Radiative properties of atoms in plasma

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Outline

- Motivation
  - Photoexcitation
  - Photoionization
- Computational method
  - Model potential Method
- Modeling of potential in plasma
- Results & Discussion
  - Continuum lowering & Pressure ionization
  - Line shift
  - Shape resonance
  - Cooper minimum
- Summary & Future direction

Motivation

❑ Radiative property quantifies the interaction of photons with matter.

Radiative processes

- **Photoionization**
- Inverse Bremsstrahlung
- Thomson/Compton scattering

- **Photoexcitation**
- Line broadening
- Resonance scattering

$\sigma(cm^2)$ →

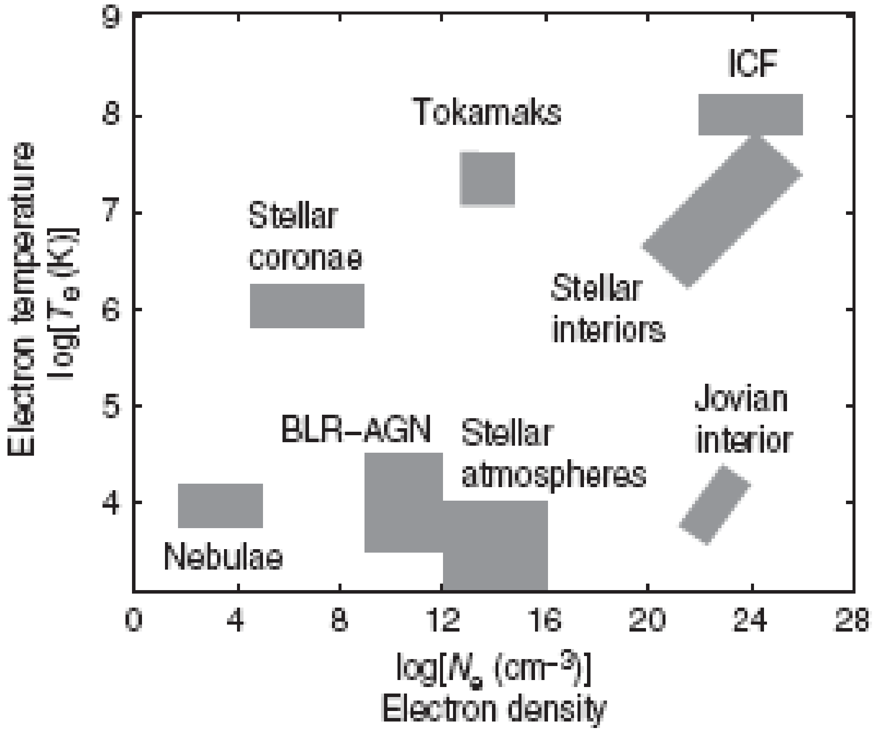
Radiative opacity

$$\Sigma(cm^2/g) = N\sigma$$

❑ Play important role in systems where radiation-matter interaction is prevalent.

- Systems at high temperature
  High radiation energy density
- Systems at high density
  small mean free path

Radiation-matter interaction in plasma



(Taken from book ***'Atomic Astrophysics and Spectroscopy'*** by **Anil K. Pradhan & Sultana N. Nahar, Cambridge University Press, 2011**)

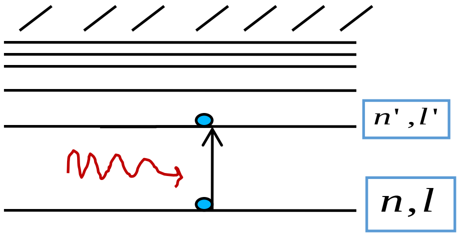
Most of the laboratory & astrophysical systems are in plasma state containing **atoms, ions and free electrons**.

Application of Radiative properties

- ❑ Radiative opacity modelling
- ❑ Study of ionization balance in plasma
- ❑ Equation of state of plasma
- ❑ Plasma diagnostics

Radiative properties of atoms/ions

Photoexcitation (Bound-Bound Transition)



Oscillator strength

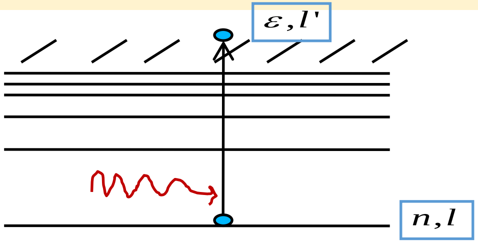
$$f_{nl\rightarrow n'l'} = \max(l,l') \frac{(E_{n'l'} - E_{nl})}{3(2l+1)E_H a_{bohr}^2} \left[R_{nl}^{n'l'}\right]^2$$

$$R_{nl}^{n'l'} = \int R_{n'l'} r R_{nl} dr$$

Requires knowledge of

- Energy of bound levels
- Wave functions of bound states
- Wave functions of Continuum states

Photoionization (Bound-Free Transition)



Differential oscillator strength

$$E_h \frac{df}{d\nu} = \frac{1}{3(2l+1)\pi} \frac{h\nu}{E_h} \left[\frac{h\nu - |E_{nl}|}{E_h}\right]^{1/2} \left[(l+1) R_{nl}^{\varepsilon l+1\,2} + l R_{nl}^{\varepsilon l-1\,2}\right]$$

$$R_{nl}^{\varepsilon l'} = \int R_{\varepsilon l'} r R_{nl} dr$$

$$H\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots\ldots, \mathbf{r}_N) = \mathbf{E}\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots\ldots, \mathbf{r}_N)$$

$$H = -\sum_{i=1,N} \frac{\nabla^2}{2} - \sum_{i=1,N} \frac{Z}{r_i} + \sum_{i,j} \frac{1}{r_{ij}}$$

Electronic structure of atomic system

$$H = -\sum_{i=1}^{N} \frac{\nabla^2}{2} - \sum_{i=1}^{N} \frac{Z}{r_i} + \sum_{i,j=1}^{N} \frac{Z}{r_{ij}}$$

- Main challenge is in dealing with the many electron-electron repulsive interaction.

