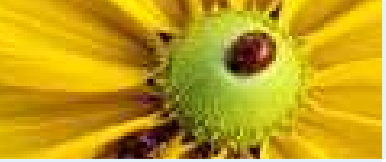
Driven Schrödinger approach to quantum scattering

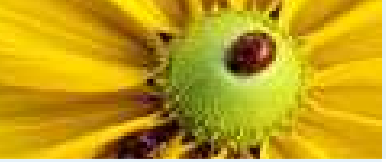
Nils Elander, Mikhail Volkov, Åsa Larson, Michael Stenrup, Zsolt Mezei,
Evgeny Yarevsky and Sergey Yakovlev

October 13, 2008



Outline

- Motivation
  - -Resonances in 3-Body Scattering



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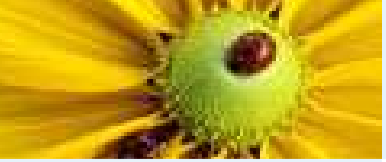

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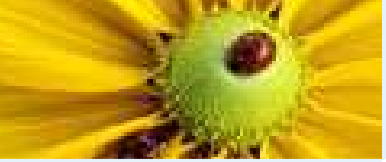

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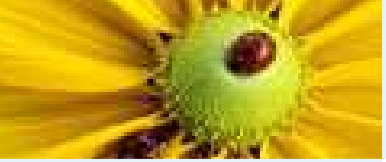

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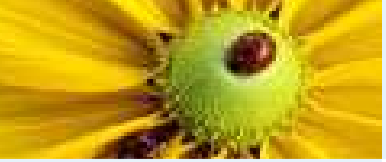

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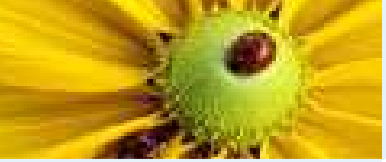

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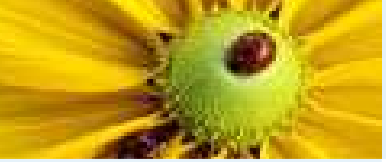

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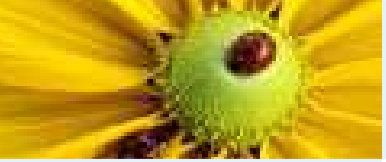

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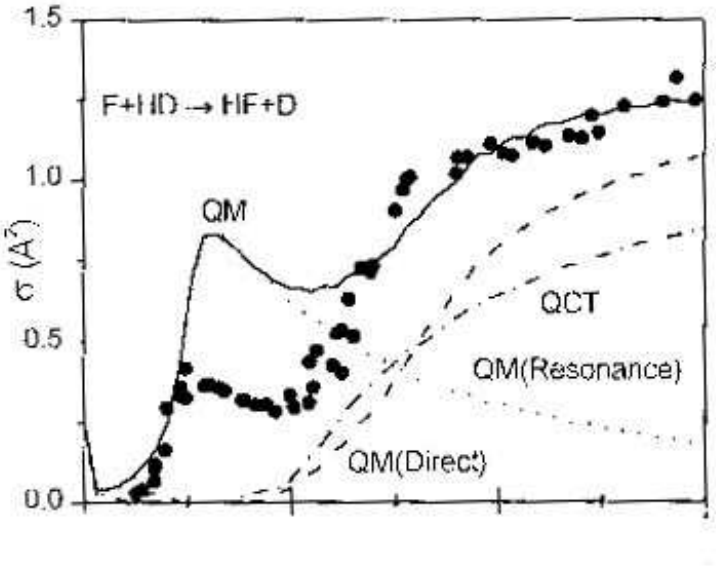
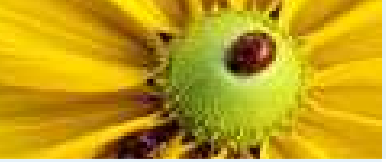
- Analysis of the Scattered wave.

- Experimental three-body atomic scattering has during the last 10 years reached high energy resolution allowing identifications of resonance structures.



Also atom-diatom collisions give evidence of resonances. Example : Measured (dots) and quantum mechanically calculated total cross sections (QM) incl. resonant and direct contributions for the channel $F + HD \rightarrow FHD \rightarrow HF + D$. (from [Phys.Chem.Comm. **5**,27(2002)].)



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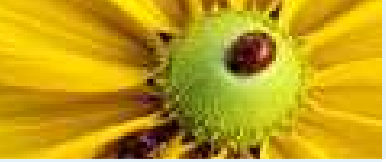

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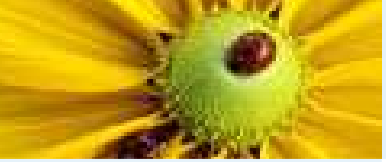
- $\longrightarrow$ Solve $H_{el}\Phi(\mathbf{r},\mathbf{R}) = W(\mathbf{R})\Phi(\mathbf{r},\mathbf{R})$ for fixed nuclear geometry - $R = R_{fixed}$ to obtain POTENTIAL ENERGY SURFACES $W(\mathbf{R})$



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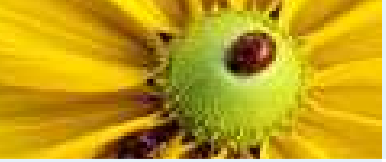

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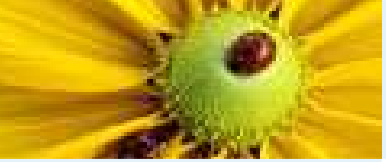

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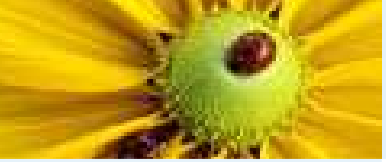

