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Numerical and Theoretical Treatment of Electron-Impact Ionization

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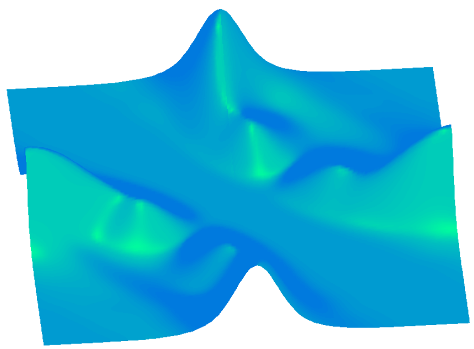

Electron-Impact Ionization

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simplest example: ionization of atomic hydrogen

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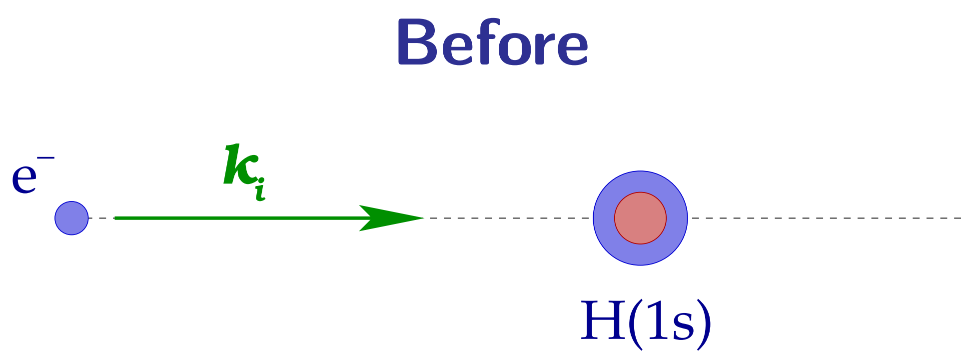
simplest example: ionization of atomic hydrogen

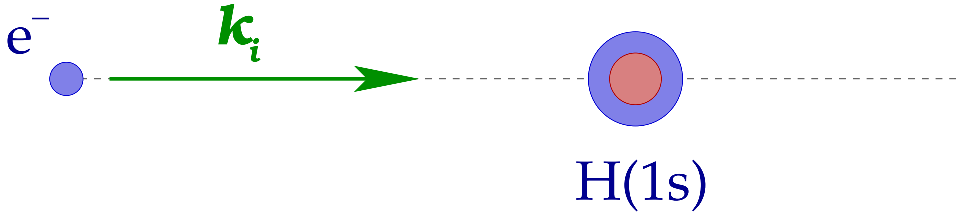
$$\mathbf{e^- + H \longrightarrow H^+ + e^- + e^-}$$

- Initial State: free electron incident on ground state hydrogen
- Final State: two free electron's outgoing from a proton
  - three-body problem
  - long-range Coulomb forces



Free electron (momentum $\hbar k_i$) incident on a ground state hydrogen atom.