- **Central field approximation** : Electron moves independently in the average field created by all other electrons & nucleus.

Electronic structure methods:

- Effective one electron potential method
  - **Model potential method**
- Self-consistent field methods
  - Hartree-Fock method with correlation treatment
  - Density Functional theory based methods etc…

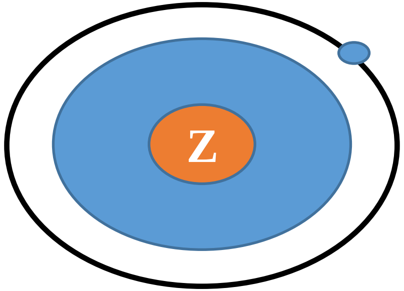
Model potential method

- The multi-electron interaction is modeled via effective one electron potential.

- The valance electron experiences the effective nuclear attraction due to screening of nuclear charge by core electrons.

$$\sum_i V(r_i) = -\sum_i \frac{Z}{r_i} + \sum_{i \neq j} \frac{1}{r_{ij}} \Longrightarrow V_{eff}(r) = -\frac{Z_{eff}}{r} = -\frac{N_c + (Z - N_c)e^{-\alpha r} + \beta r e^{-\gamma r}}{r}$$

- Parameters (α, β, γ) give information regarding many electron effect.
- These are optimized to take into account the effect of core electrons.



Numerical integration of radial Schrodinger equation for Bound state

$$\frac{d^2P_{nl}(r)}{dr^2}+\left(2E_{nl}-2V_{eff}(r)-\frac{l(l+1)}{r^2}\right)P_{nl}(r)=0$$

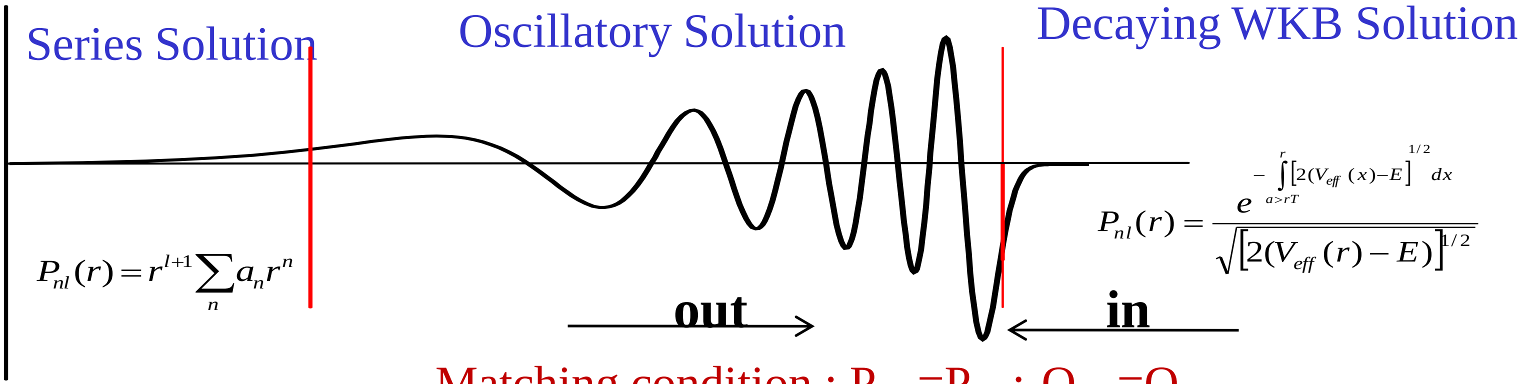
$$\Psi_{nlm}(r)=\frac{P_{nl}(r)}{r}Y_m^l(\theta,\varphi)$$

$$\frac{dP_{nl}}{dr}=Q_{nl}$$

$$\frac{dQ_{nl}}{dr}=-\left(2E_{nl}-2V_{eff}-\frac{l(l+1)}{r^2}\right)P_{nl}$$

Classically allowed region | Classically forbidden region

$$P_{nl}(r=0)=0$$



$$P_{nl}(r)=r^{l+1}\sum_n a_n r^n$$

$$P_{nl}(r)=\frac{e^{-\int_{a>rT}^{r}\left[2(V_{eff}(x)-E)\right]^{1/2}dx}}{\sqrt{\left[2(V_{eff}(r)-E)\right]^{1/2}}}$$

Matching condition : $P_{out}=P_{in}$; $Q_{out}=Q_{in}$

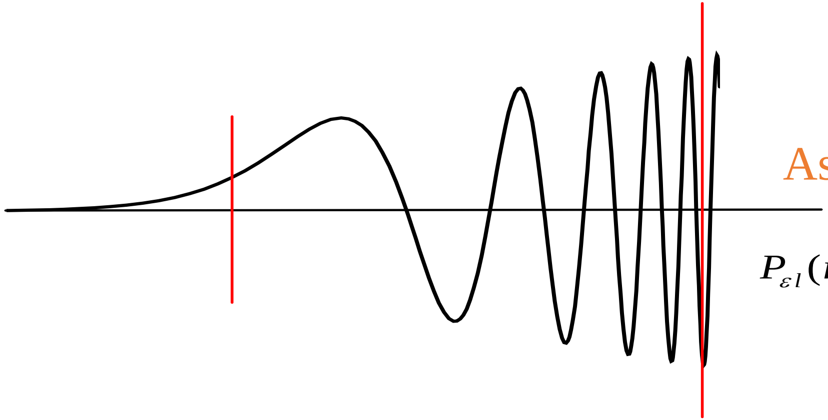
Numerical integration of radial Schrodinger equation for free state

$$\frac{d^2P_{\varepsilon l}(r)}{dr^2}+\left(2\varepsilon-2V_{D/IS}(r)-\frac{l(l+1)}{r^2}\right)P_{\varepsilon l}(r)=0$$

$$\Psi_{\varepsilon lm}(r)=\frac{P_{\varepsilon l}(r)}{r}Y_m^l(\theta,\varphi)\;;\;\varepsilon=\frac{k^2}{2}$$

$$\frac{dP_{\varepsilon l}}{dr}=Q_{\varepsilon l}$$

$$\frac{dQ_{\varepsilon l}}{dr}=-\left(2\varepsilon-2V_{D/IS}-\frac{l(l+1)}{r^2}\right)P_{\varepsilon l}$$



