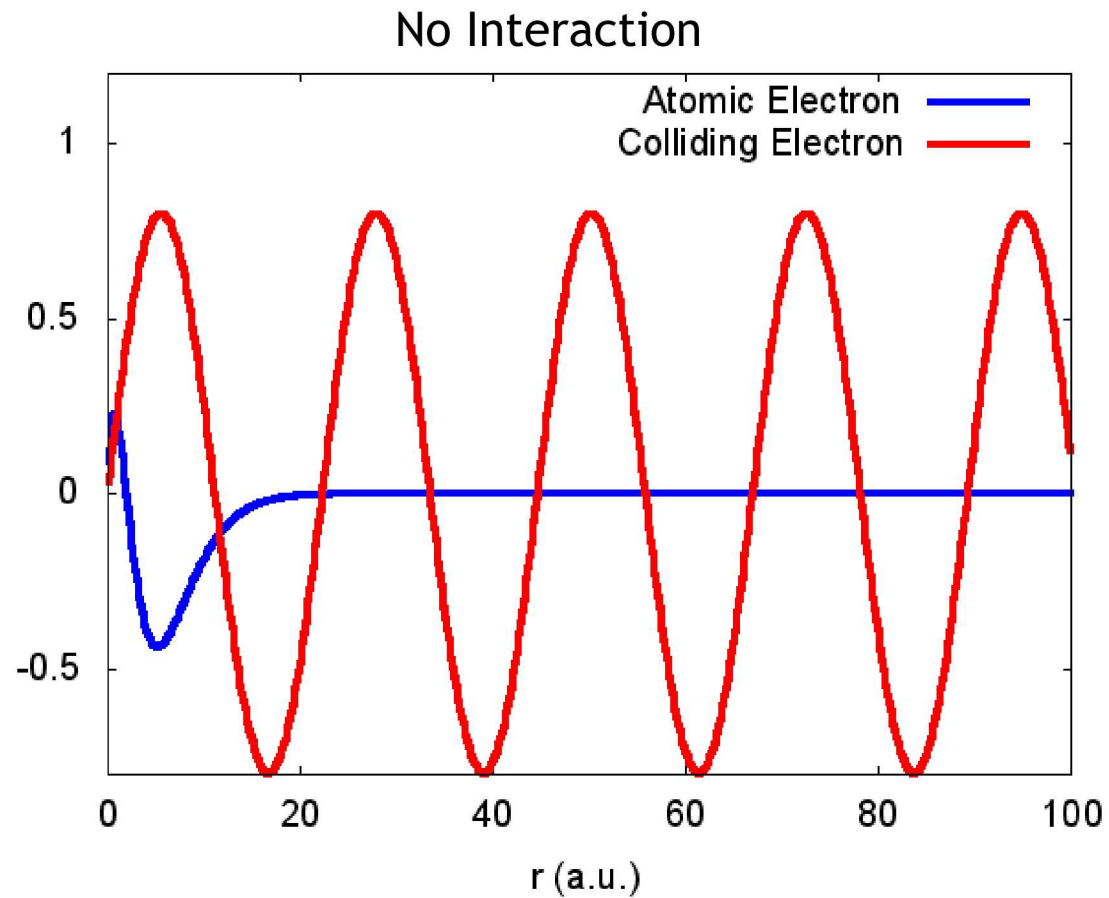


## Exchange Interactions

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



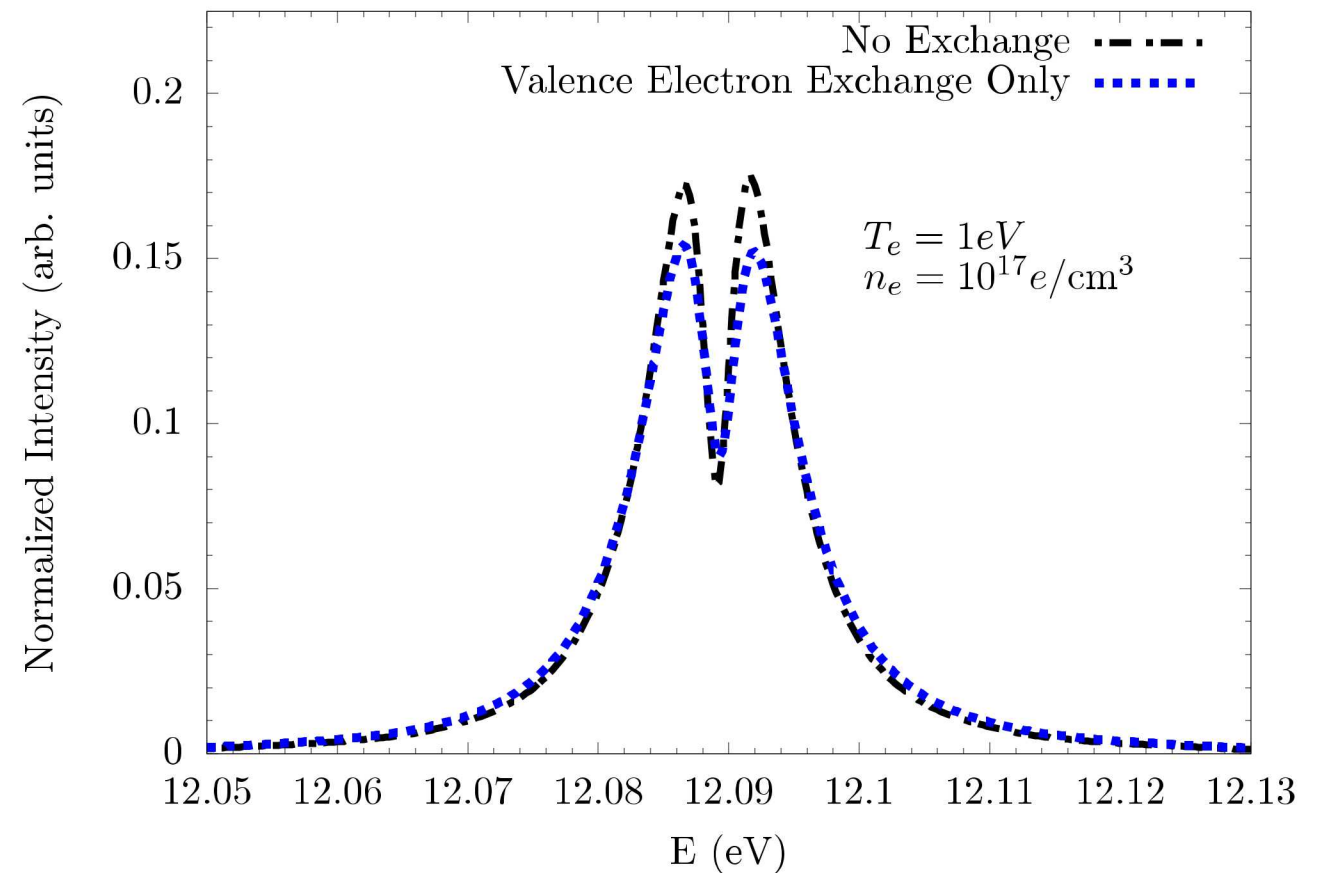