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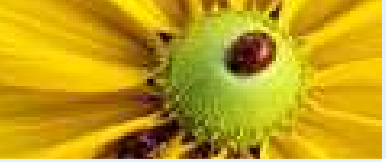
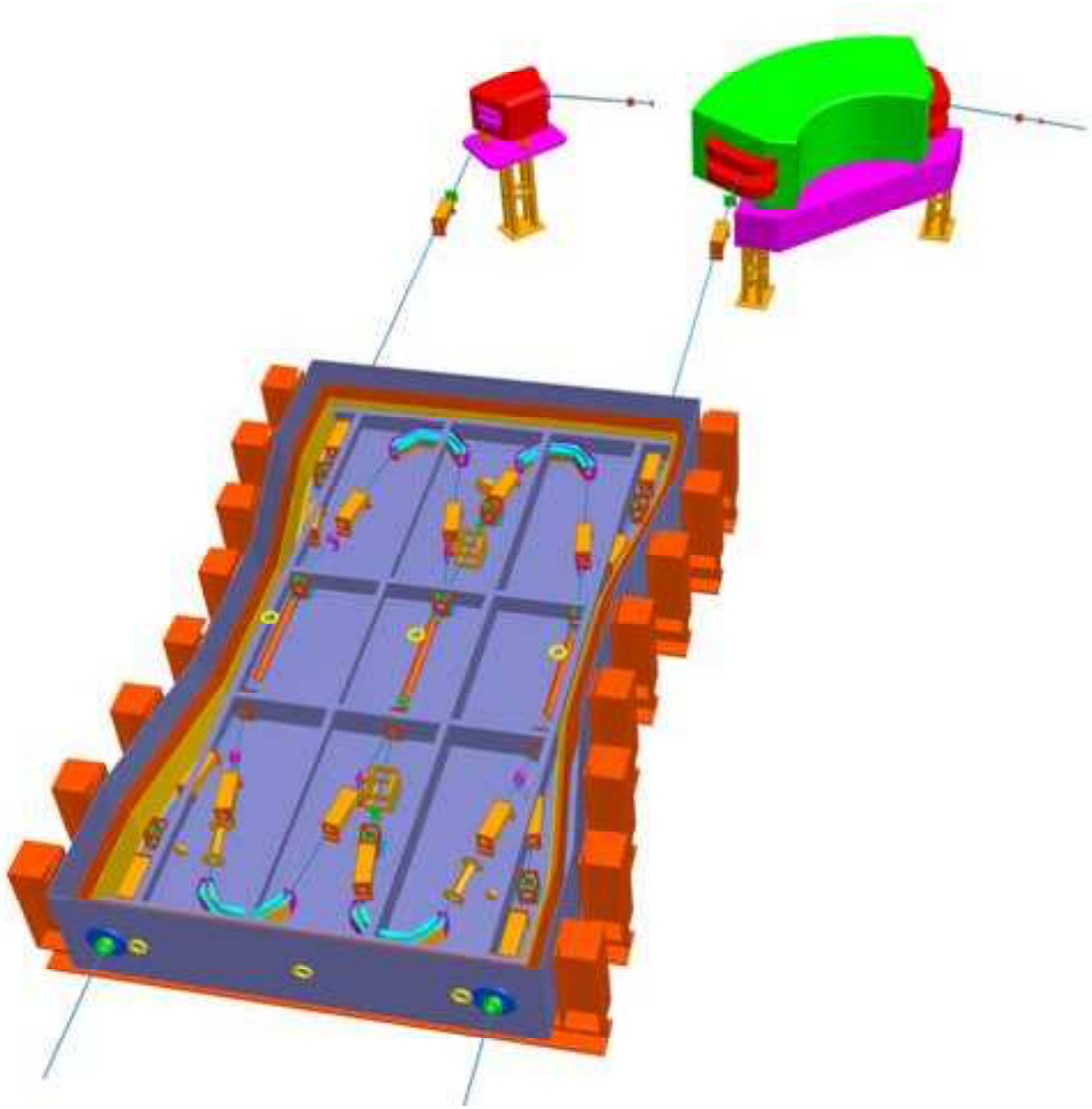
• Atomic and molecular scattering involve **nuclei moving on the electronic potential energy surfaces** and **jumping between them**.

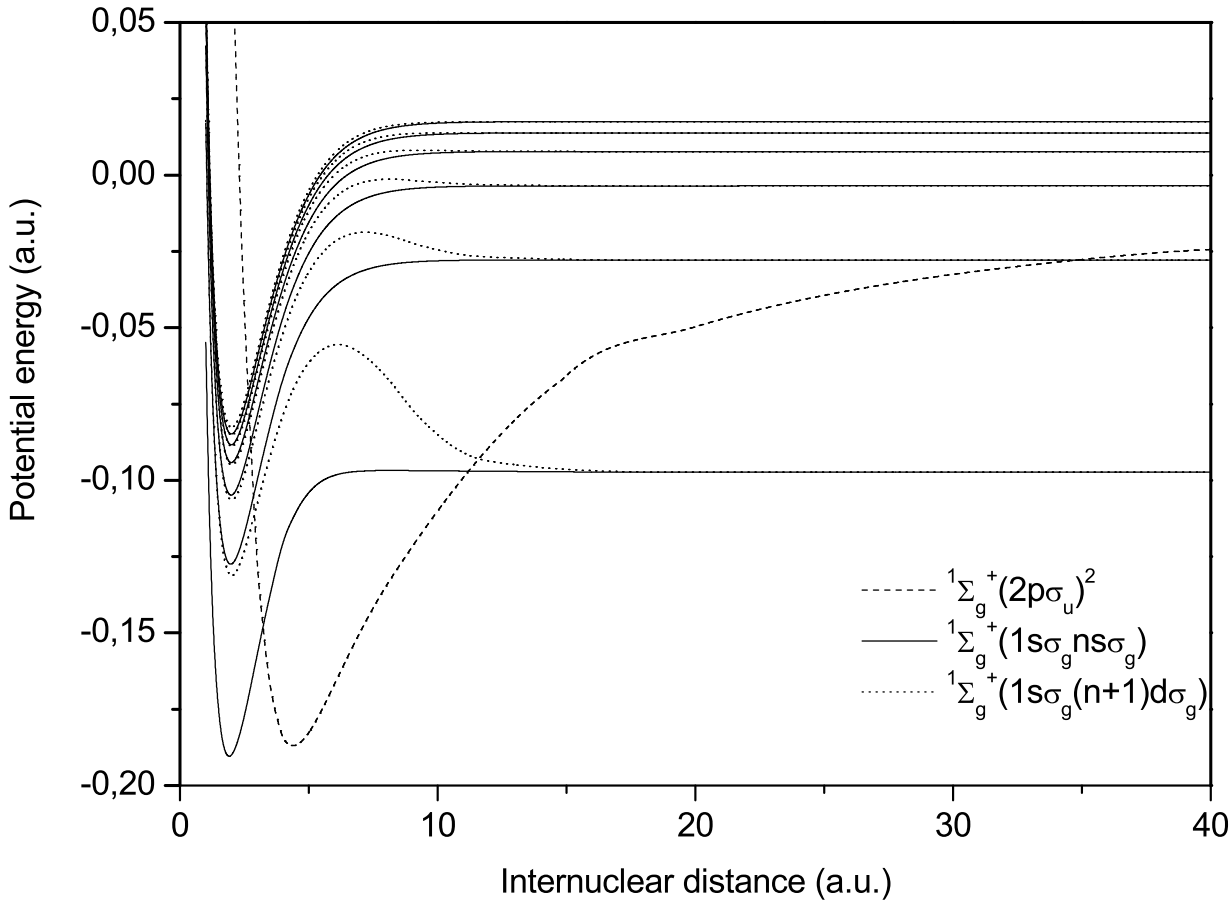
• The nuclear motion is represented as a potential scattering problem where $W(\mathbf{R})$ is a continuous set of potential energy surface matrices - one for each nuclear geometry - **R**.