Before



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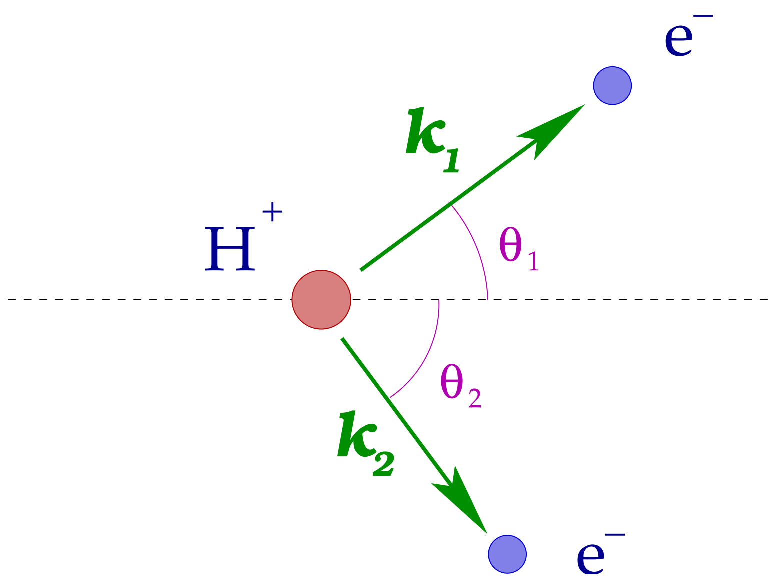
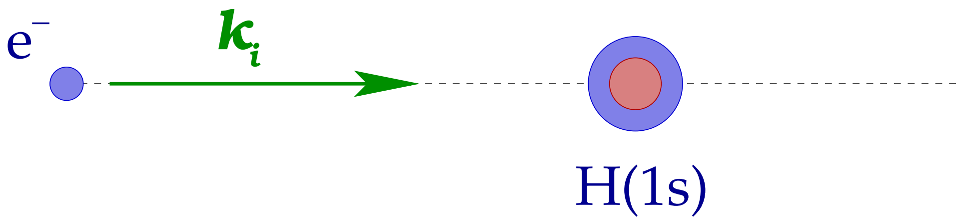


- Two outgoing electrons
- Two scattering angles
- Energy shared continuously between two outgoing electrons

Colinear Model

Before



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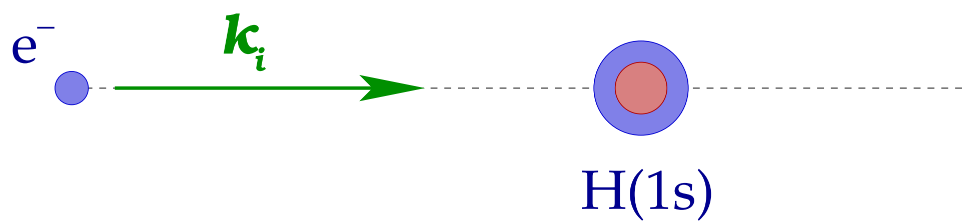

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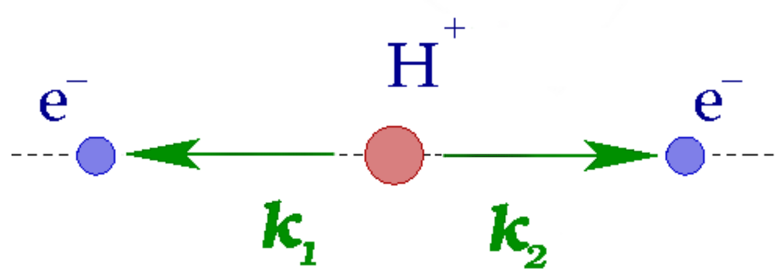

- Two outgoing electrons
- Constrained to a π scattering angle, thus no angular momentum
- Energy shared continuously between two outgoing electrons

Importance of Boundary Conditions

- Cross sections are calculated by extracting scattering information from quantum mechanical wave functions.
- Calculating the correct wave function is, by far, the most computationally intensive step.
- $\approx$35 years of research overcoming formal difficulties.

