# Theoretical analysis of high-order interference in energetic ion-molecule collisions

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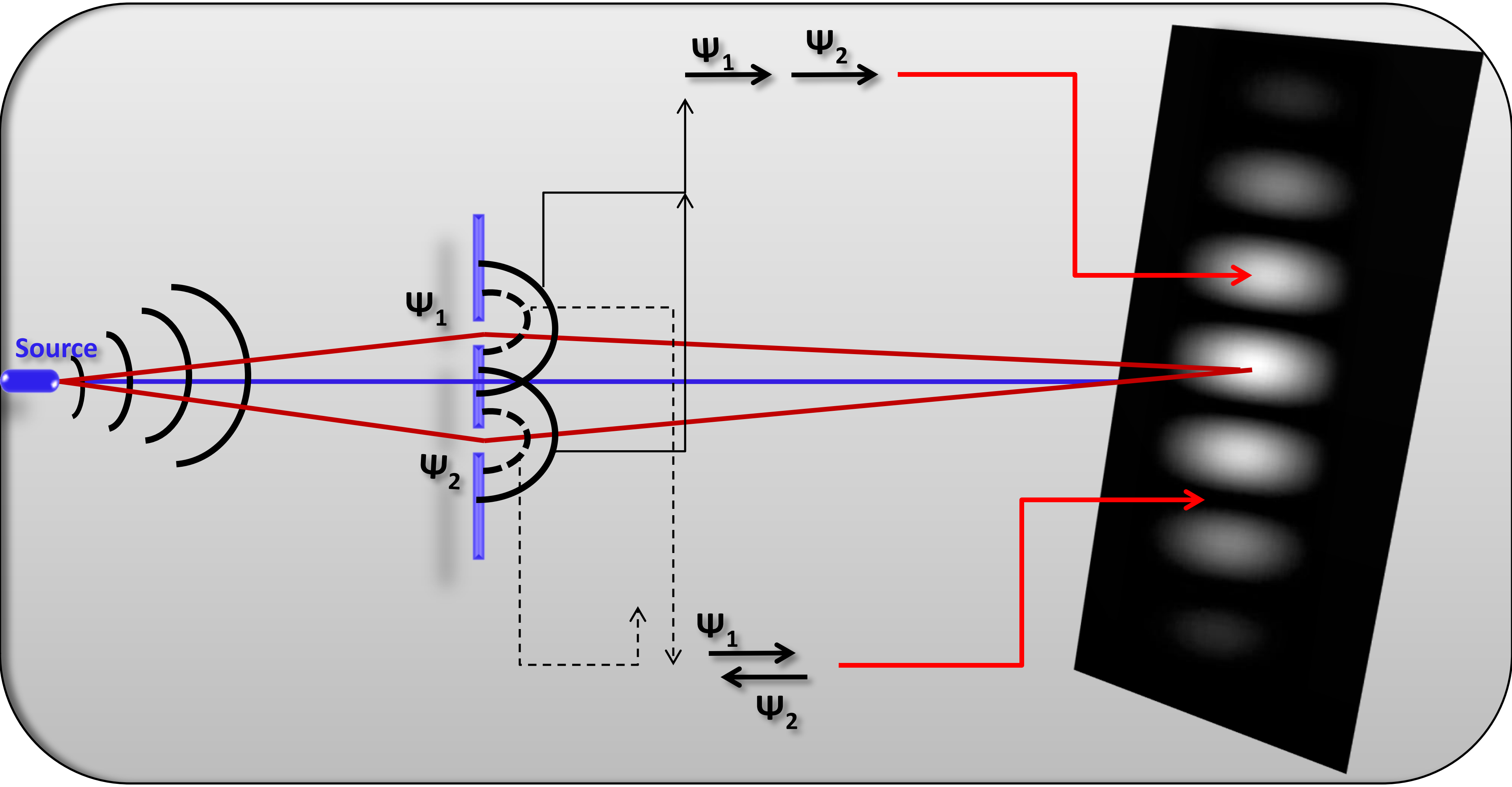
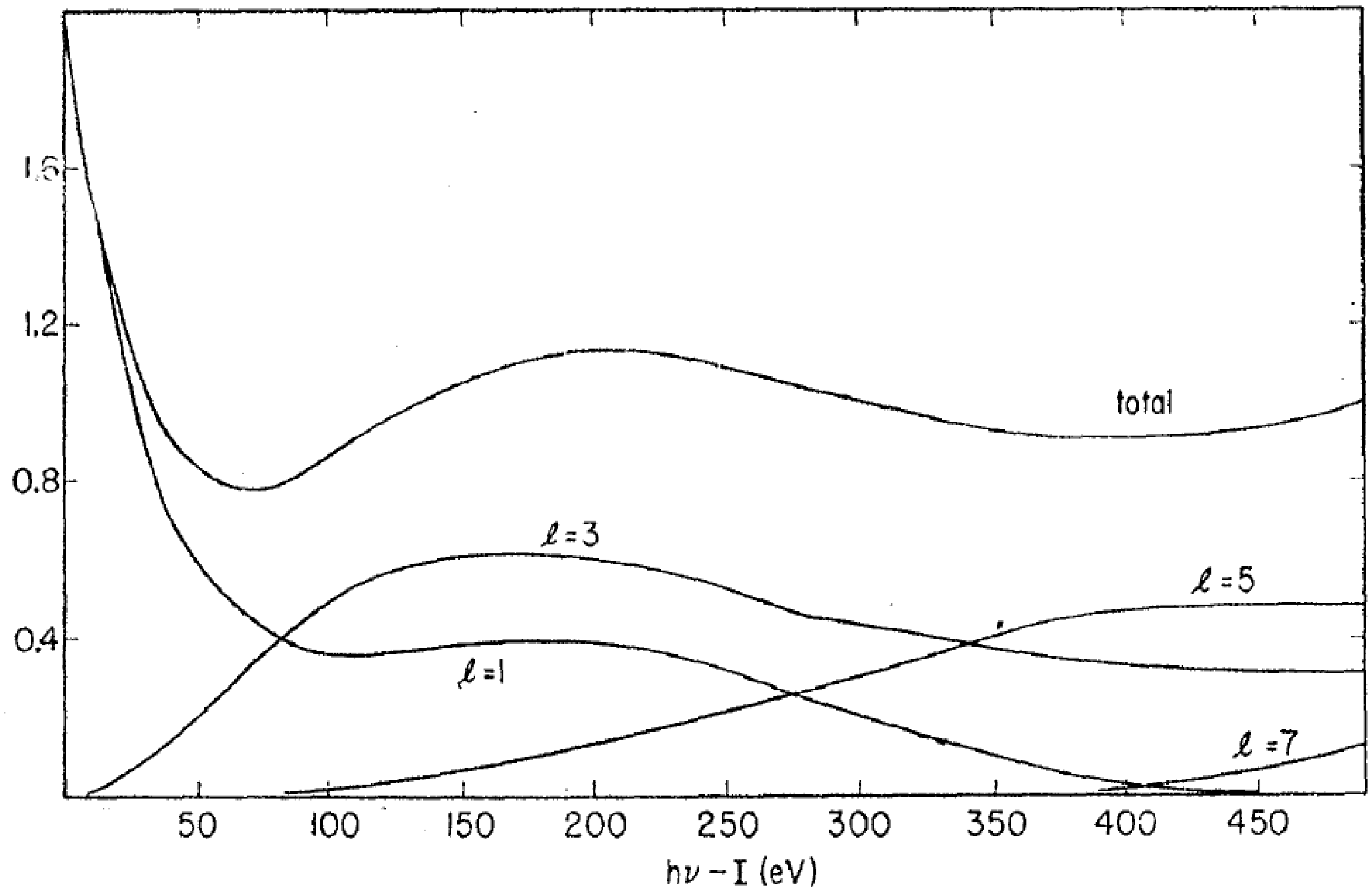
# Young's double-slit