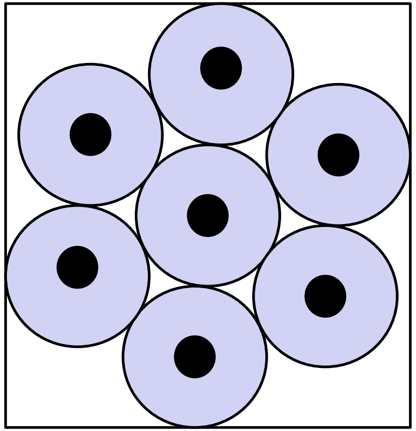
Series Solution

$$P_{\varepsilon l}(r=0)=0$$

Asymptotic Solution

$$P_{\varepsilon l}(r=\infty)\sim\sqrt{\frac{2}{\pi k}}Sin(kr-l\frac{\pi}{2}+\delta_{\varepsilon})$$

Modeling of effective potential in plasma



- Free electrons & neighboring ions modify the field in vicinity of ion.

- Modified Hamiltonian in plasma

$$H = -\sum_{i=1}^{N} \frac{\nabla^2}{2} - \sum_{i=1}^{N} \frac{Z}{r_i} + \sum_{i,j=1}^{N} \frac{Z}{r_{ij}} + V_{be} + V_{bi}$$

- Model potentials for plasma can be devised using static screening approximation
- Plasma effects:
  - ✓ Plasma free electrons ➔ **Screening of** nuclear charge seen by bound electrons
  - ✓ Finite density ➔ Confinement due to neighboring ions

Static screening is valid when plasma fluctuation takes place over a longer time.

Effective potential in plasma

Short range plasma potentials under static screening approximation

$$\Gamma = \frac{\text{Coulomb energy}}{\text{Thermal Energy}} = \frac{(Z^2 e^2 / a)}{k_B T}$$

$$a = \left(\frac{3}{4\pi n_{ion}} \right)^{1/3} = \text{interatomic distance}$$

Debye-Huckel Potential (DHP)

- Valid for weakly coupled plasma ($\Gamma < 1$)
- Plasma particles are non-degenerate

$$V_D(r) = -\frac{Z_{eff}\, e^{-r/\lambda_D}}{r}$$

$$\lambda_D = 1/\mu_D = \sqrt{\frac{k_B T}{4\pi n_e e^2}}$$

Effective potential in strongly coupled plasma

Ion Sphere Potential (ISP)

- For strongly coupled plasma ($\Gamma \geq 1$)
- plasma particles are non-degenerate ($T > T_F$)

$$V_{IS}(r) = -\frac{Z_{eff}}{r} + \frac{Z_0}{2R_{IS}}\left(3 - \left(\frac{r}{R_{IS}}\right)^2\right) \quad ; \quad r \leq R_{IS}$$

$$R_{IS} = \left(\frac{3}{4\pi n_{ion}}\right)^{1/3}$$

Quantum plasma Potential (QP)

- For strongly coupled plasma ($\Gamma \geq 1$)
- plasma particles are degenerate ($T<T_F$)

$$V_Q(r) = -\frac{Z_{eff}}{r} e^{-r/k} \cos(r/k)$$

$$k = \left(\frac{4m^2\omega_{pe}^2}{\hbar^2}\right)^{1/4} \qquad \omega_{pe} = \sqrt{4\pi n_e e^2 m}$$

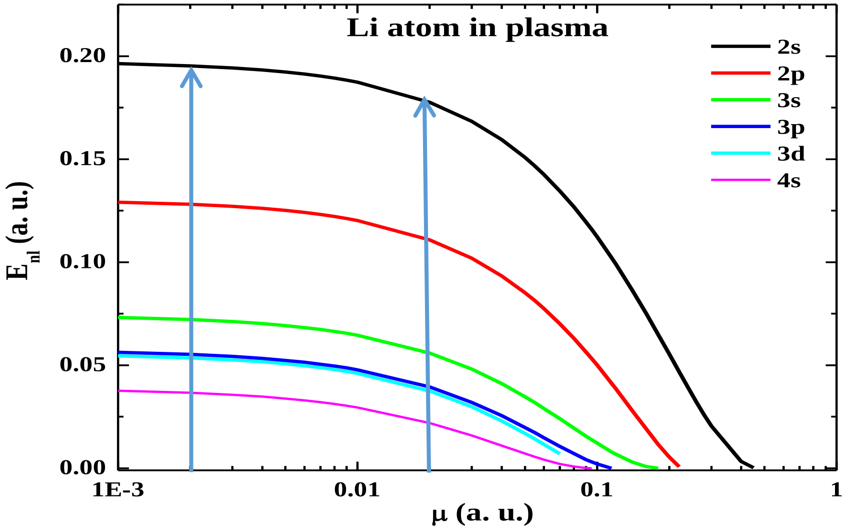
Results & Discussion

Effect of plasma on energy level

Continuum lowering : Phenomenon of decrease of ionization potential of bound levels