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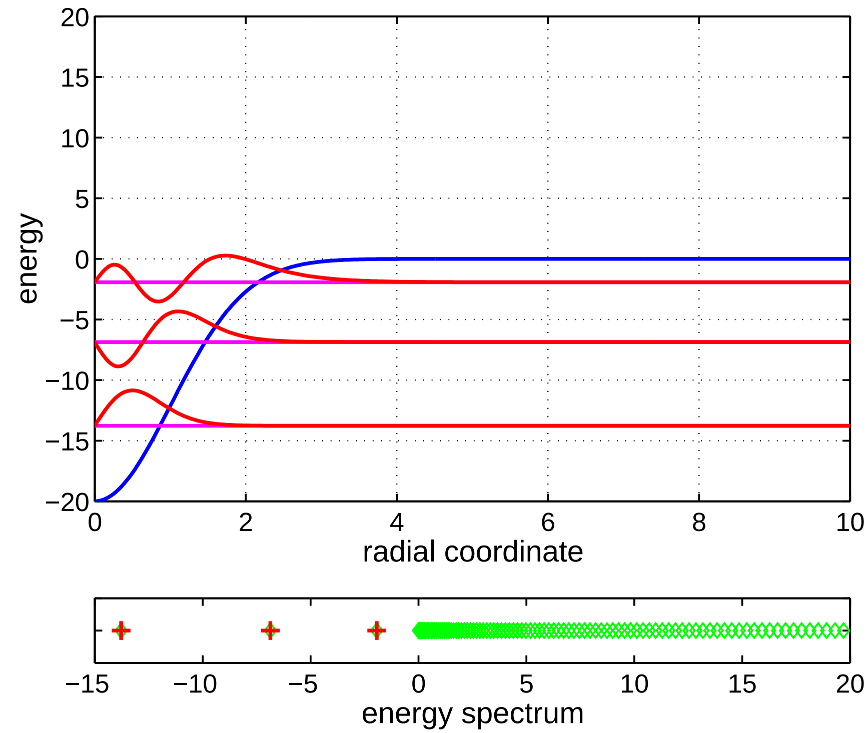
Specifying Boundary Conditions

- Describing electron-impact ionization:
  - two electrons "in the continuum",
  - energy can be shared continuously between them,
  - existence of long-range Coulomb forces.
- Difficult to even specify correct boundary conditions, let alone implement them in a calculation.

Boundary Conditions Refresher

- Short-range potential well
- One-dimensional (radial) problem
- Find solutions to $H\psi = E\psi$ (eigenvalue problem)



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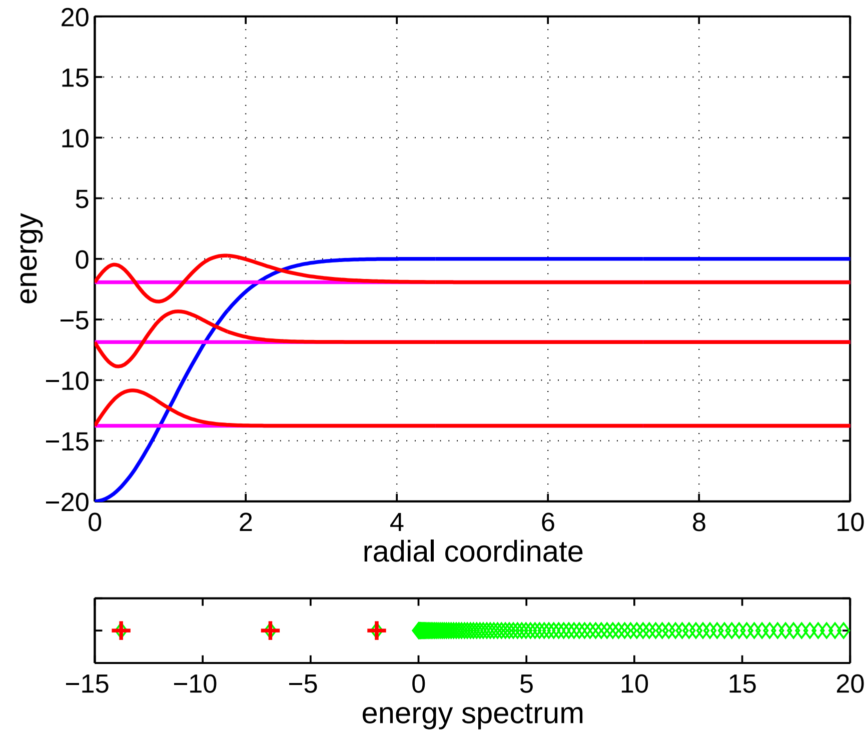