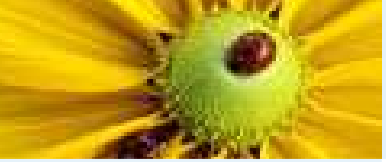


Motivation at home : The Storage ring Desiree under construction at the Manne Siegbahn laboratory in Stockholm



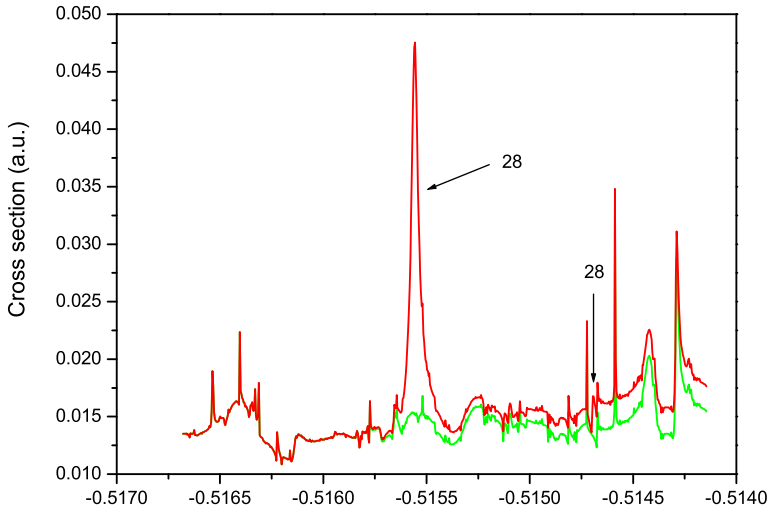
The lowest diabatic ${}^1\Sigma_g^+$ potential energy curves for the $H^+ + H^-$ mutual neutralization reaction.





Example 1: Mutual neutralization $H^+ + H^-$

The red curve illustrates the full channel cross section for the channel $\mathbf{H^+ + H^- \rightarrow H_2(^1\Sigma_g^+) \rightarrow H(n=1) + H(n=5)}$ as a function of the relative collision energy



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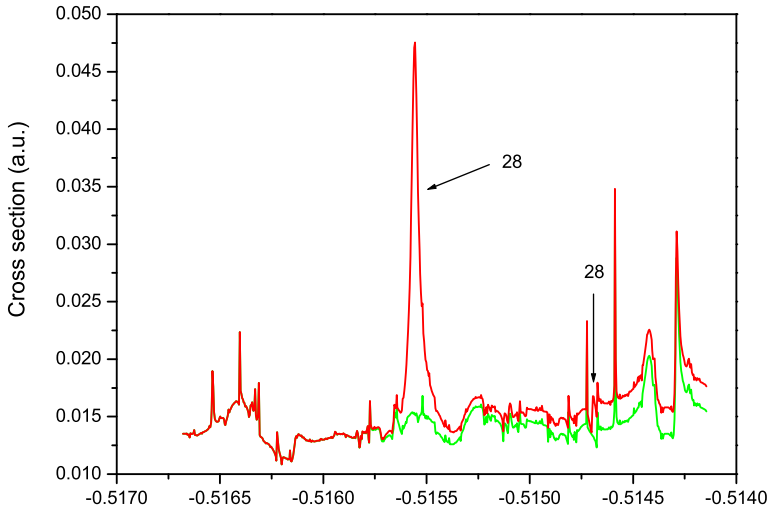
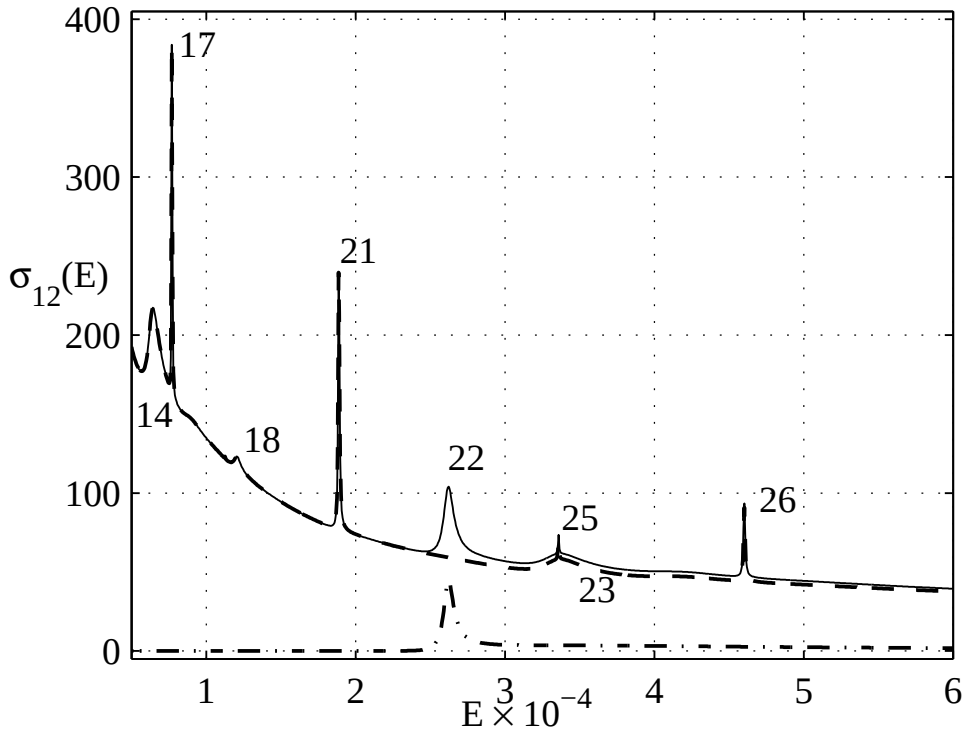
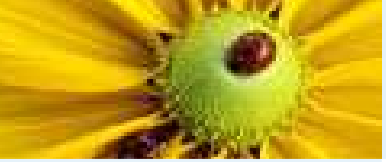


while the green curve shows the corresponding cross section when the contribution from the partial wave $J = 28$ is subtracted. This identifies the origin of two peaks in the full channel cross section.