- due to nuclear charge screening by free electrons bound electrons feel less attraction.
- bound levels are lifted up in energy and hence the ionization potential is lowered.
- Higher excited states are affected by screening as well as quantum confinement due to plasma ions.
- For critical screening strength, levels merge into continuum leading to pressure ionization of levels

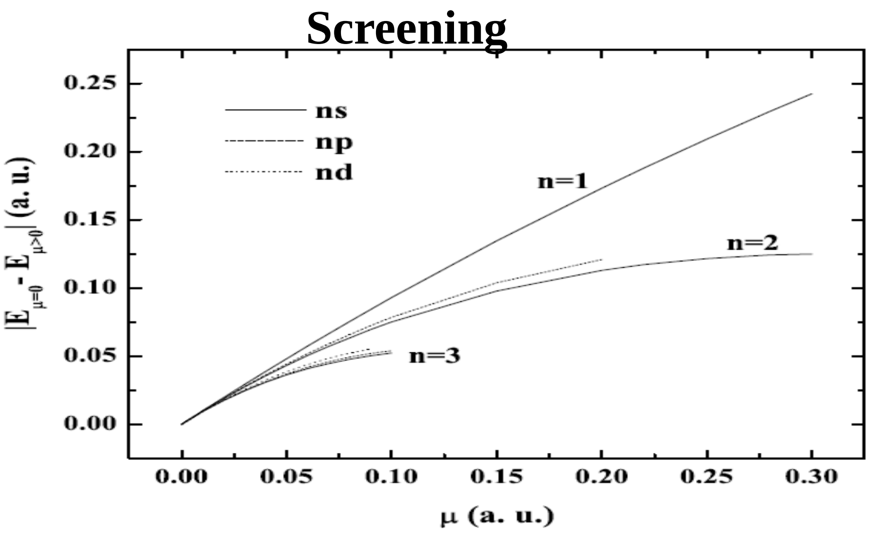
$$V_{eff}(r) = -\frac{Z_{eff}}{r} e^{-\mu_D r} = -\frac{N_c + (Z - N_c)e^{-\alpha r} + \beta r e^{-\gamma r}}{r} e^{-\mu_D r}$$

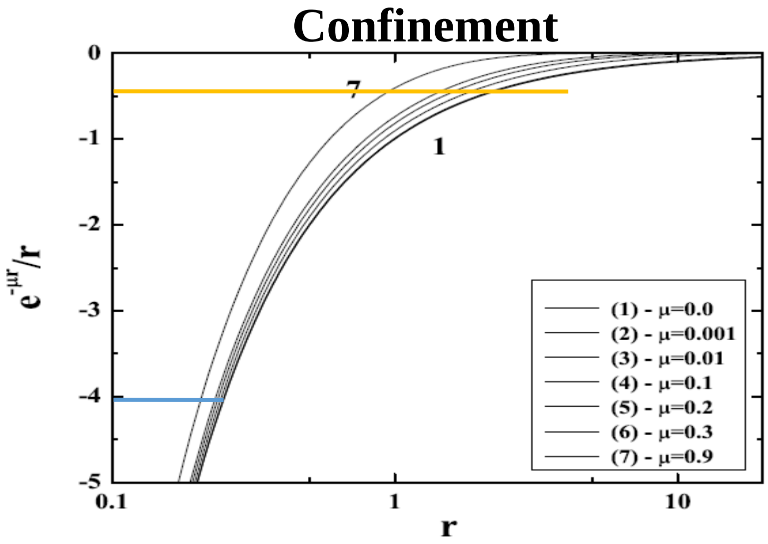


Pressure ionization: Phenomenon of merging of bound levels into continuum as a result of confinement

- Due to overlap of wave functions of neighboring ions

Effect of plasma on energy level





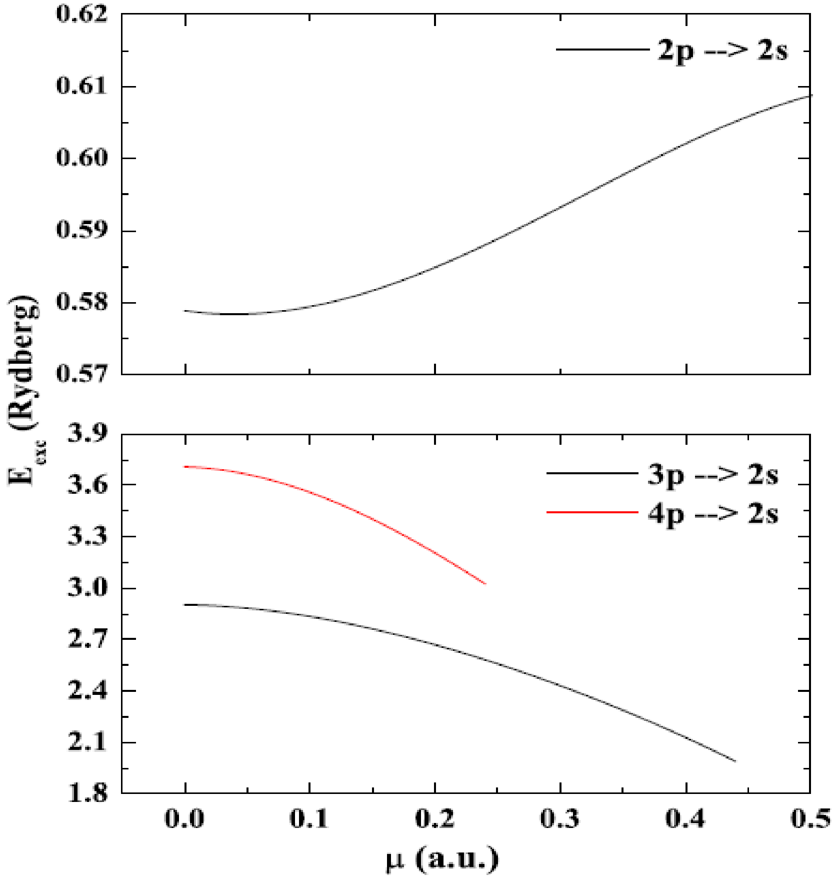
- Effect of Screening depends on principal quantum number '*n*'.
  - ✓ ***Shift in energy of lower 'n' states are more***
- Effect of Confinement depends on angular momentum quantum number '*l*'.
  - ✓ ***Higher 'l' states lie close to the edge of potential and are lifted up more for same 'n'***