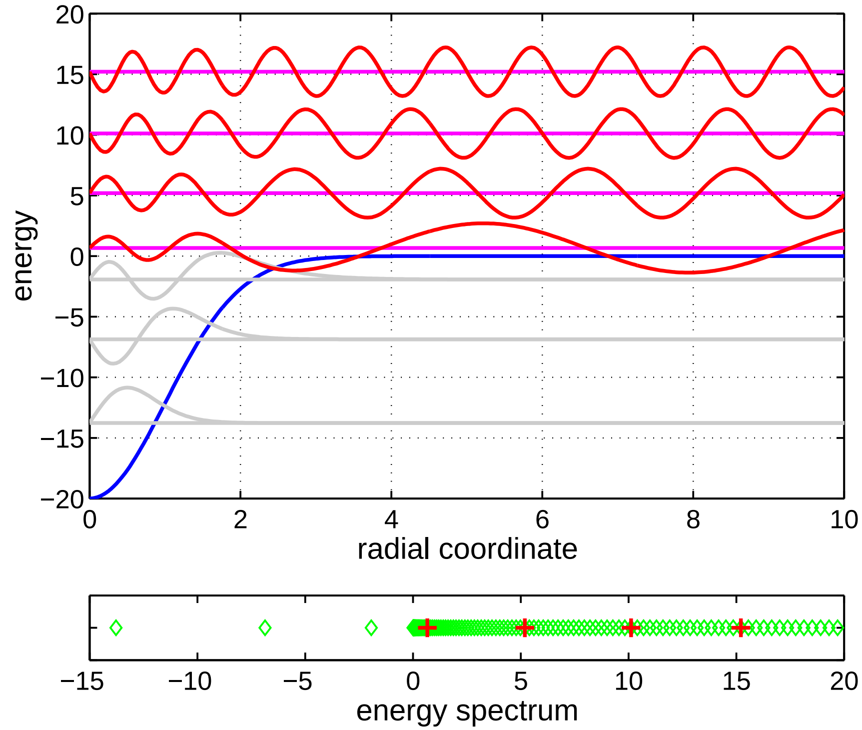
Bound States

- Energies are less than zero.
- Energies are restricted to discrete values.
- Wave functions go to zero as $r \longrightarrow \infty$.

Free Particle Wave Functions

Positive energies correspond to the particle being free.

- Positive energy spectrum is a continuum, not quantized.
- Wave functions are unbounded
- but they do have a well-defined (large r) asymptotic form.



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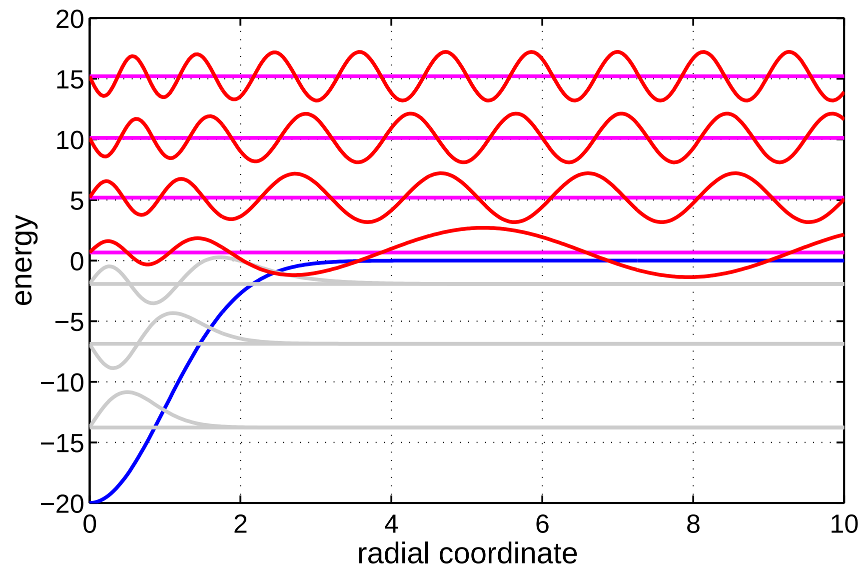

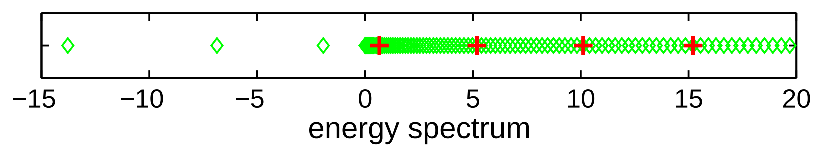

Ionization Problem

- Two electrons are free — “double continuum”.
- Asymptotic form is difficult to define and is reached only for very large separations of all three particles due to presence of Coulomb forces.