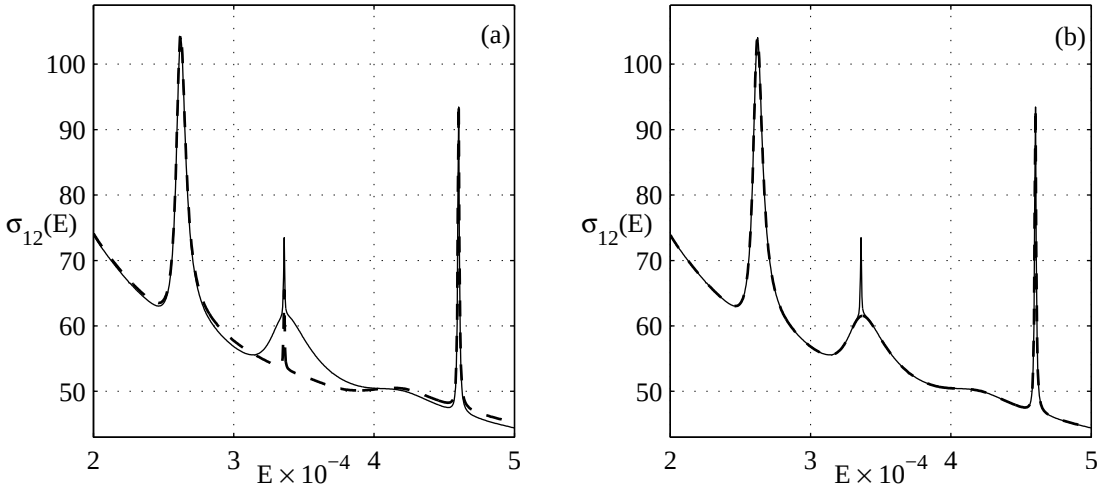
The $\mathbf{N^{3+} + H \rightarrow (NH)^{3+} \rightarrow N^{2+} + H^{+}}$ charge transfer cross section (channel $1 \rightarrow 2$) in then region $5 \cdot 10^{-5} - 6 \cdot 10^{-4}$ atomic energy units. The full drawn line shows the converged cross section, $\sigma_{tot,12}(E)$. The dash-dotted line illustrates the partial wave cross section $\sigma_{22,12}(E)$ while the dashed line displays the cross section described by $\sigma_{tot,12}(E) - \sigma_{22,12}(E)$



Now : Identification of the double bump labeled 23 and 25



Identifying resonances in a partial wave cross section ($\ell = 23$ and 25)



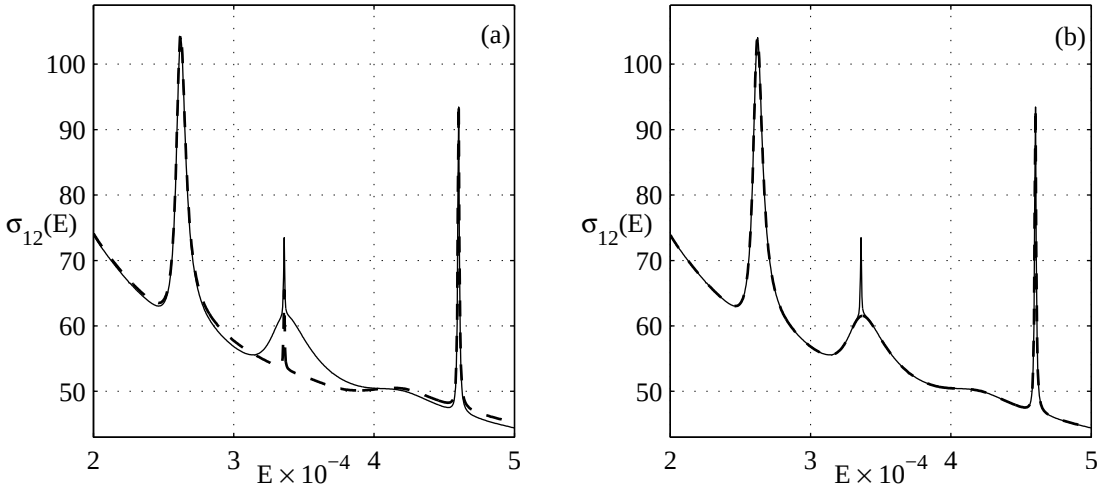
- The reduced partial wave S-matrix

$\tilde{S}_{\ell,ij}(E, E_k) = S_{\ell,ij}(E) - \ \mathcal{R}es\ [\ S_{\ell,ij}(E_k)\ ]/(E - E_k).$

- The reduced partial wave cross section

$\tilde{\sigma}_{\ell,ij}(E, E_k) = 4\pi(2\ell + 1)\left|(\tilde{S}_{\ell,ij} - \delta_{ij})/(2\imath k_i)\right|^2$

The full line describes the total cross section in the region of interest. The dashed lines shows in (a) the reduced cross section $\sigma_{tot,12}(E) - \tilde{\sigma}_{23,12}(E, E_{23})$



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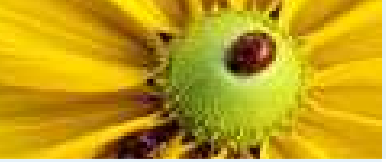


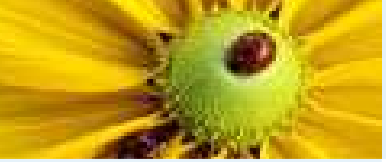
Current problem

$$H_2^+(X, v', j') + H^- \rightarrow H_3 \rightarrow H_2(Y, v'', j'') + H(n)$$

or $$HD^+(X, v', j') + H^- \rightarrow DH_2 \rightarrow H_2(Y, v'', j'') + D(n)$$

or $$HD^+(X, v', j') + H^- \rightarrow DH_2 \rightarrow HD(Y, v'', j'') + H(n)$$

$X(Y)$ -Electronic state of H_2 or HD etc.
v -Vibrational quantum number
j -Rotational quantum number