## Exchange is Important Even for Hydrogen

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





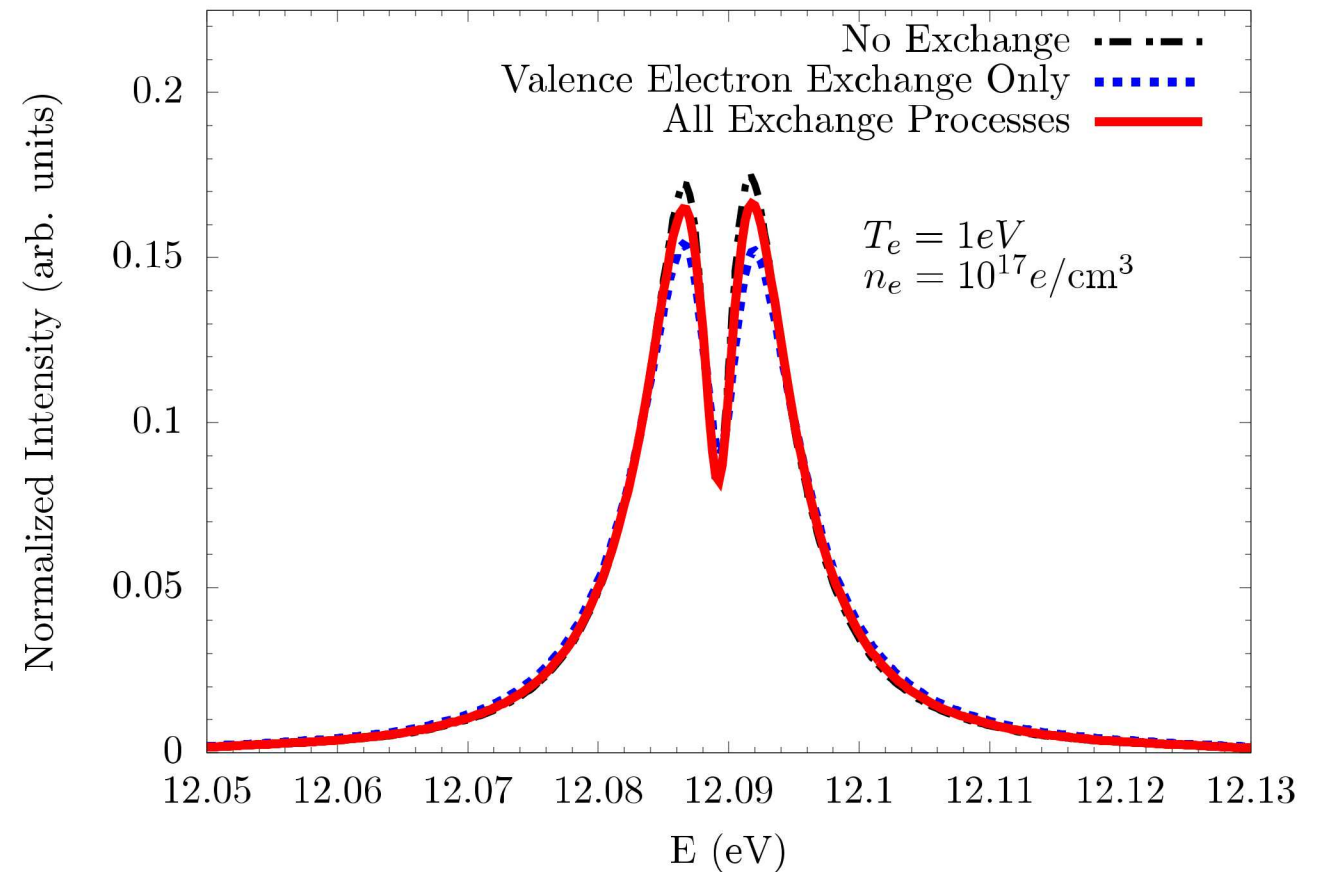
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