Scattering Boundary Conditions

- Scattered electron is moving outward in r.
- Asymptotic form of wave function $\sim e^{ikr}$
- momentum of scattered electron is $\hbar k$.

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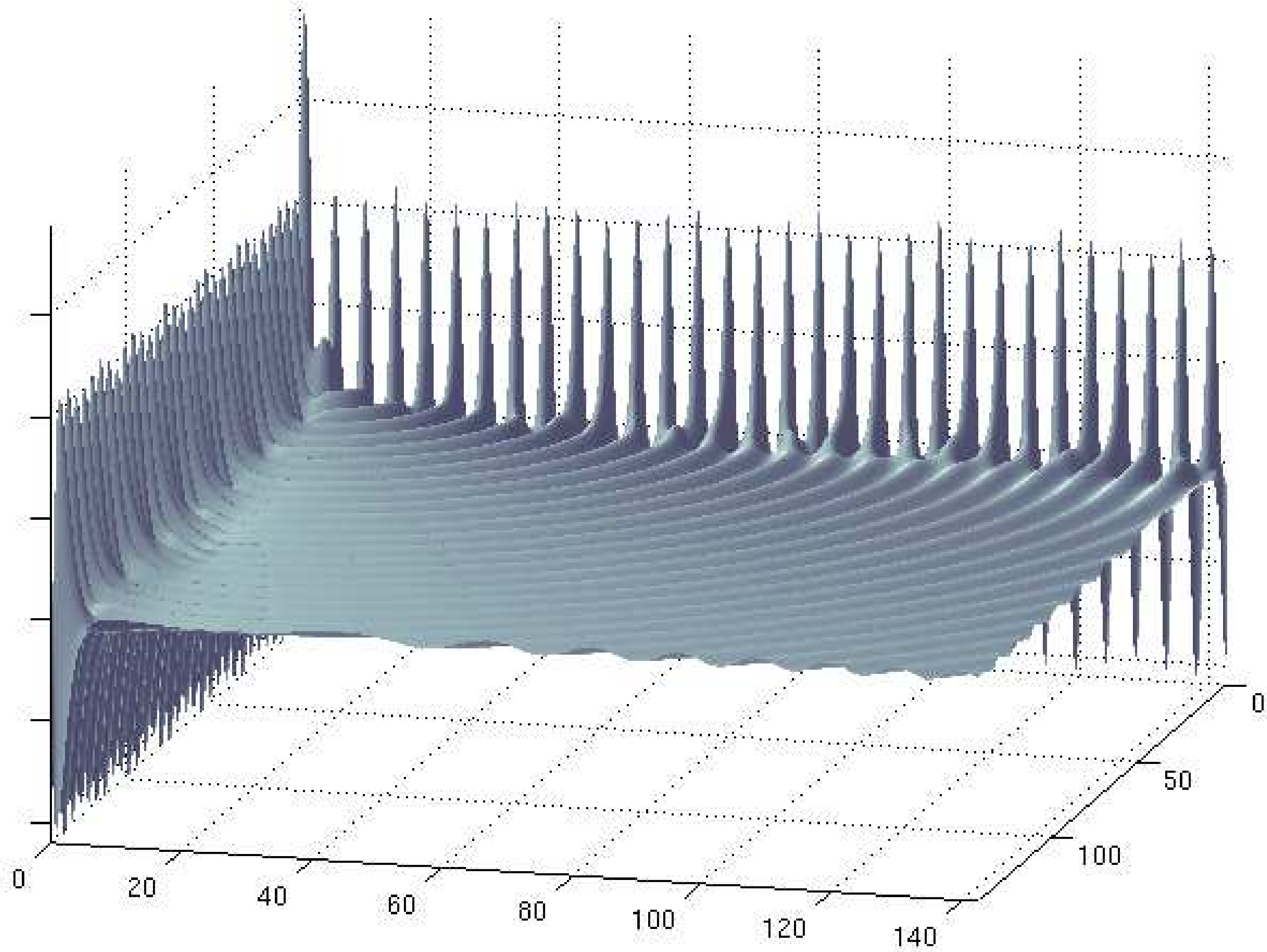
Electron-Impact Ionization