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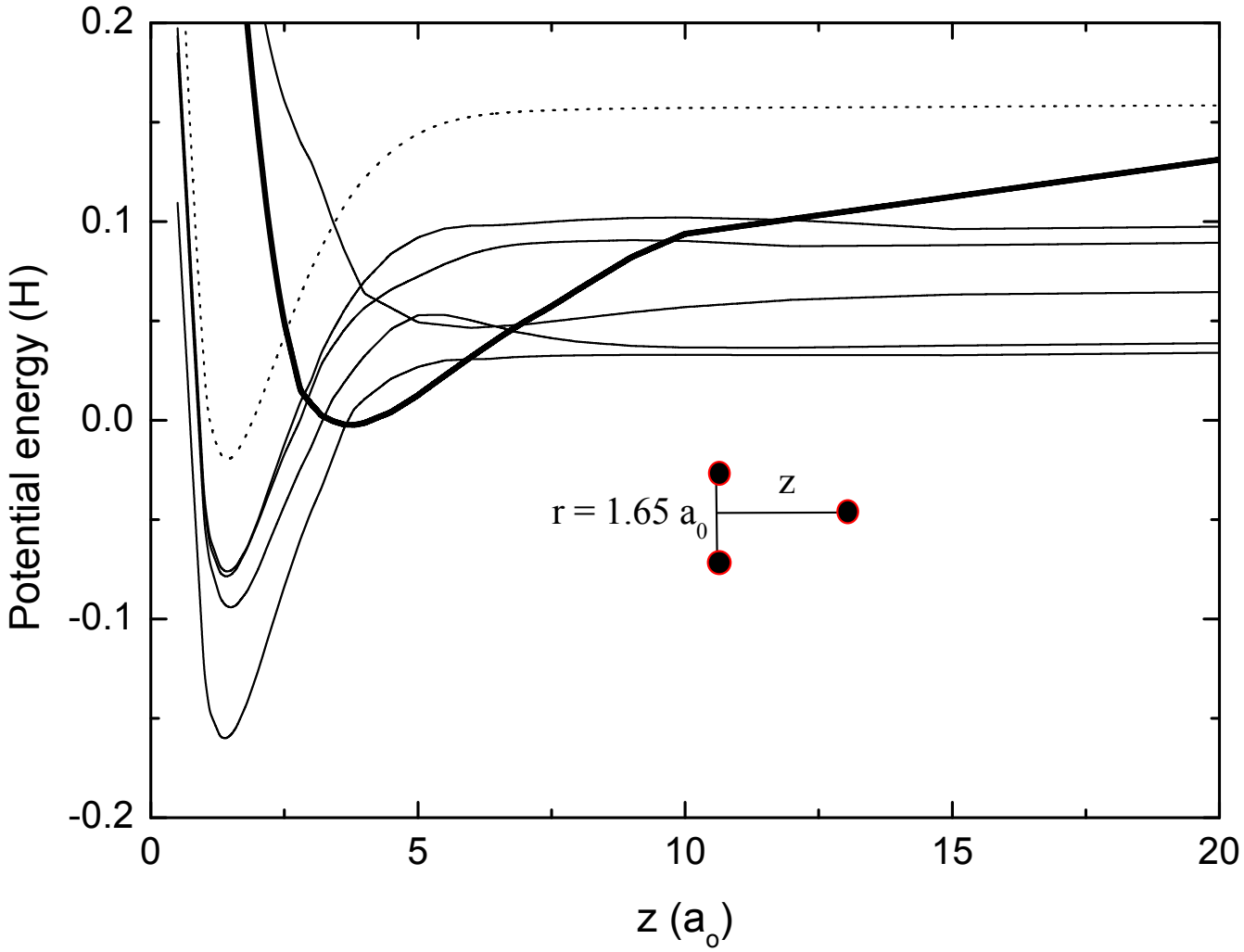
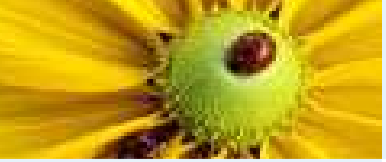
• We want a theory which allows us to assign the **Quantum states of resonances** as in the two-body H_2 or $(NH)^{3+}$ examples.





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$$(H-E)\Psi = 0 \quad \text{with} \quad \Psi = \Psi_{in} + \Psi_{scat}$$

$$\Rightarrow \qquad (H-E)\Psi_{in} = -(H-E)\Psi_{scat}$$

$$\Rightarrow \quad \left\{ H = T + V \right\} \Rightarrow \qquad -V\Psi_{in} = (H-E)\Psi_{scat}$$

Known

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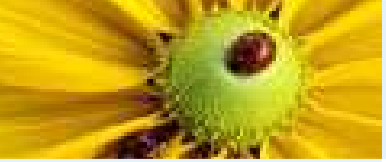

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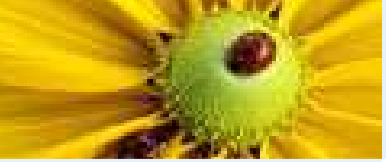

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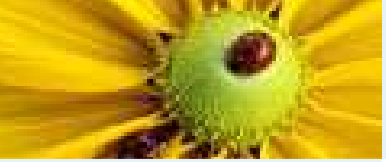