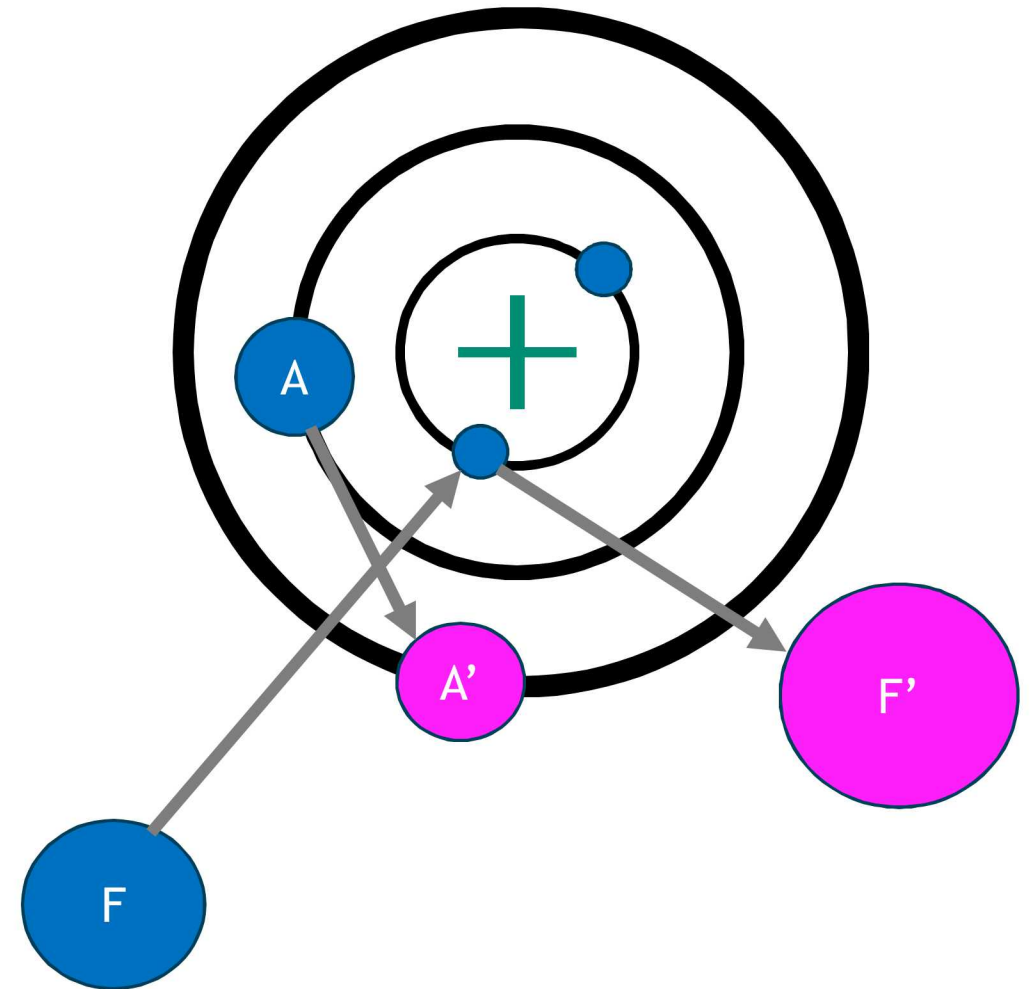
But because exchange can also occurs with nuclear interactions, the effect of exchange is largely cancelled for hydrogen