- Long-Range Coulomb Forces
  - Outgoing asymptotic form is a bit more complicated.
  - Asymptotic form is reached more slowly.
- "Double-Continuum"
  - Outgoing asymptotic form is much more complicated.
  - Asymptotic form is reached much more slowly.

Need to avoid having to specify the correct asymptotic form.

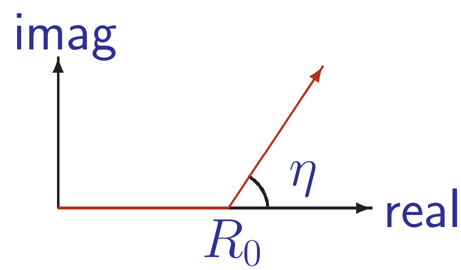
Example Radial Function:



Simplify Boundary Conditions with Exterior Complex Scaling

We do not need to explicitly specify the correct asymptotic form if we simplify the scattering boundary conditions using exterior complex scaling.

The wave function is calculated on a complex coordinate system defined by rotating the radial coordinates into the upper-half of the complex plane beyond some distance R_0.



Mathematically, this complex contour is defined as

$$r \rightarrow \begin{cases} r, & r < R_0, \\ R_0 + (r - R_0)e^{i\eta}, & r \geq R_0, \end{cases}$$

where η is the complex coordinate rotation angle.

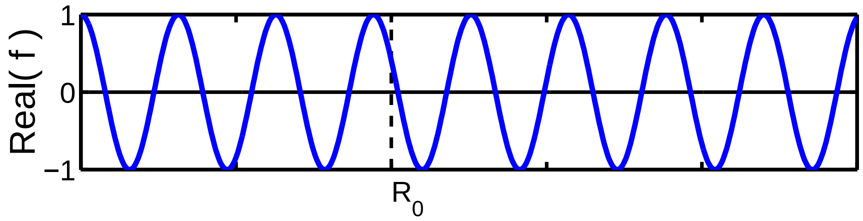
Any outgoing wave will decay exponentially on the complex contour.

Simplify Boundary Conditions with Exterior Complex Scaling

To see how ECS simplifies the outgoing wave boundary conditions consider the canonical asymptotic form of an outgoing wave.

$$f(r) = e^{ikr}$$

Without ECS: $f(r) = e^{ikr}$ has infinite range.