Effect of plasma on energy level

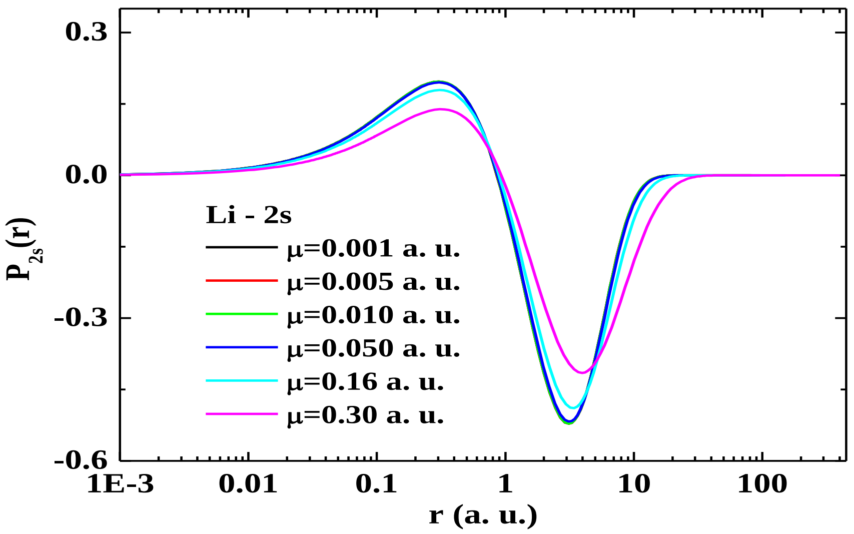
Shift in transition line:

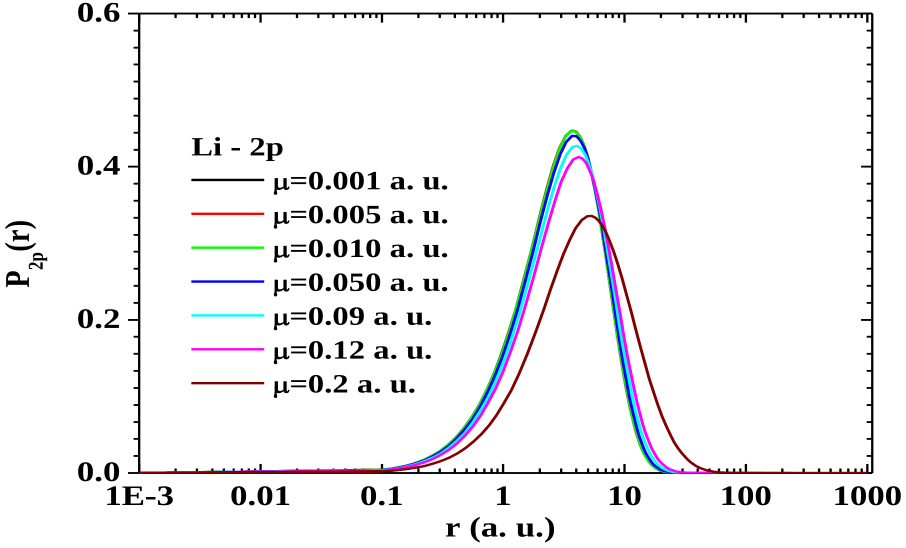
Due to different effect of screening and confinement on (*n*,*l*) states, behavior of line shift due to plasma is different.

- Δn=0 transition ➔ Lines shift towards higher energy (Blue shift)
- Δn ≠ 0 transition ➔ Lines shift towards lower energy (Red shifted)