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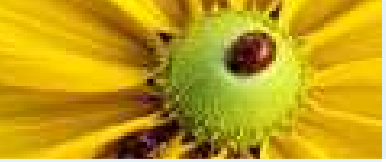
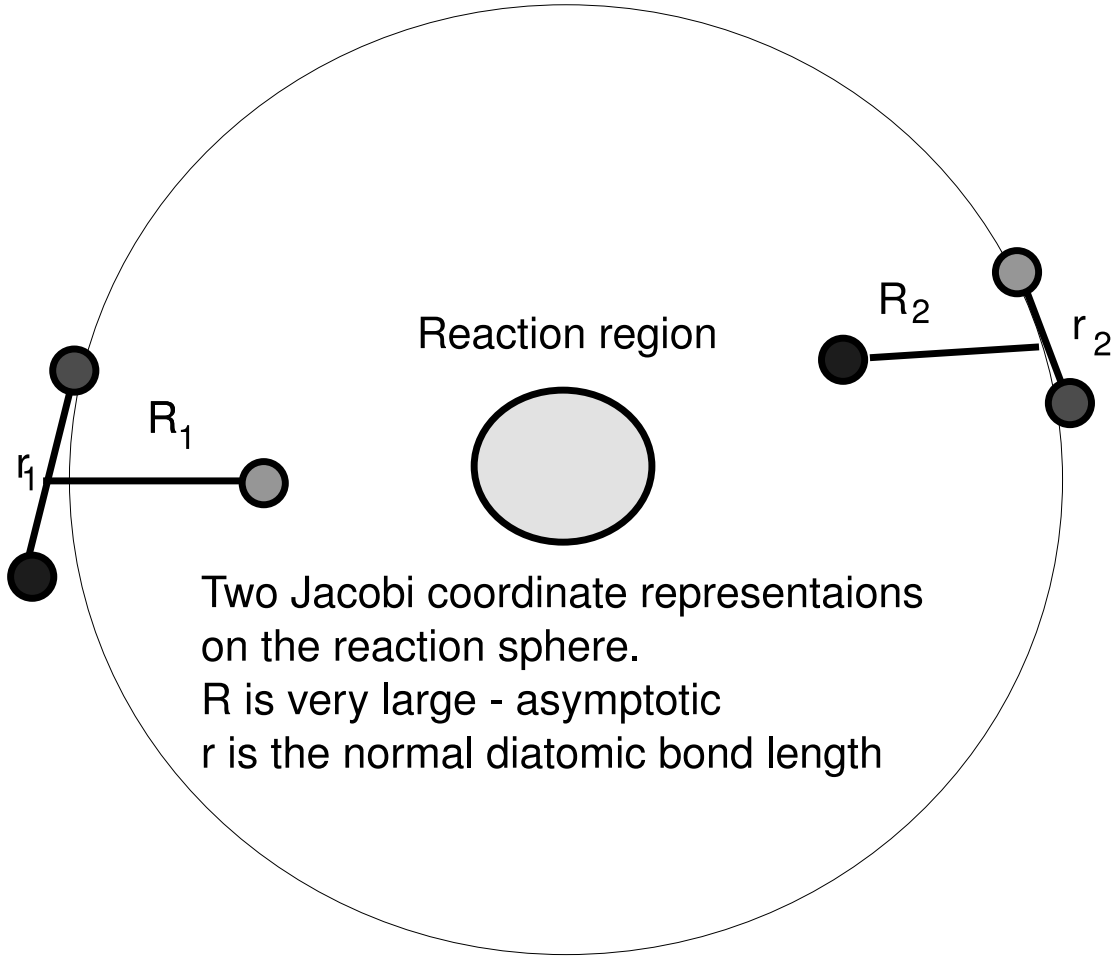
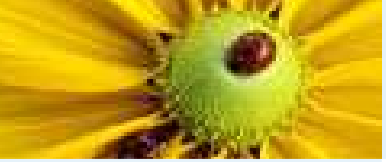
Unknown to be computed $\Rightarrow \Psi_{scat}$ The Scattered wave.



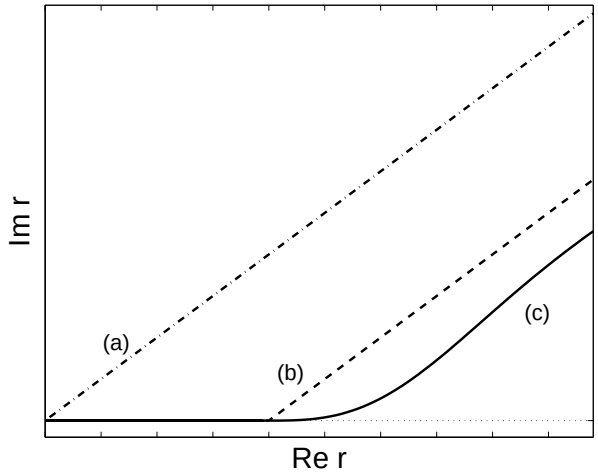
Coordinate system - Jacobi

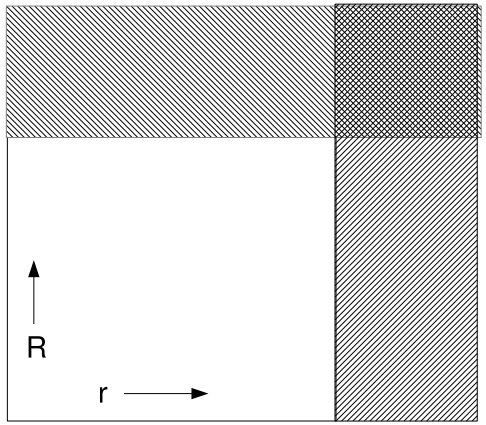




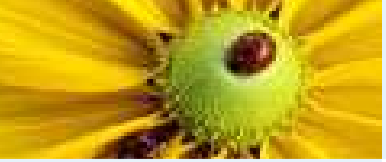
Boundary conditions etc.

Incoming wave : $\Psi_{in}(\mathbf{r},\mathbf{R},\phi) = \varphi(r)\exp(i(k_{in}R - \ell\pi/2))$ **Use Exterior Complex Scaling !**





Scattered wave : $\Psi_{scat}(\mathbf{r},\mathbf{R},\phi) \to 0$ as r or $R \to \infty$



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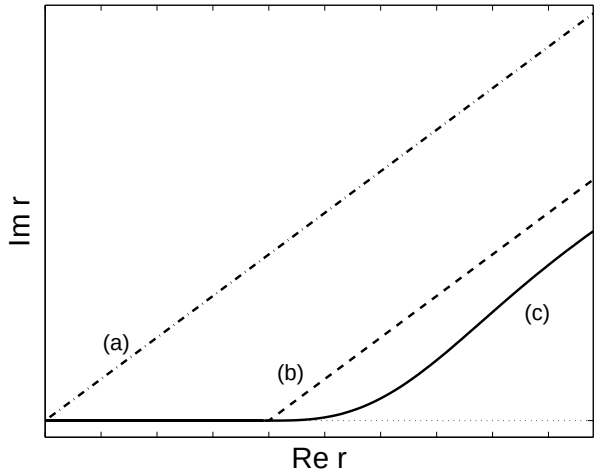