## Exchange Interactions for Multi-Electron Atoms

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

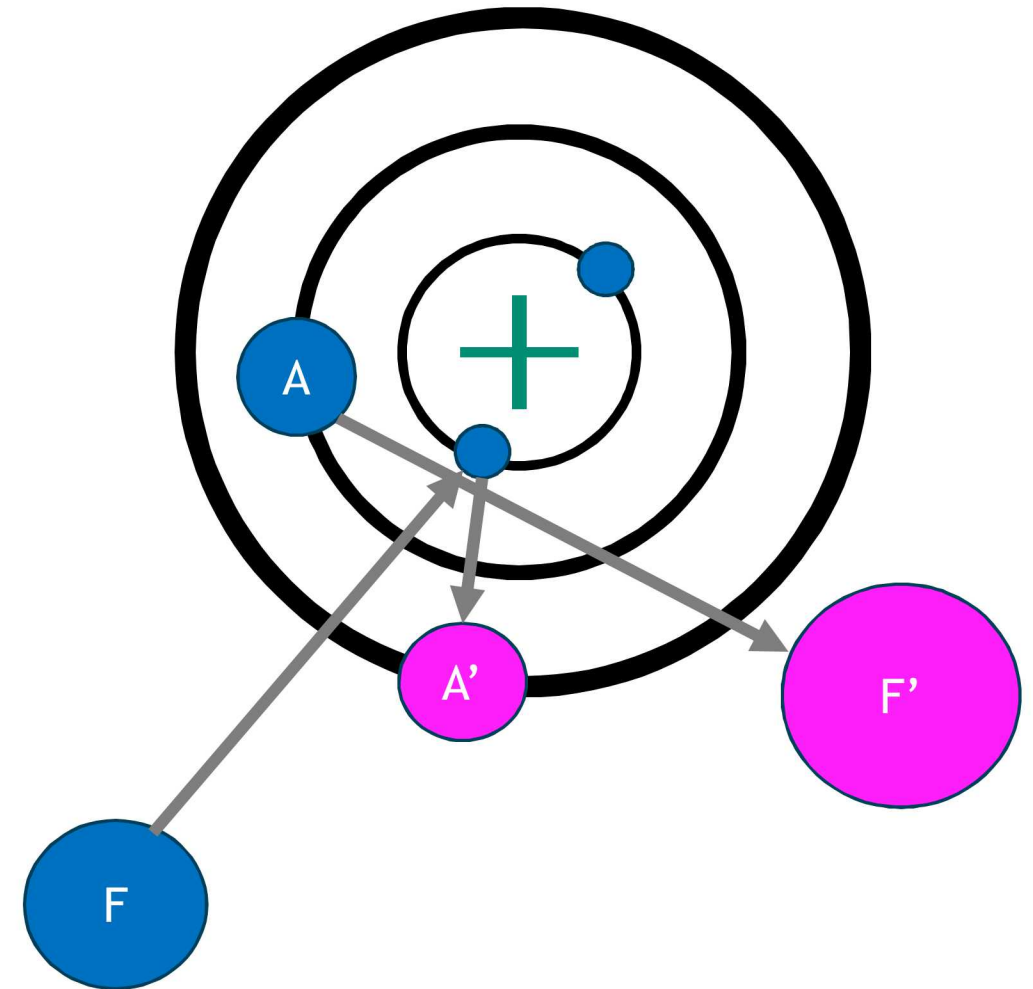