Effect on bound state wave function

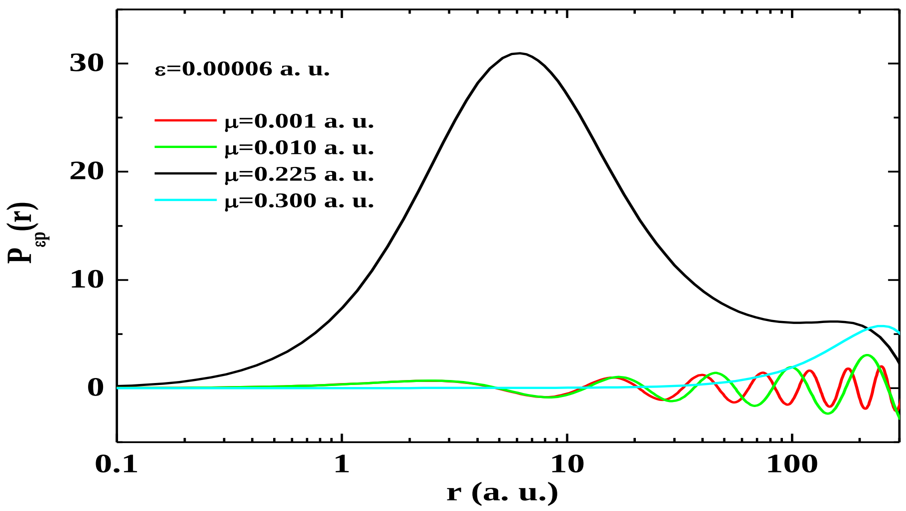


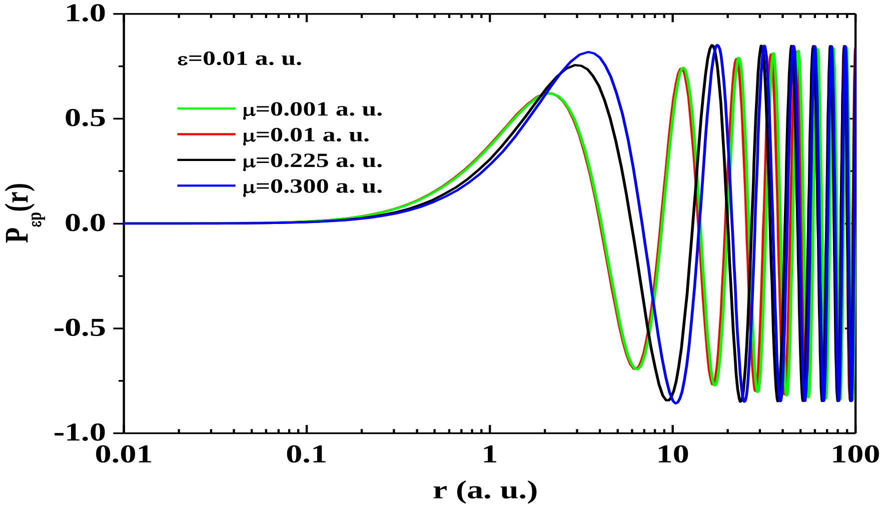


- Wave functions spread in space leading to delocalization of bound levels.

- Outer excited wave functions are affected more.

Effect on continuum state wave function





- Amplitude and phase are affected by plasma environment.
- The variation is prominent for low energy states which are in the field of nuclear potential
- Modified nuclear potential has **no appreciable** effect on high energy continuum electrons

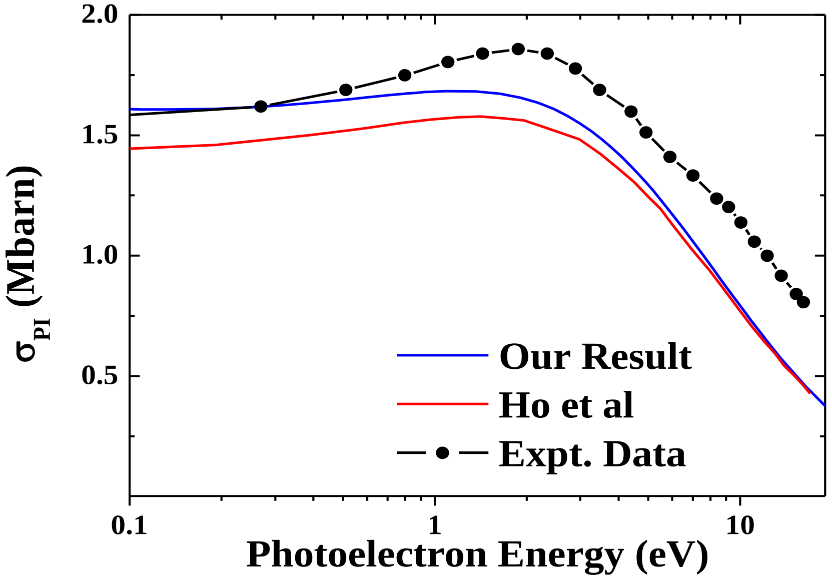
Ground state photoionization cross section of isolated Lithium atom

In non-relativistic dipole approximation

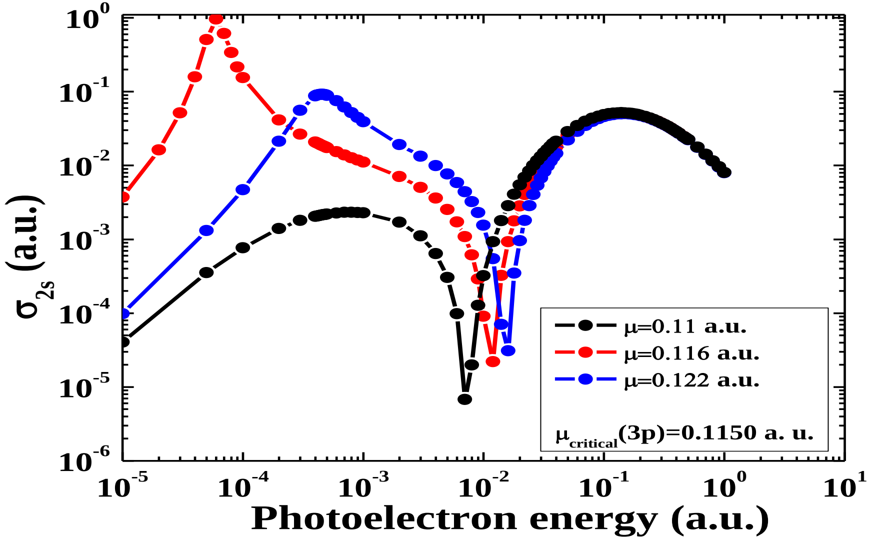
$$E_h \frac{df}{d\nu} = \frac{1}{3(2l+1)\pi} \frac{h\nu}{E_h} \left[\frac{h\nu - |E_{nl}|}{E_h} \right]^{1/2} \left[(l+1) R_{nl}^{\varepsilon l+1^2} + l R_{nl}^{\varepsilon l-1^2} \right]$$