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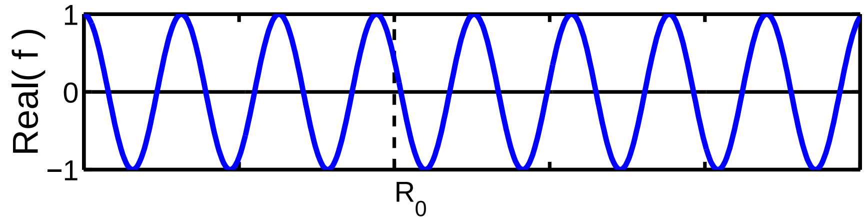
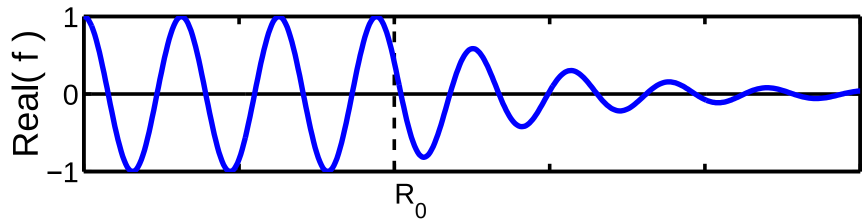
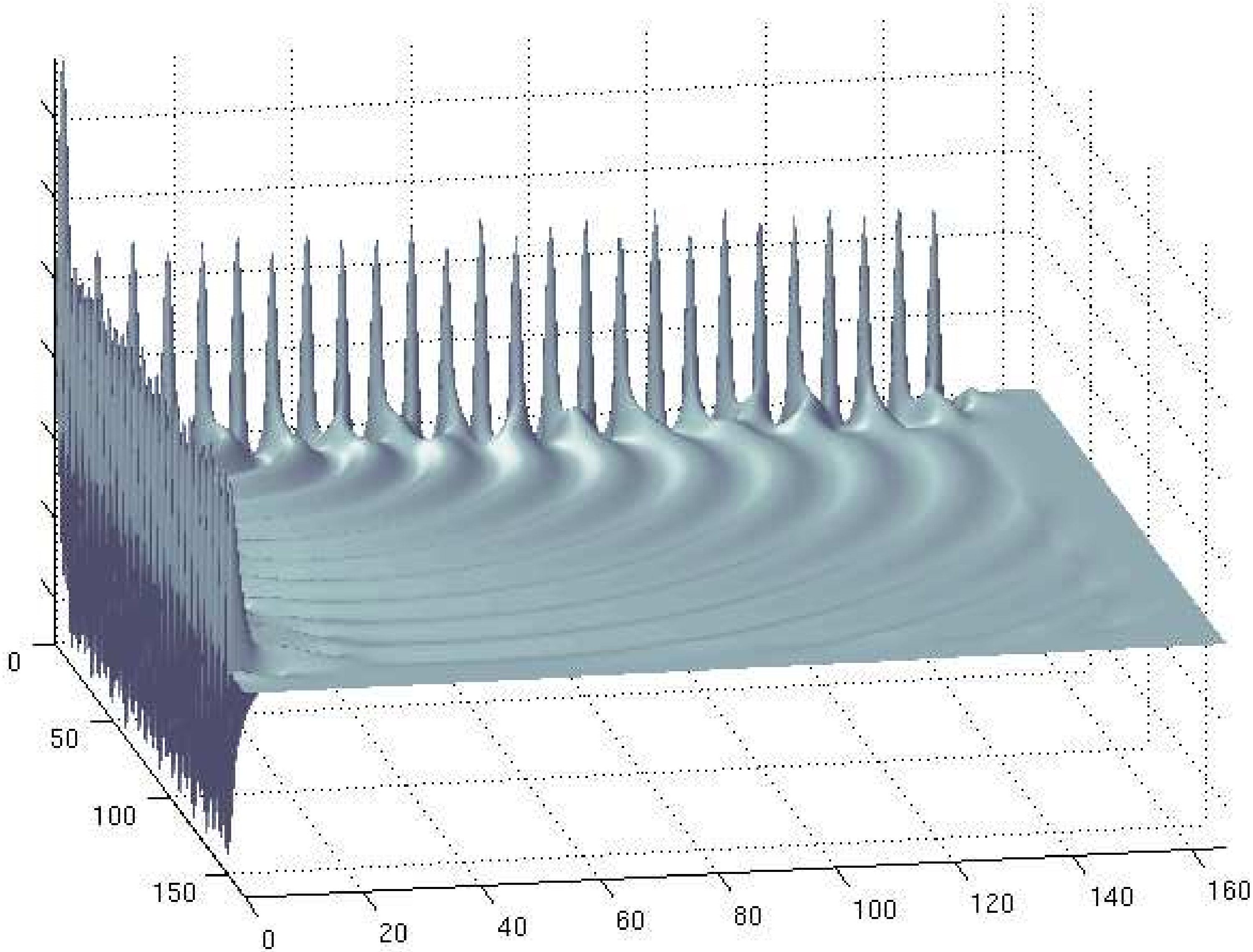


With ECS: $f(r)$ decays exponentially beyond R_0.



The same holds true for any outgoing wave.

Example Radial Function:



Future Work

- Calculate the crossectional area of the wave function using the DVR basis.
- Expand our DVR implementation from the colinear model to the full 3 dimensional problem
- On to collisions with multi-electron atoms.