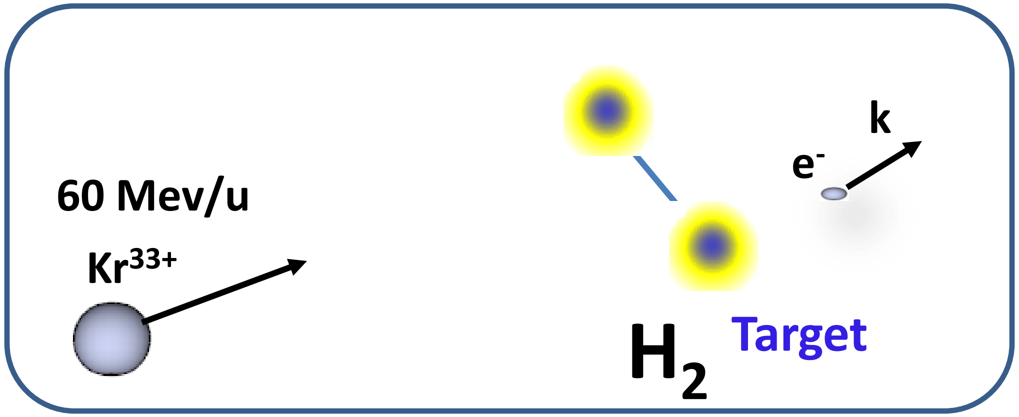
# Fano Interference

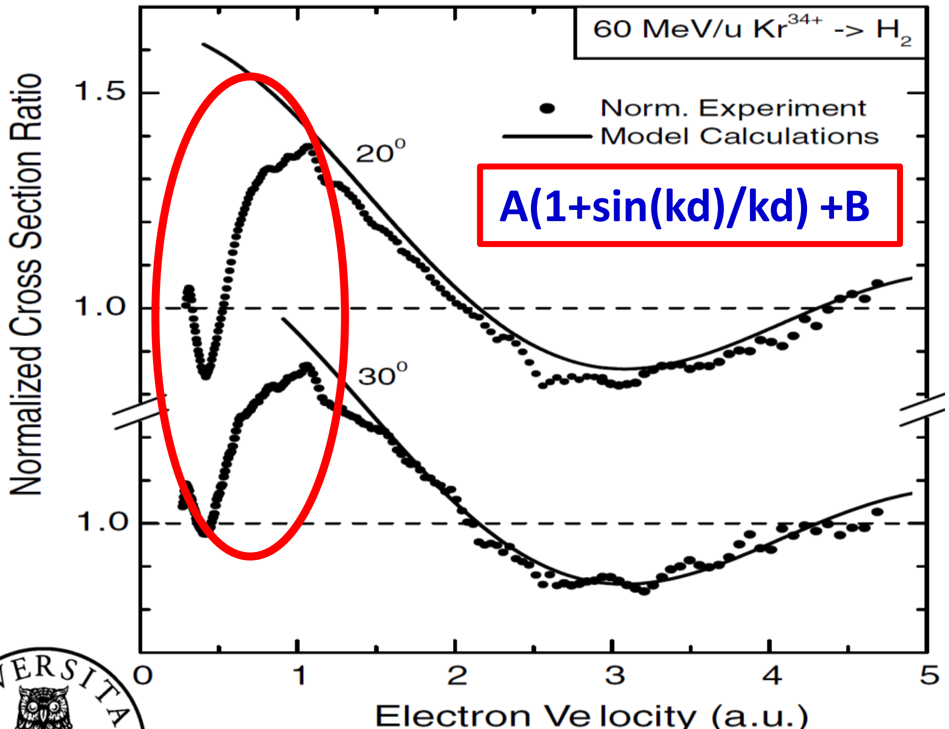


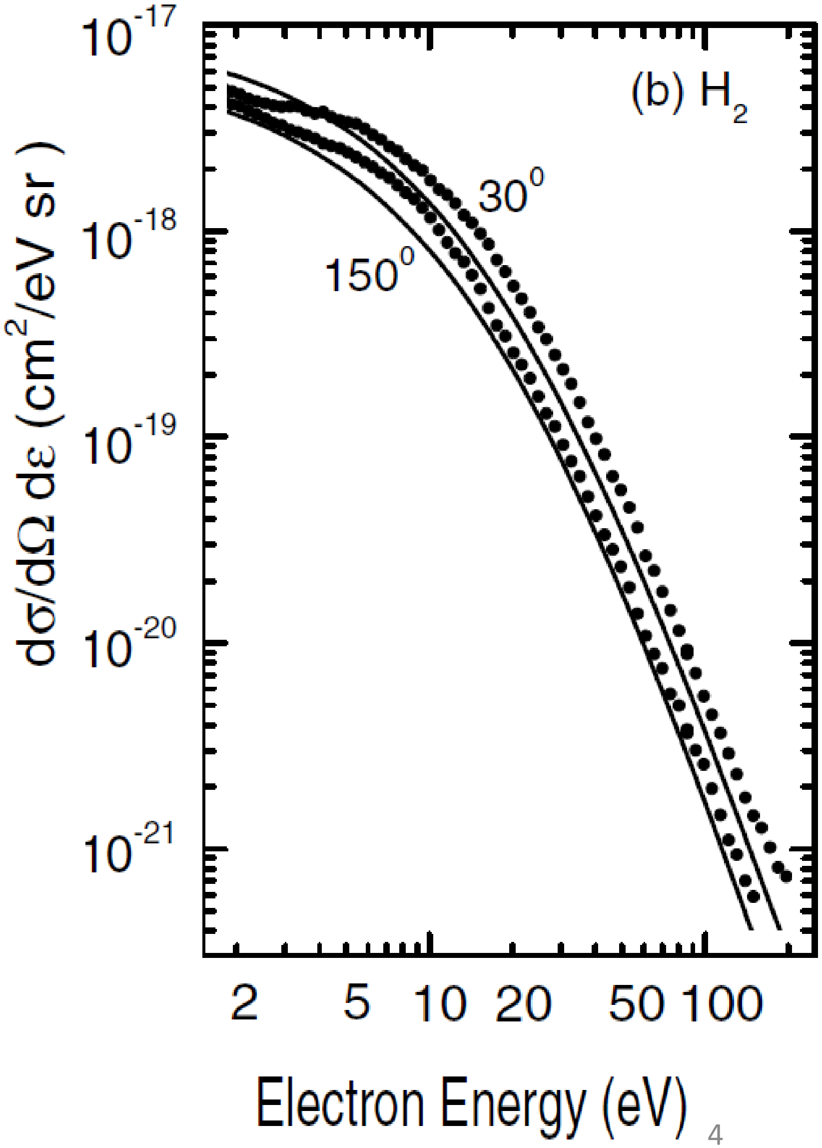

$$\sigma=\sum_l \sigma_l=\sigma_H(Z^*)[1+(\sin kR)/kR]/(1+S)$$

*Cohen and Fano Phys. Rev. 150, 30 (1966)*

# Interference effects in electron emisssion $Kr^{33+}$ -$H_2$

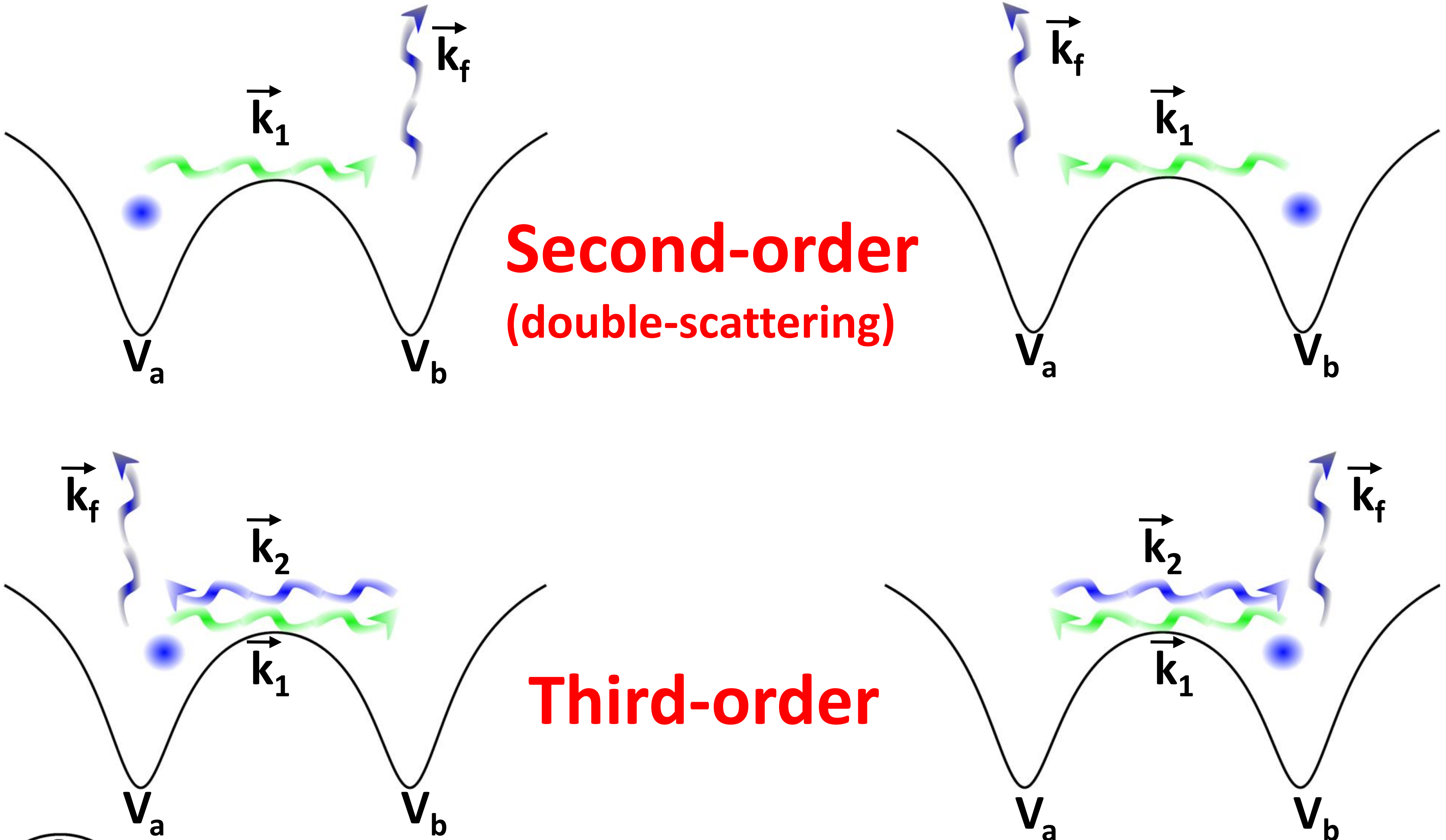


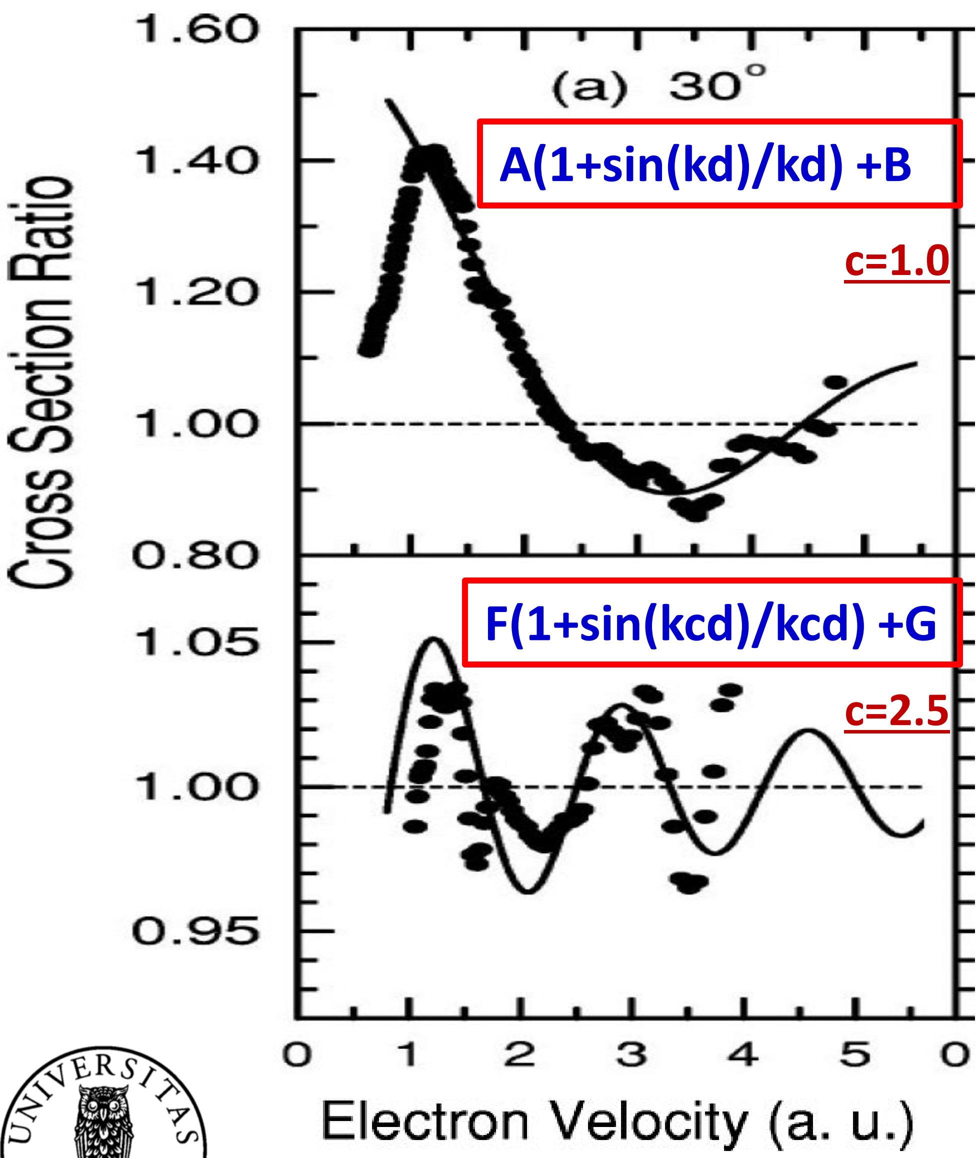




Stolterfoht *et al. Phys. Rev. Lett. 87, 023201 (2001)*

# High-order interference mechanisms



# Interference effects in electron emisssion $Kr^{33+}$ -$H_2$



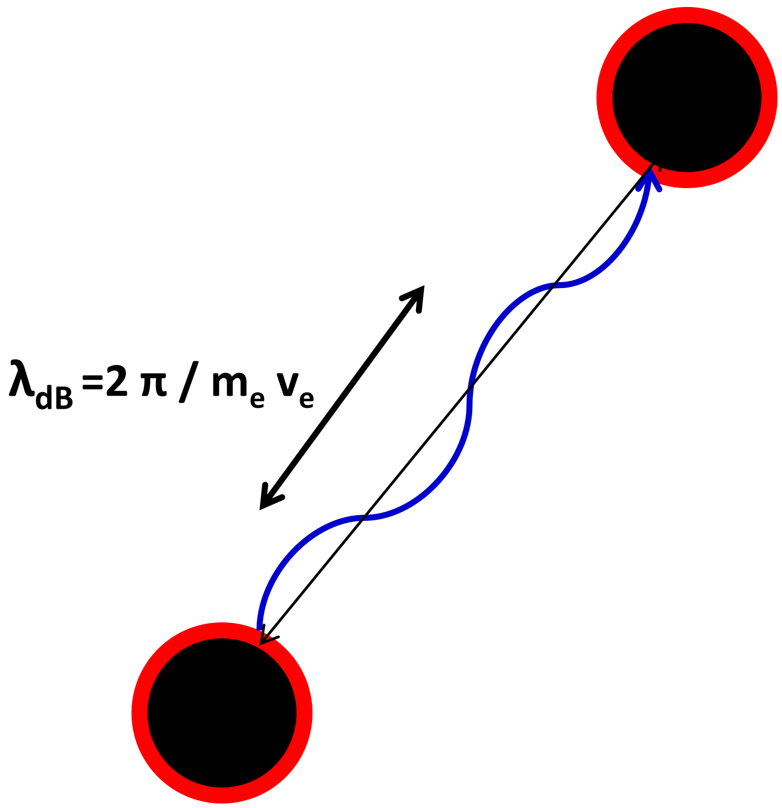