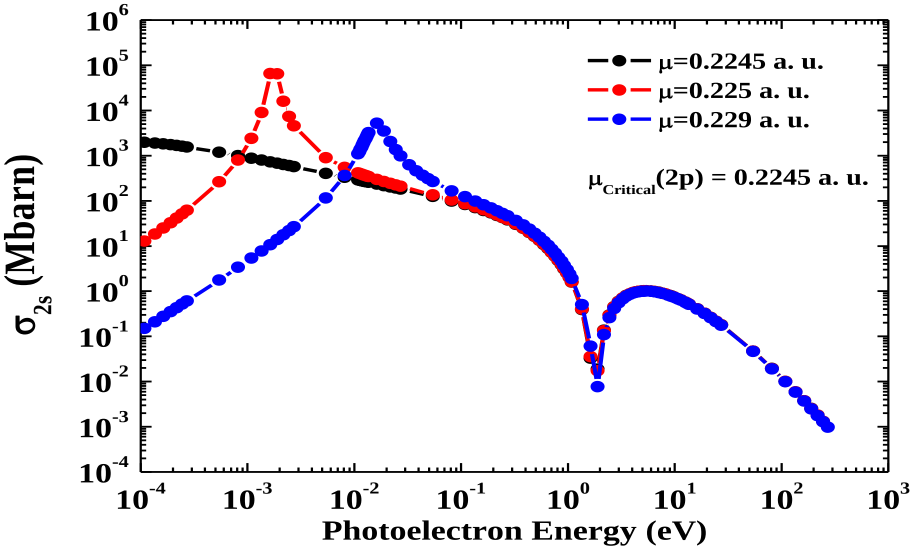
	[1]	[2]	[3]	[4]
σ^{Th}(Mb)	1.6	1.4	1.5	1.54 $\pm$ 0.23
σ^{Peak}(Mb)	1.72	1.58	1.66	1.86 $\pm$ 0.28
E^{Peak}(eV)	1.5	1.4	1.4	1.9

1. ***This work.***
2. ***S. Sahoo, Y, K. Ho, Phys. Plasmas, 13 (2006)063301***
3. ***G. Peach, H. E. Saraph et al. J. Phys. B, 21 (1988) 3669.***
4. ***R. D. Hudson, V. L. Carter, J. Opt. Soc. Am., 57 (1967) 657.***



Lithium atom in Debye plasma





- ❖ Appearance of Resonance structures at specific values of screening

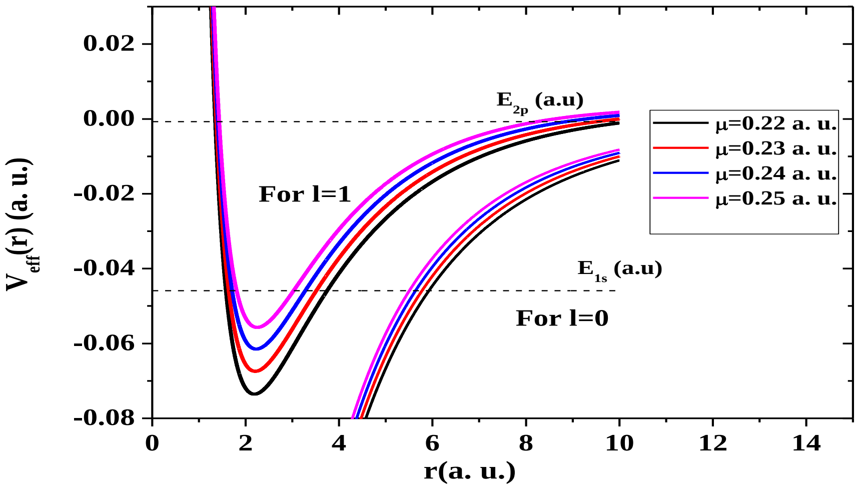
  Shape Resonance :Due to presence of quasi-bound 'p' level.

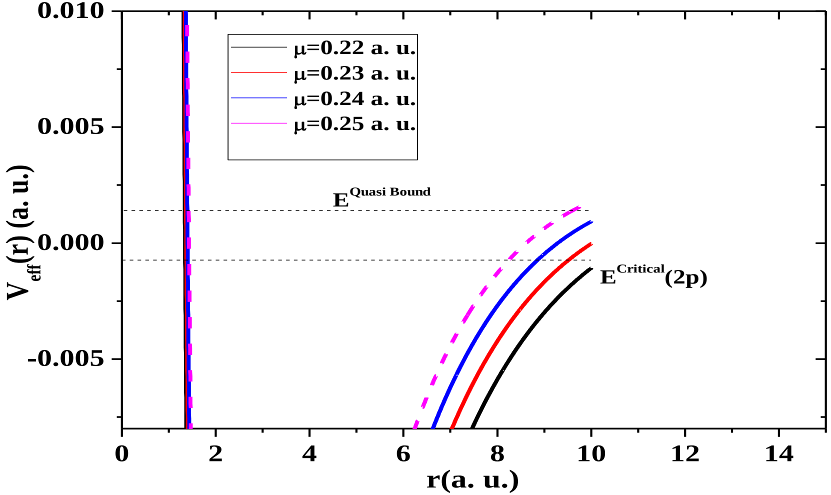
- ❖ Appearance of Minimum for certain photoelectron energy