These include not only two-body exchange, but three-body exchange as well (assuming atomic wavefunctions are roughly orthogonal)



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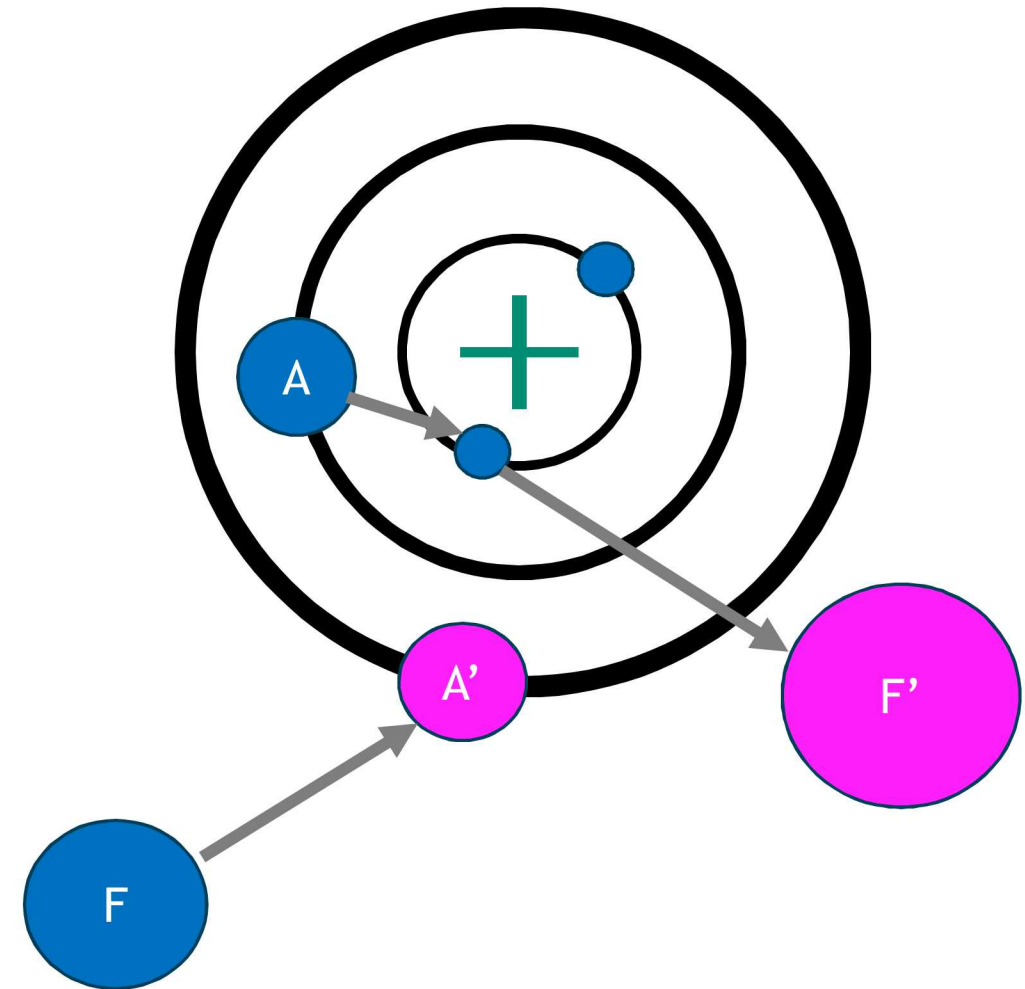
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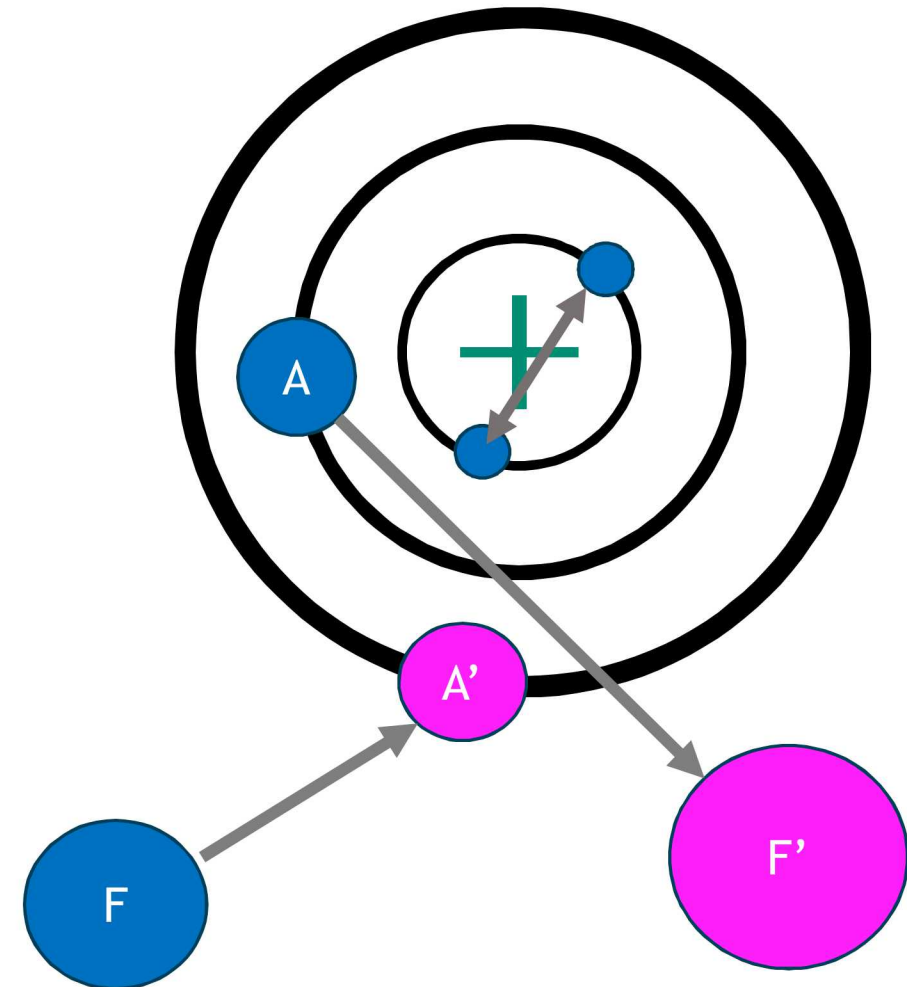
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