Stolterfoht *et al. Phys. Rev. A 69, 012701 (2004)*

## List of papers


1. S. Hossain et al Phys. Rev. A **72** 010701 (2005)
2. S. Hossain et al Nucl. Instrum. Meth. Phys. Res. B. **233**, 201 (2005)
3. J. A. Tanis et al Phys. Rev. A **74** 022707 (2006)
4. J. L. Baran et al Phys. Rev. A **78** 012710 (2008)
5. D. Misra et al Phys. Rev. A **80** 062701 (2009)
6. N. Sisourat et al Phys. Rev. A **76** 012718 (2007)
7. L. Salen et al Phys. Rev. A **81** 022718 (2010)


Existence of the double-scattering effect is not yet fully established !!! WHY!

# Difficulty to observe double-scattering effects




A critical parameter for the second and higher order mechanisms to be pronounced is the internuclear distance $R_{ab}$: for $H_2$ ($R_{ab}$ =1.4 au)

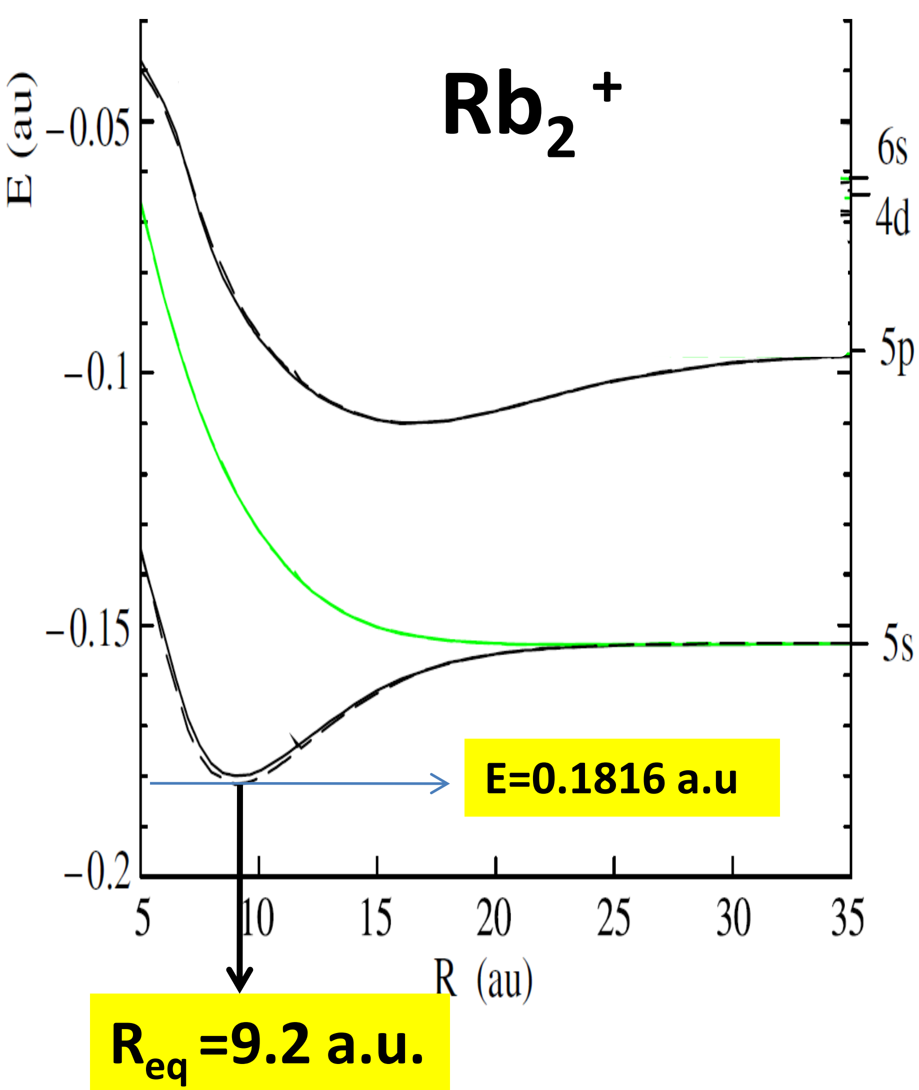
$\lambda_{dB}$ : 1.3-6 au

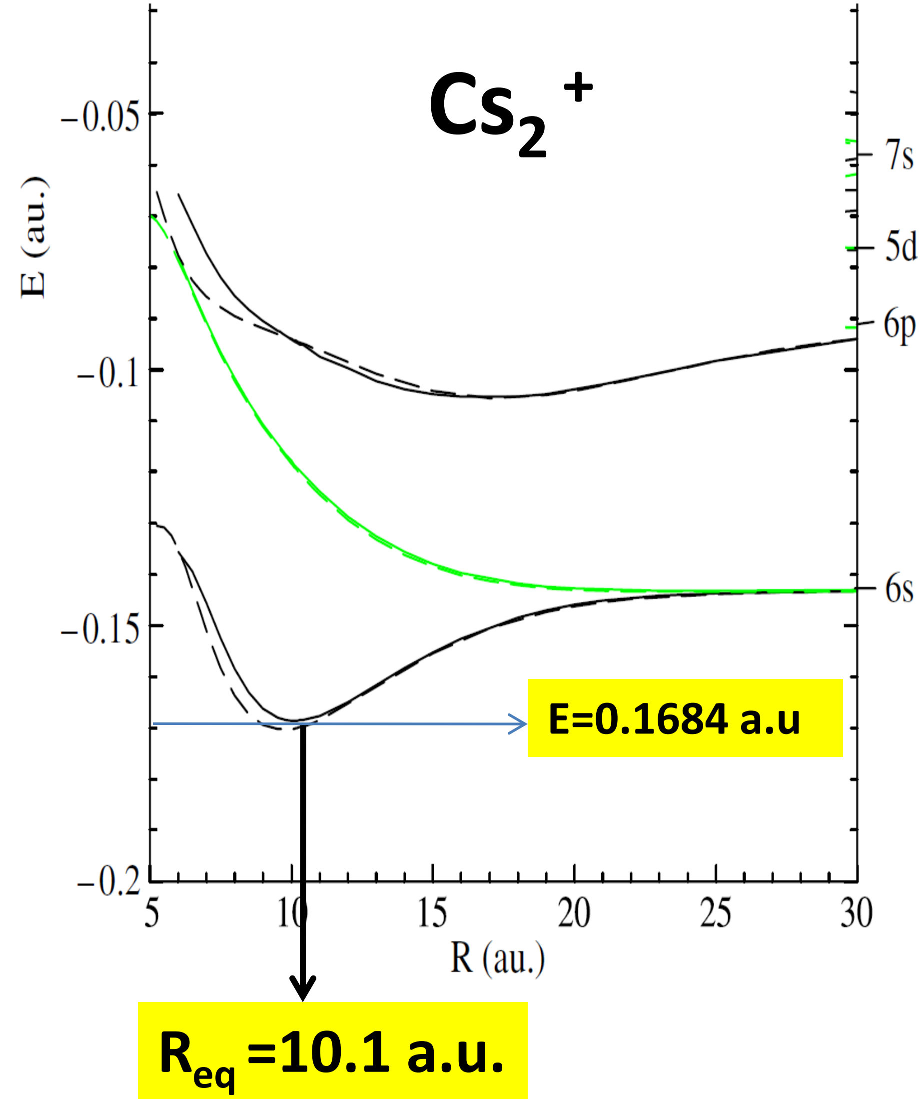
$$R_{eq} << \lambda_{dB}$$

The situation could be repaired by analyzing oscillations at higher electron energies: 2nd order process vanish