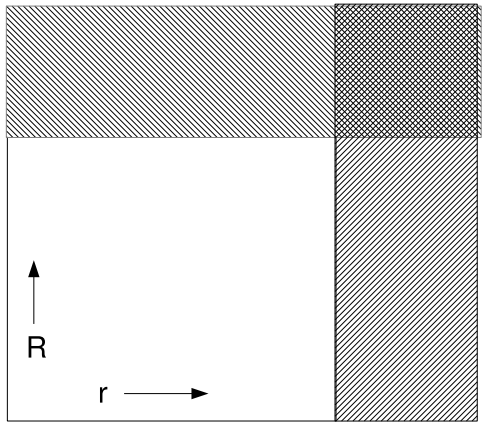

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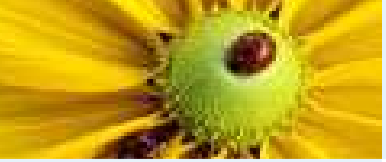
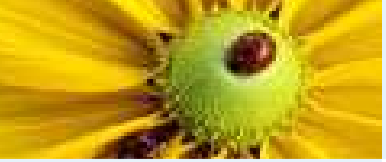
$\Rightarrow$ Zero boundary cond. for $\mathbf{r} = 0$ and $\mathbf{R} = 0$ and at **practical infinity**



Analysis of Scattered wave

- Three different Jacobi coordinate systems $(\mathbf{R}_\alpha, \mathbf{r}_\alpha, \phi_\alpha)$ where $\phi_\alpha = \hat{\mathbf{R}}_\alpha \cdot \hat{\mathbf{r}}_\alpha$.



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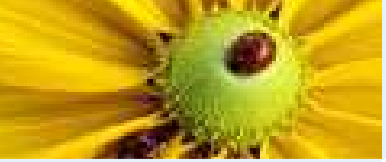

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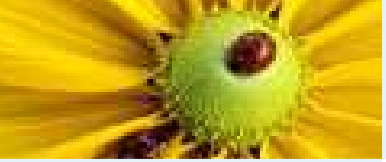

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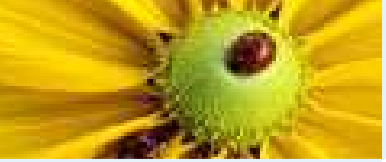

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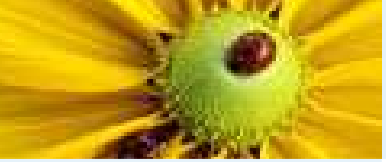

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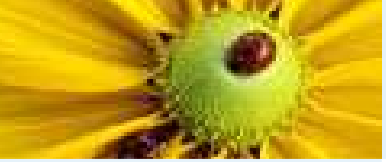

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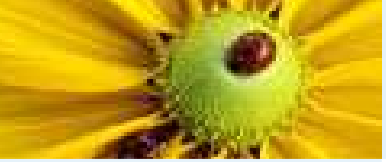
- yielding the total energy $E = (q_\alpha^j)^2 + \kappa_\alpha^j$ and the third particle momentum q_α^j.



The inhomogeneous (Driven) Schrödinger equation - Scattering Amplitudes

Substituting $\Psi(\mathbf{R}_\alpha, \mathbf{r}_\alpha)$ into the Schrödinger equation above we obtain

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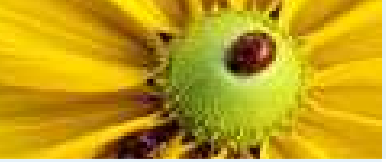

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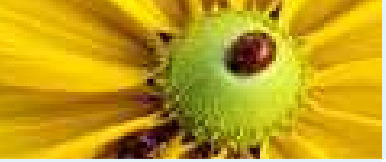

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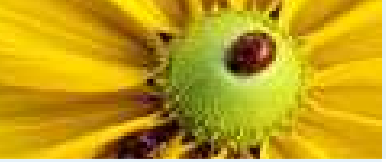

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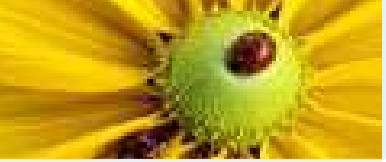
• the **breakup amplitude** is obtained from the sum of amplitudes $A_\alpha^0(\hat{\mathbf{r}}_\alpha, \hat{\mathbf{R}}_\alpha, \phi_\alpha)$.



Scattering amplitudes from the solution $\Phi(\mathbf{R}_\alpha, \mathbf{r}_\alpha)$

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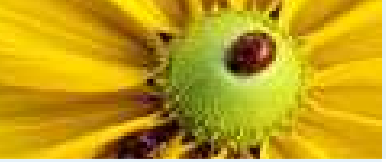

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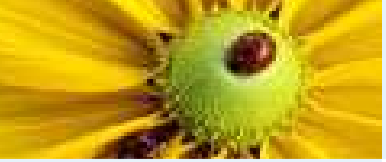

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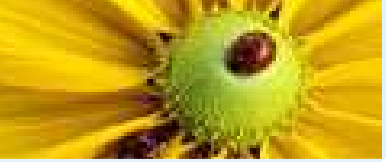

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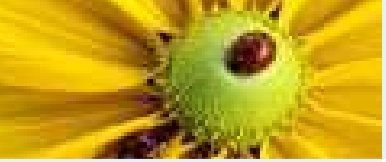
• In the same channel, the vibrational eigenfunctions are orthogonal, so we have

$$\int d\mathbf{r}_\alpha \varphi_\alpha^k(\mathbf{r}_\alpha)\Phi(\mathbf{R}_\alpha, \mathbf{r}_\alpha) \sim A_\alpha^k(\hat{\mathbf{R}}_\alpha)\frac{e^{iq_\alpha^k R_\alpha}}{R_\alpha}. \tag{4}$$



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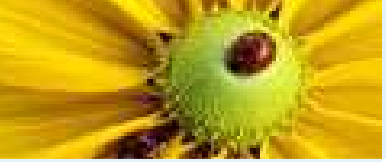
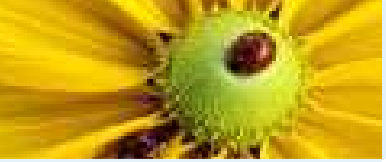
$\Rightarrow$ With the last equation, we can asymptotically find both the elastic and rearrangement amplitudes.



Finite element realization - Compare to the corresponding eigenvalue problem

Eigenvalue problem : $\mathbf{Hc} - \mathbf{ESc} = \mathbf{0}$

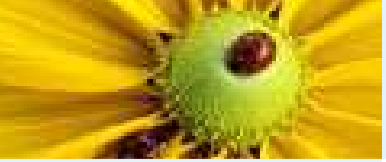


Finite element realization - Compare to the corresponding eigenvalue problem

Eigenvalue problem : $\mathbf{Hc} - \mathbf{ESc} = \mathbf{0}$

Scattering problem : $-\mathbf{Vb} = \mathbf{Hc} - \mathbf{ESc}$

- $\mathbf{H}$: Hamiltonian matrix
- $\mathbf{S}$: Overlap matrix
- $\mathbf{V}$: Potential matrix
- $\mathbf{c}$: Scattered wave vector
- $\mathbf{b}$: Incoming wave vector.