  Cooper Minimum: Due to variation in phase of continuum state

Shape resonances in Lithium atom in Debye plasma

Due to centrifugal barrier, potential can support positive energy bound states



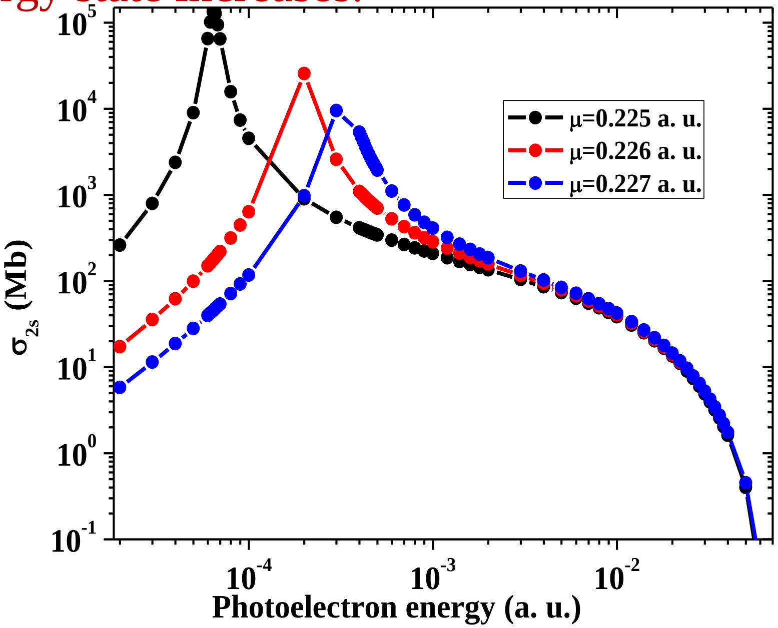


- At μ_c bound level enters into continuum due to pressure ionization ➔ quasi-bound state is formed.
- Ionized electrons are trapped in these QB state for finite time ➔ enhancement in bound-free transition probability.

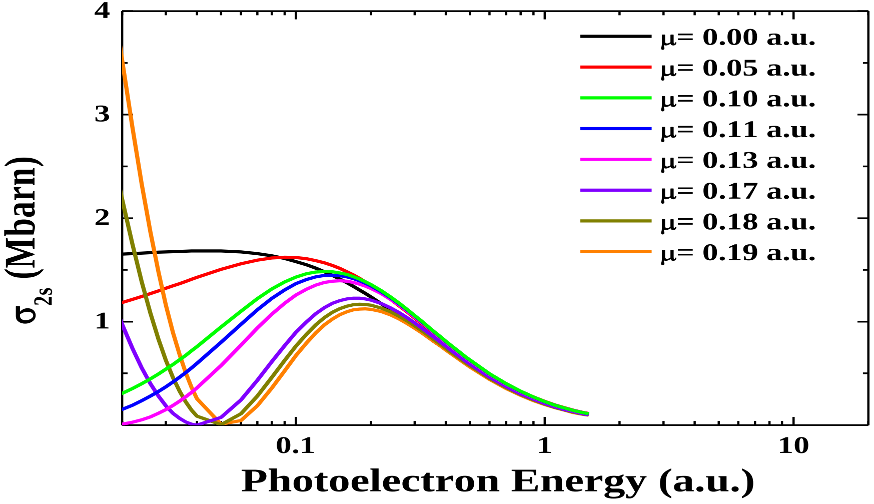
Shape resonances are related to the shape of potential and hence can be a measure of size of the system.

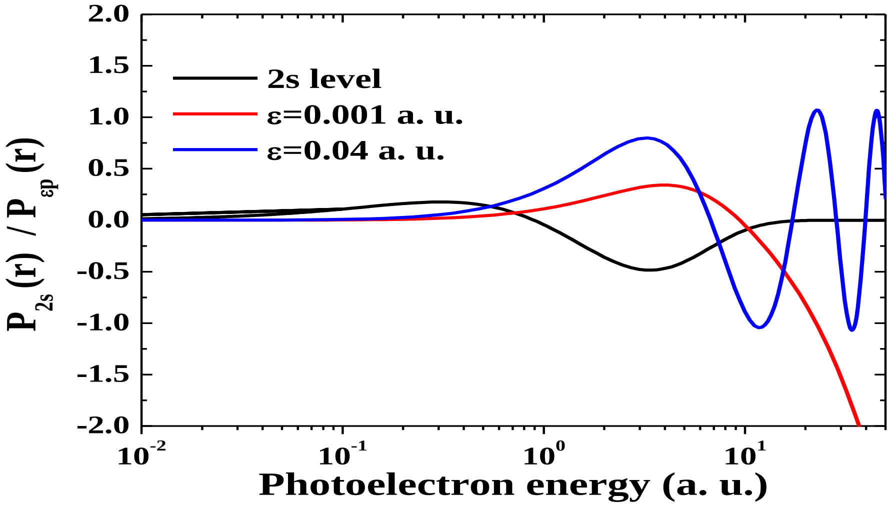
Shape resonances in Lithium atom in Debye plasma

- For $\mu > \mu_c$, quasi bound states move towards peak of centrifugal barrier.
- The shape resonance gradually shifts to higher energies.
- The probability of tunneling from higher energy state increases.
- Resonance peak gets broadened



Cooper minimum in Lithium atom in Debye plasma





- For particular μ_{Cooper}, zeros appear in bound-free matrix element **(termed as Cooper minimum)**
- Modification in core interaction due to plasma screening results in **constructive and destructive interference of dipole matrix elements** for different regime of photon energy.
- *Appears for states having at least one node i.e. n-l-1 >0*

Summary & Future Direction

- ❑ Effect of plasma on energy level
  - ❖ Continuum lowering & pressure ionization
  - ❖ Red and Blue shift in transition lines
- ❑ Effect of plasma on wave function
  - ❖ Delocalization of bound & continuum wave function
  - ❖ Phase shift in continuum wave function
- ❑ Effect of plasma on photoionization cross section
  - ❖ Shape resonances due to quasi bound pressure ionized states
  - ❖ Cooper minimum due to phase shift in continuum wave

Future Direction

- ❖ Model potential method for plasma is fast and can be used in-line to get radiative properties of plasma.
- ❖ It is more accurate than the widely used Screened hydrogenic model in radiative opacity modeling.
- ❖ We aim at employing this methodology to improve the radiative opacity modeling.

Acknowledgements

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Thank You