Remaining alternative is to consider molecules with large internuclear distance

# Heavy diatomic molecules




M. Aymar *et al*. J. *Phys. B 36, 4799 (2003)*

# Non-perturbative approach

- **1D-1e-TDSE**

$$[\mathcal{H}_e(t) - i\frac{\partial}{\partial t}]\psi(t) = 0$$

$$\mathcal{H}_e(t) = -\frac{1}{2}\nabla^2 + V_a(x) + V_b(x) + V_p(t)$$

$$V_i(x) = -\frac{1 + (Z_i - 1)e^{-a_1 x_i} + a_2 x_i e^{-a_3 x_i}}{\sqrt{x_i^2 + \alpha^2}} \quad x_i = |x - R_i|, \quad i = a, b$$

$$V_p(t) = -\frac{Z_p}{\sqrt{|x - R(t)|^2 + \beta^2}}$$

# Non-perturbative approach

- **Time-propagation**

  **(Predictor-corrector)**

$$\psi(t) = \sum_i c_i(t) f_i(x)$$

- **To check** Finite-difference & Crank-Nicolson

- **Analysis**

  - **Ionization wave-function**

$$|\phi_{ioniz}(x)\rangle = [1 - \sum_{i\,\text{bound}} |\Psi_i(x)\rangle\langle\Psi_i(x)|]|\psi(t \to \infty)\rangle$$

  - **Momentum distribution**

$$|\,\phi_{ioni}(p_x)\,|^2 = |\,\mathcal{F}(\phi_{ioni}(x))\,|^2$$

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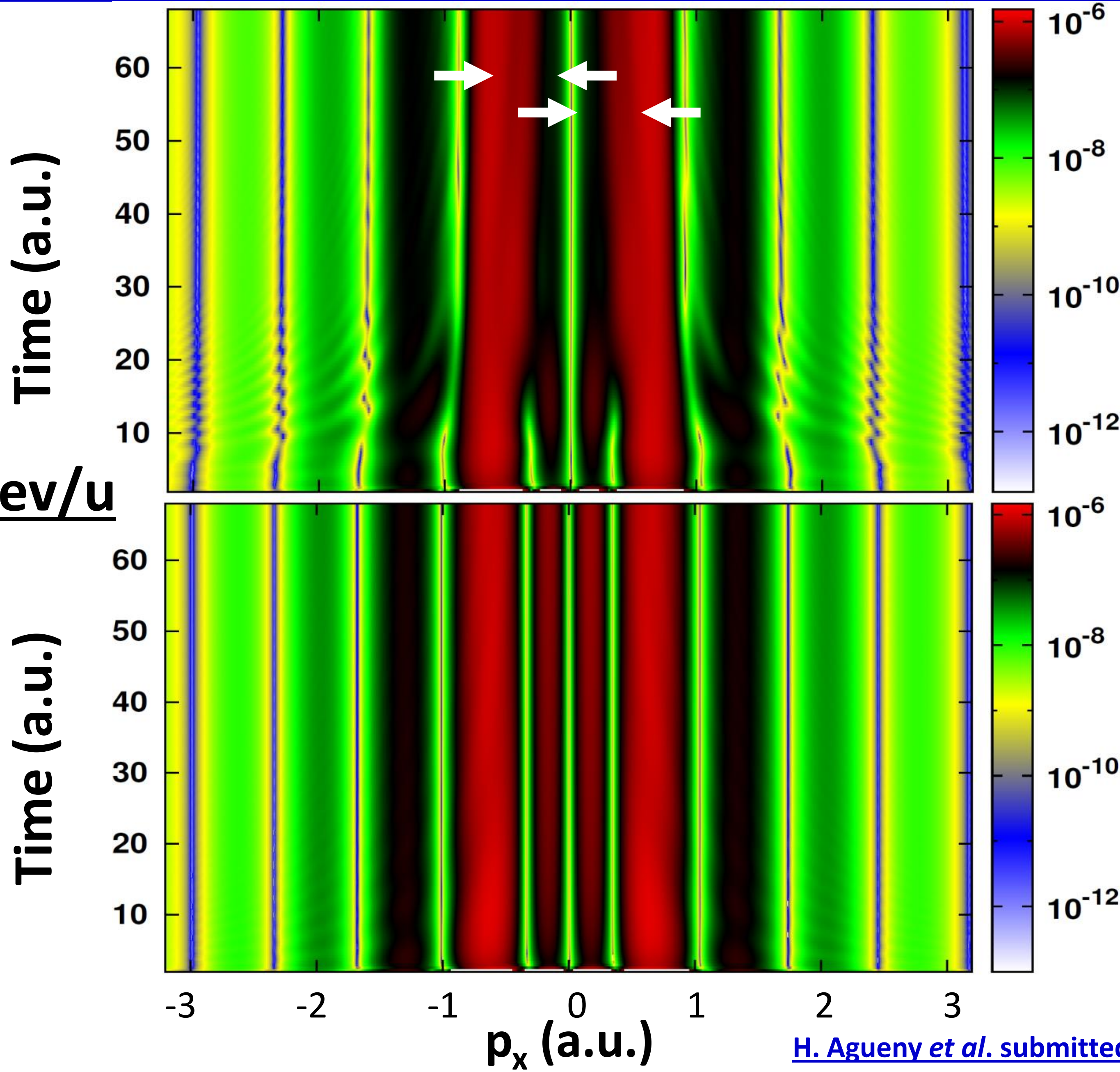
# Coherent Electron Emission Beyond Young-type Interference: $H^{+}$- $Rb_2^{+}$