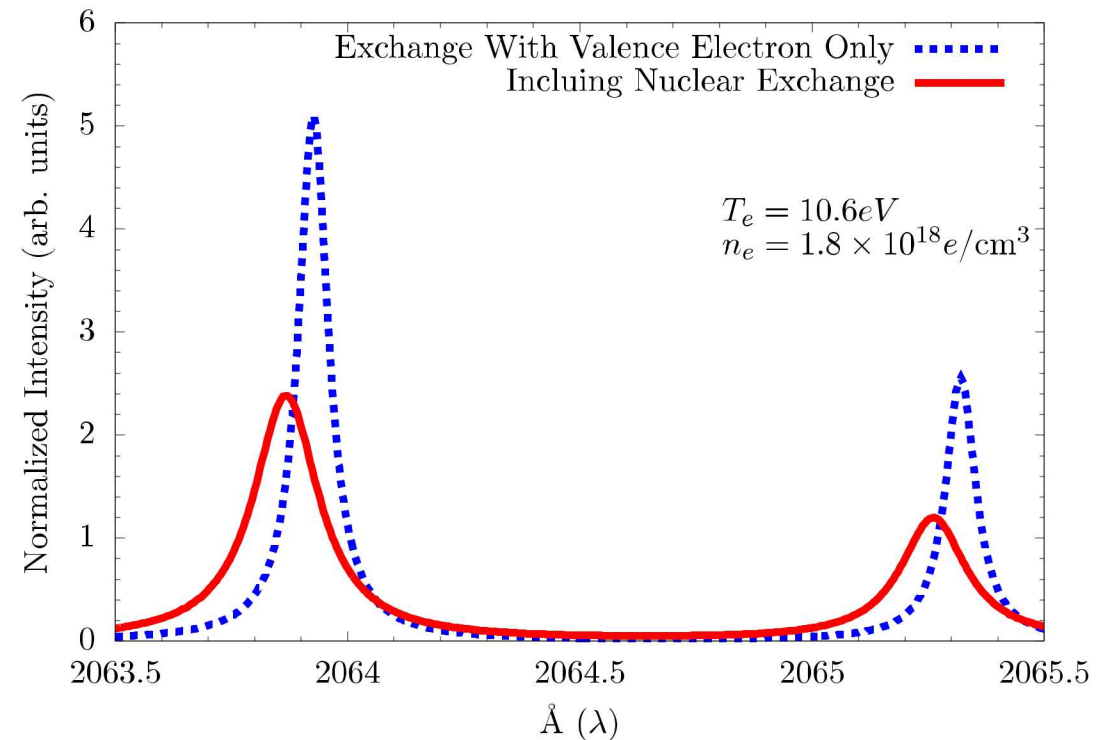


## These Exchange Terms are Large

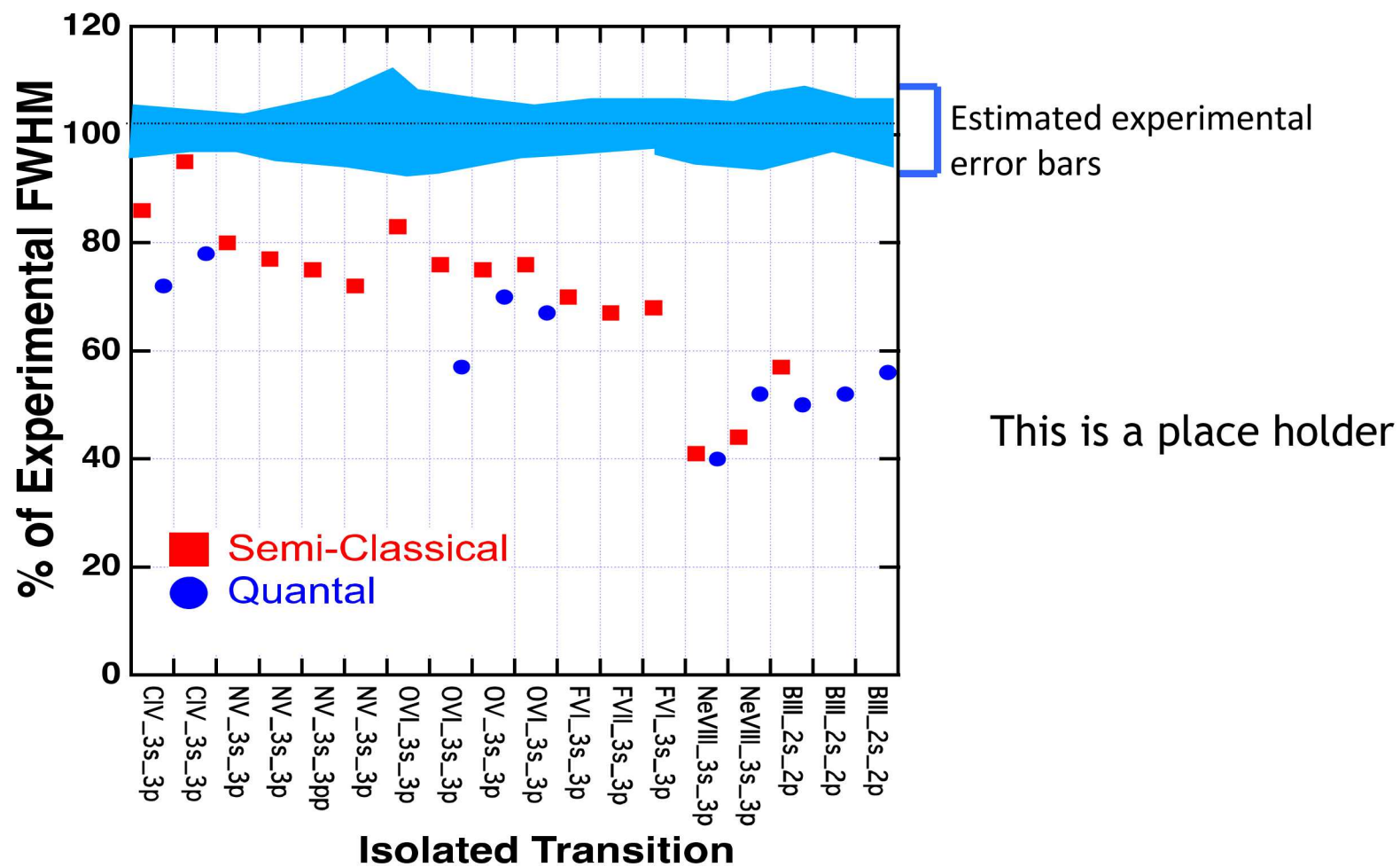
One exchange process—such as the nuclear contribution—can contribute a factor of two in the line shape

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 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)