Finite element realization - Compare to the corresponding eigenvalue problem

Eigenvalue problem : $\mathbf{Hc} - \mathbf{ESc} = \mathbf{0}$

Scattering problem : $-\mathbf{Vb} = \mathbf{Hc} - \mathbf{ESc}$

- $\mathbf{H}$: Hamiltonian matrix
- $\mathbf{S}$: Overlap matrix
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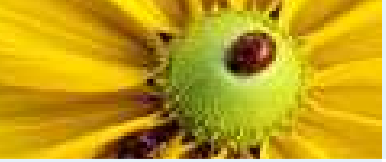
- Our "smooth exterior complex scaling full angular momentum code can solve the eigenvalue problem."



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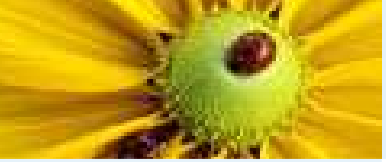
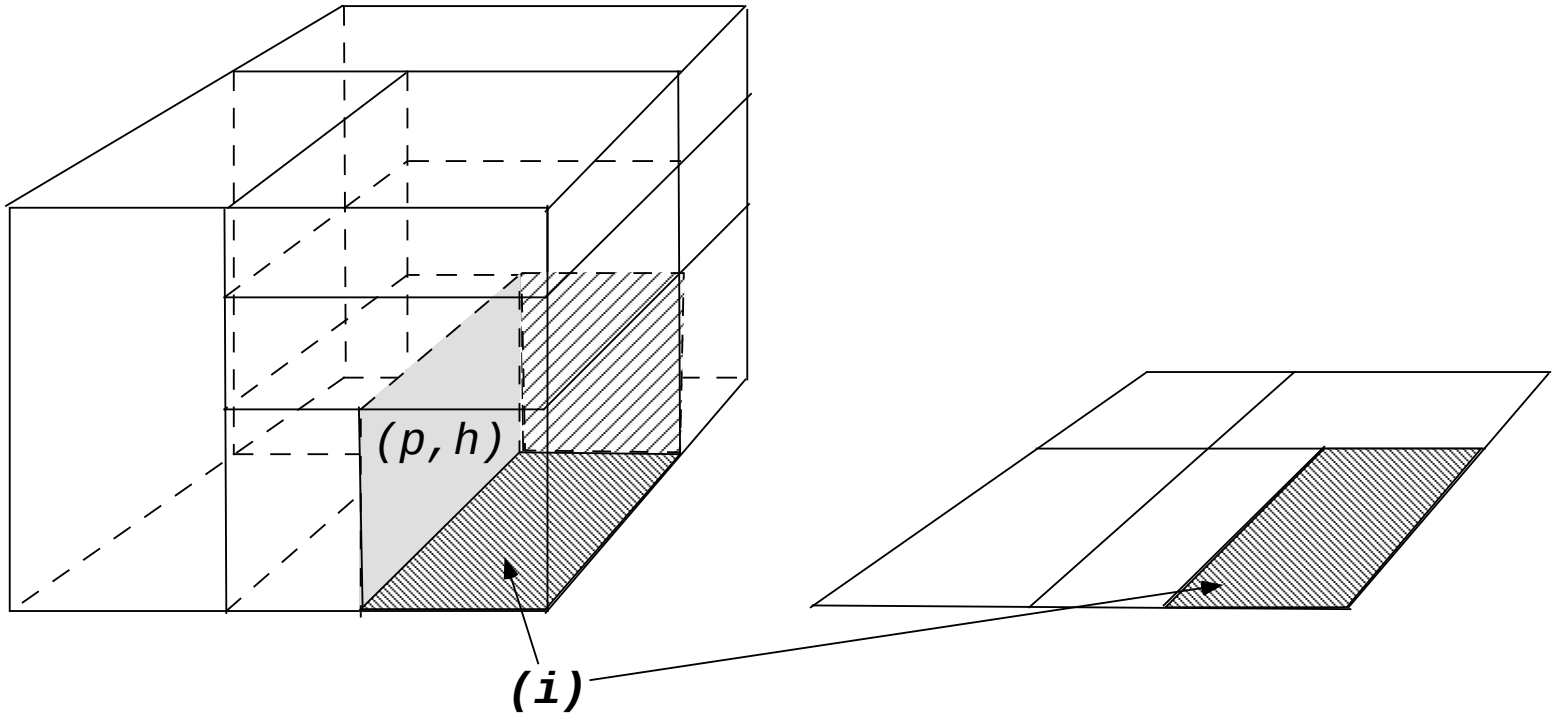
- Our "smooth exterior complex scaling full angular momentum code can solve the eigenvalue problem."
- $\Rightarrow$ We can use this code as a start for a scattering code.



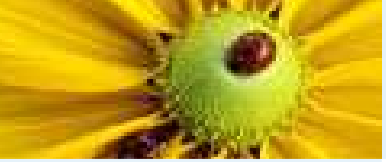
FEM expansion

Here the wave function ($c_{i,j}$) and the incoming wave ($b_{i,j}$) is expanded in FEM-basis functions in each rectangular box.

$$\Phi(\mathbf{r}_\alpha, \mathbf{R}_\alpha) = \sum_{i,j} d_{i,j} f_R^{i,j}(R) f_r^{i,j}(r) f_\phi^{i,j}(\phi)$$



- We are HOME $\Longleftrightarrow$ We can probably manage to code this !!



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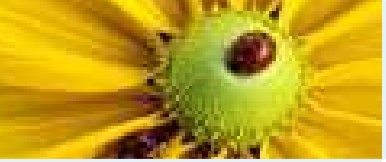

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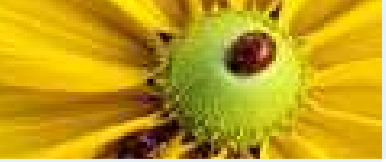

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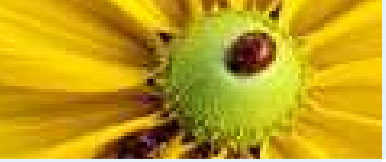

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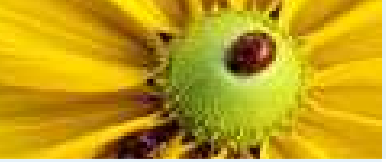

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!! Younger a well as Older Post Docs

are welcome to apply for two year contracts !!