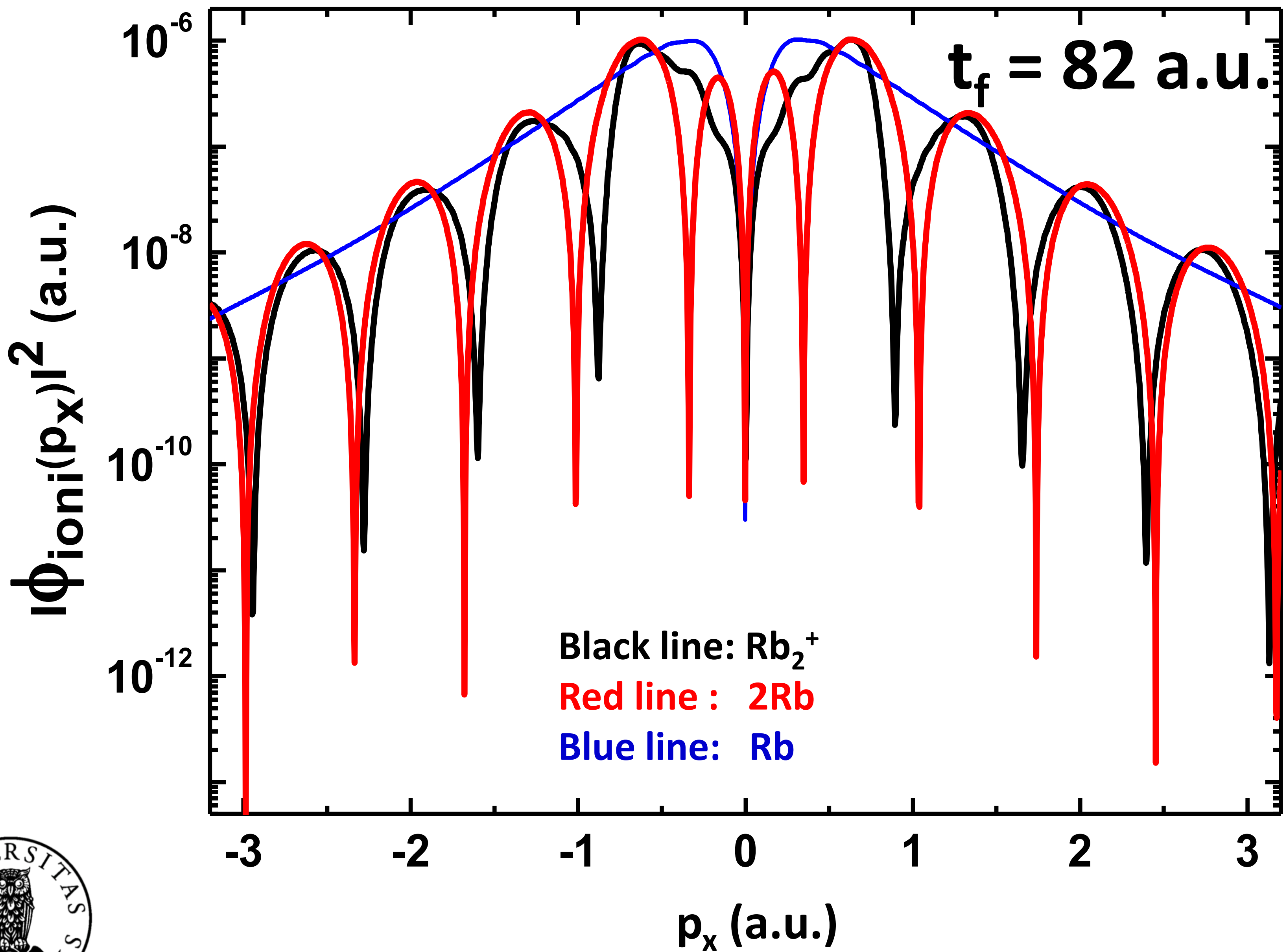



**E=63 Mev/u**



H. Agueny *et al*. submitted to *Phys. Rev. Lett.*

# Coherent Electron Emission Beyond Young-type Interference: $H^+$- $Rb_2^+$



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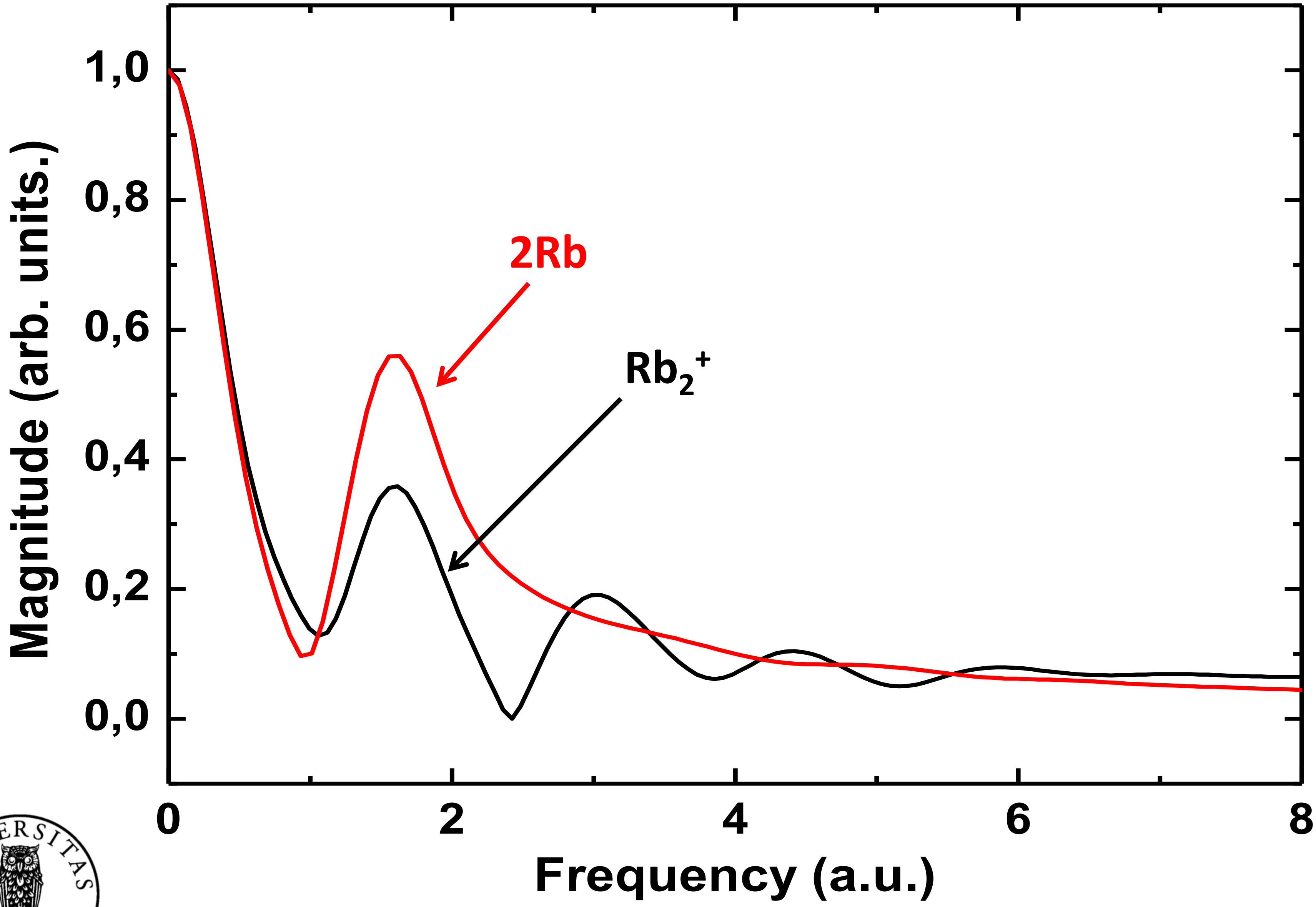




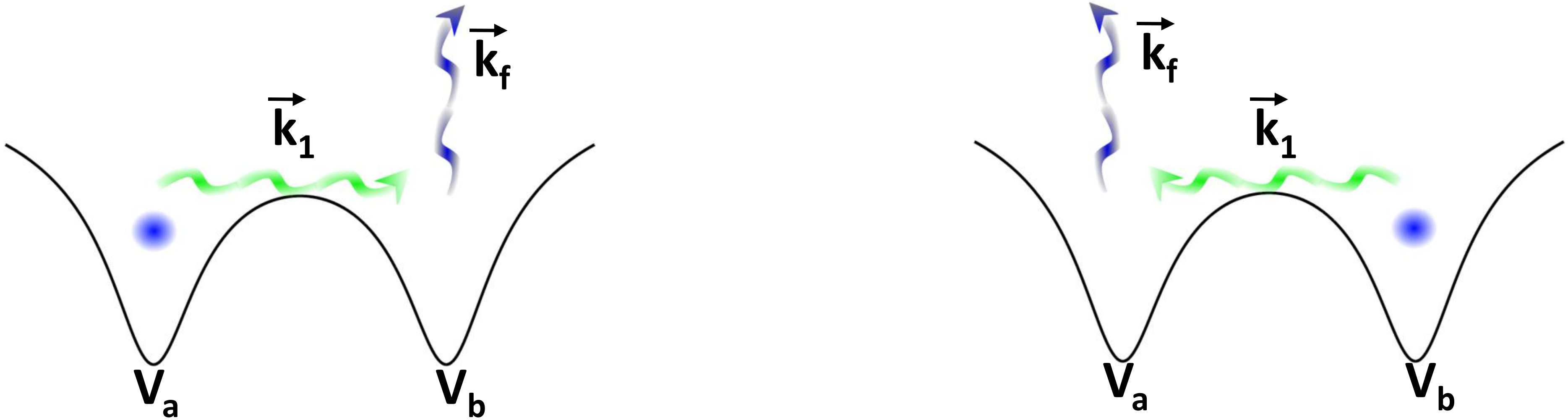


H. Agueny *et al*. submitted to *Phys. Rev. Lett.*

# Second-order Born Approximation

## 2nd order scattering amplitude

$$a^{(2)}(\vec{k}_f) = \int d^3k_1 [a^{(2),+}(\vec{k}_1, \vec{k}_f) + a^{(2),-}(\vec{k}_1, \vec{k}_f)]$$



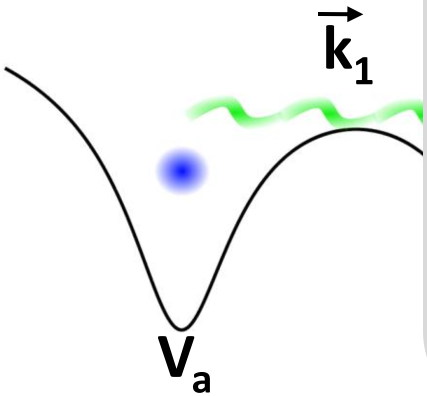

$$a^{(2),\pm}(\vec{k}_1,\vec{k}_f) \sim \int_{-\infty}^{\infty} dt_2 e^{i\Delta E_2 t_2} \langle \psi_{k_f}(\vec{r}_2,\vec{k}_f)|V_s(r_2)|\psi^{\pm}_{k_1}(\vec{r}_2,\vec{k}_1)\rangle$$

$$\times \int_{-\infty}^{t_2} dt_1 e^{i\Delta E_1 t_1} \langle \psi^{\pm}_{k_1}(\vec{r}_1,\vec{k}_1)|V(r_1,t_1)|\psi_i(r_1,\vec{R}_{ab})\rangle$$

# Second Born Approximation

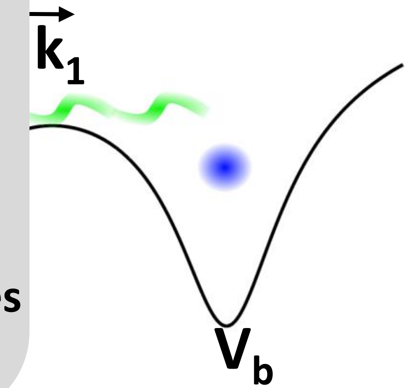
## 2nd order scattering amplitude

$$a^{(2)}(\vec{k}_f) = \int d^3k_1 [a^{(2),+}(\vec{k}_1, \vec{k}_f) + a^{(2),-}(\vec{k}_1, \vec{k}_f)]$$




**To evaluate the amplitude:**

- **Vs=Va+Vb: screened Coulomb (e-T)**
- **V: constant (e-P)**
- **Initial state: LCAO**
- **Final and intermediate wavefunctions: Plane waves**




$$a^{(2),\pm}(\vec{k}_1, \vec{k}_f) \sim \int_{-\infty}^{\infty} dt_2 e^{i\Delta E_2 t_2} \langle \psi_{k_f}(\vec{r}_2, \vec{k}_f) | V_s(r_2) | \psi^{\pm}_{k_1}(\vec{r}_2, \vec{k}_1) \rangle$$

$$\times \int_{-\infty}^{t_2} dt_1 e^{i\Delta E_1 t_1} \langle \psi^{\pm}_{k_1}(\vec{r}_1, \vec{k}_1) | V(r_1, t_1) | \psi_i(r_1, \vec{R}_{ab}) \rangle$$

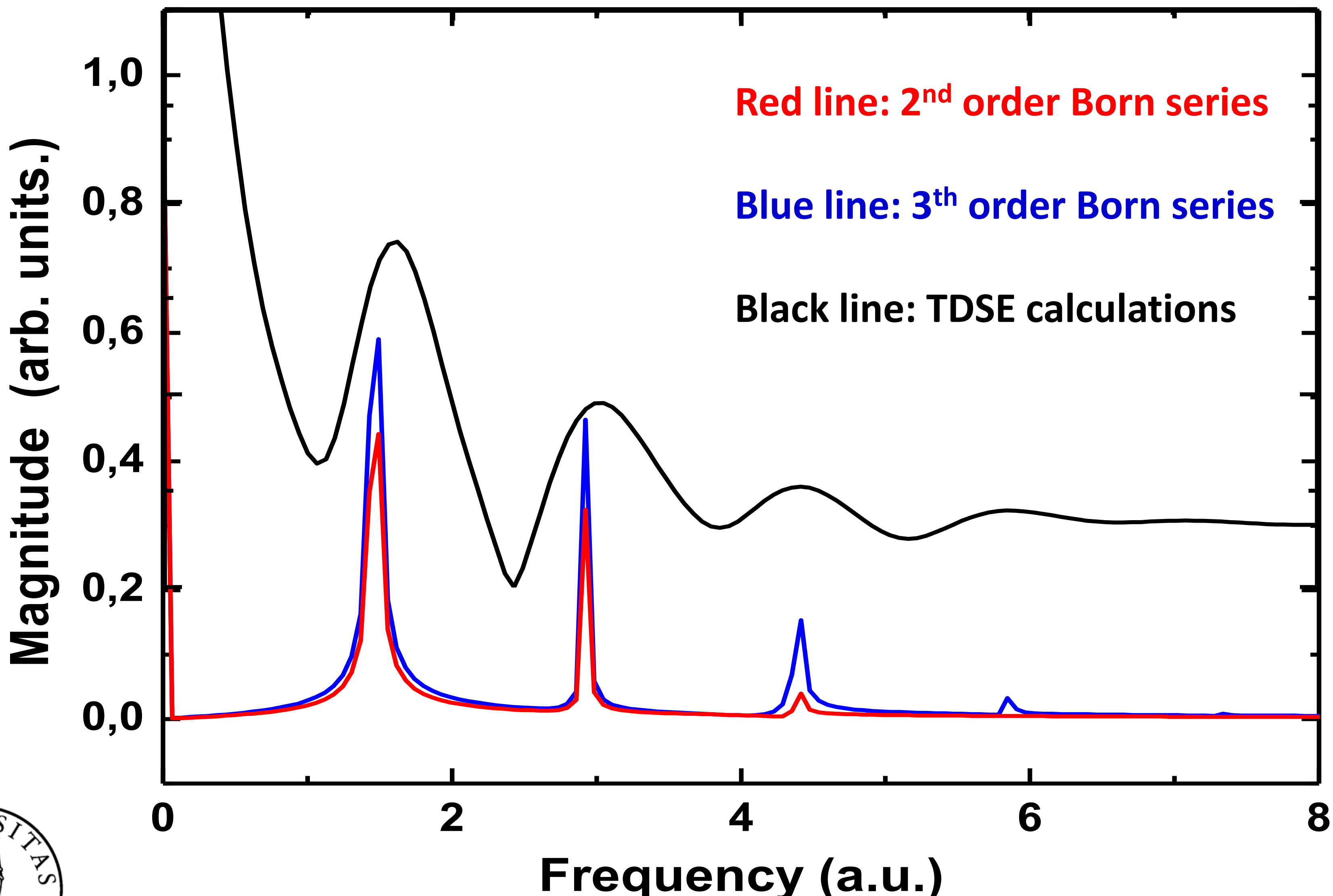
# Second Born Approximation

## 2nd order scattering probability

$$| a^{(2)} |^2 \sim | a^{(2),+} |^2 + | a^{(2),-} |^2 + 2Re(a^{(2),+,*} a^{(2),-})$$

$$|a^{(2)}(k_1, k_f)|^2 \sim |a|^2 \Big[ 3 + 3\cos(k_f R_{ab}) + 4\cos(k_1 R_{ab}) + 6\cos(k_f R_{ab})\cos(k_1 R_{ab}) + \cos(2k_1 R_{ab}) + \cos(k_f R_{ab})\cos(2k_1 R_{ab}) \Big].$$

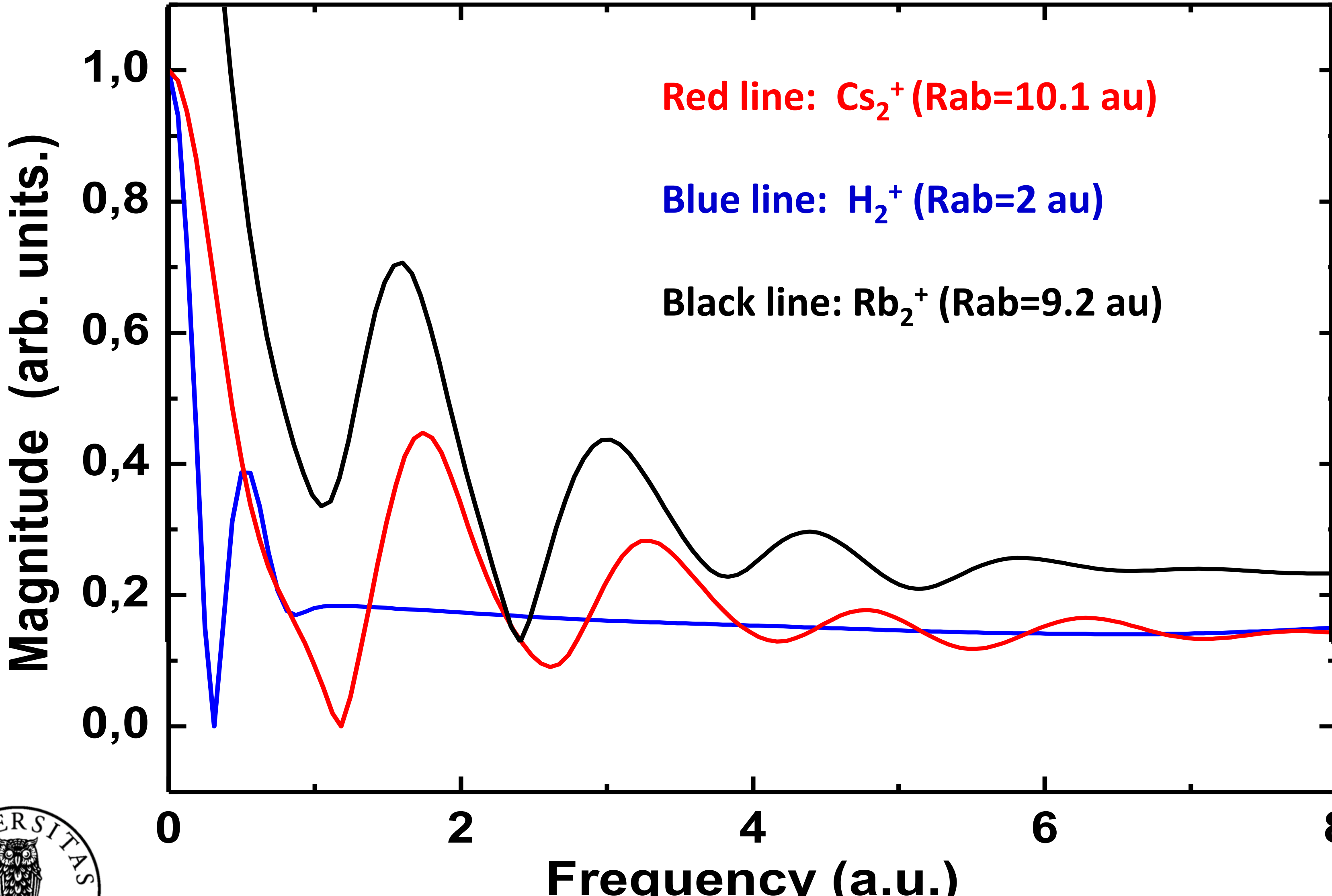
# Coherent Electron Emission Beyond Young-type Interference: $H^+$- $Rb_2^+$






H. Agueny *et al*. submitted to *Phys. Rev. Lett.*

# Coherent Electron Emission Beyond Young-type Interference: Internuclear distance effect



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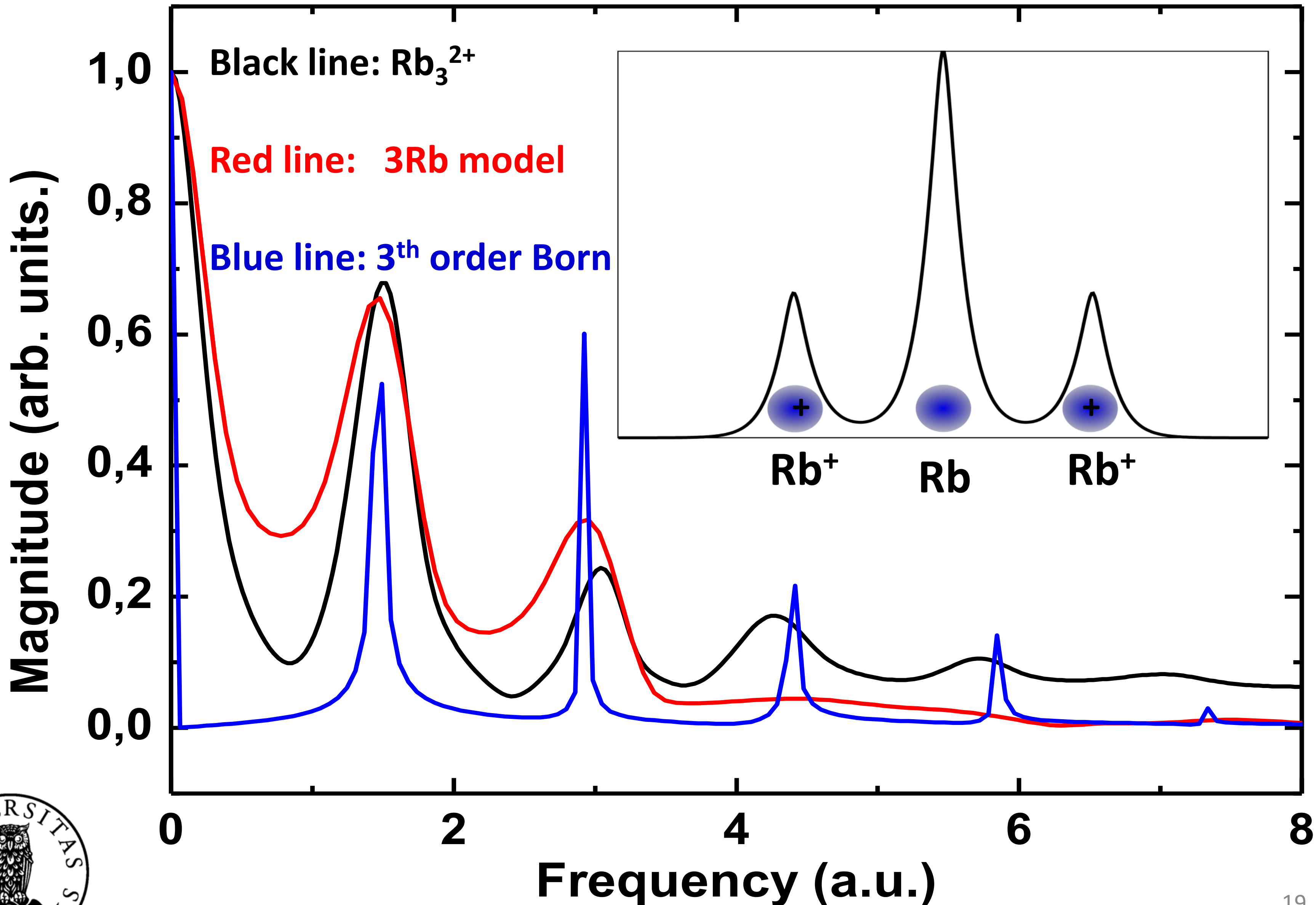
# Coherent Electron Emission Beyond Young-type Interference: $H^+$- $Rb_3^{2+}$

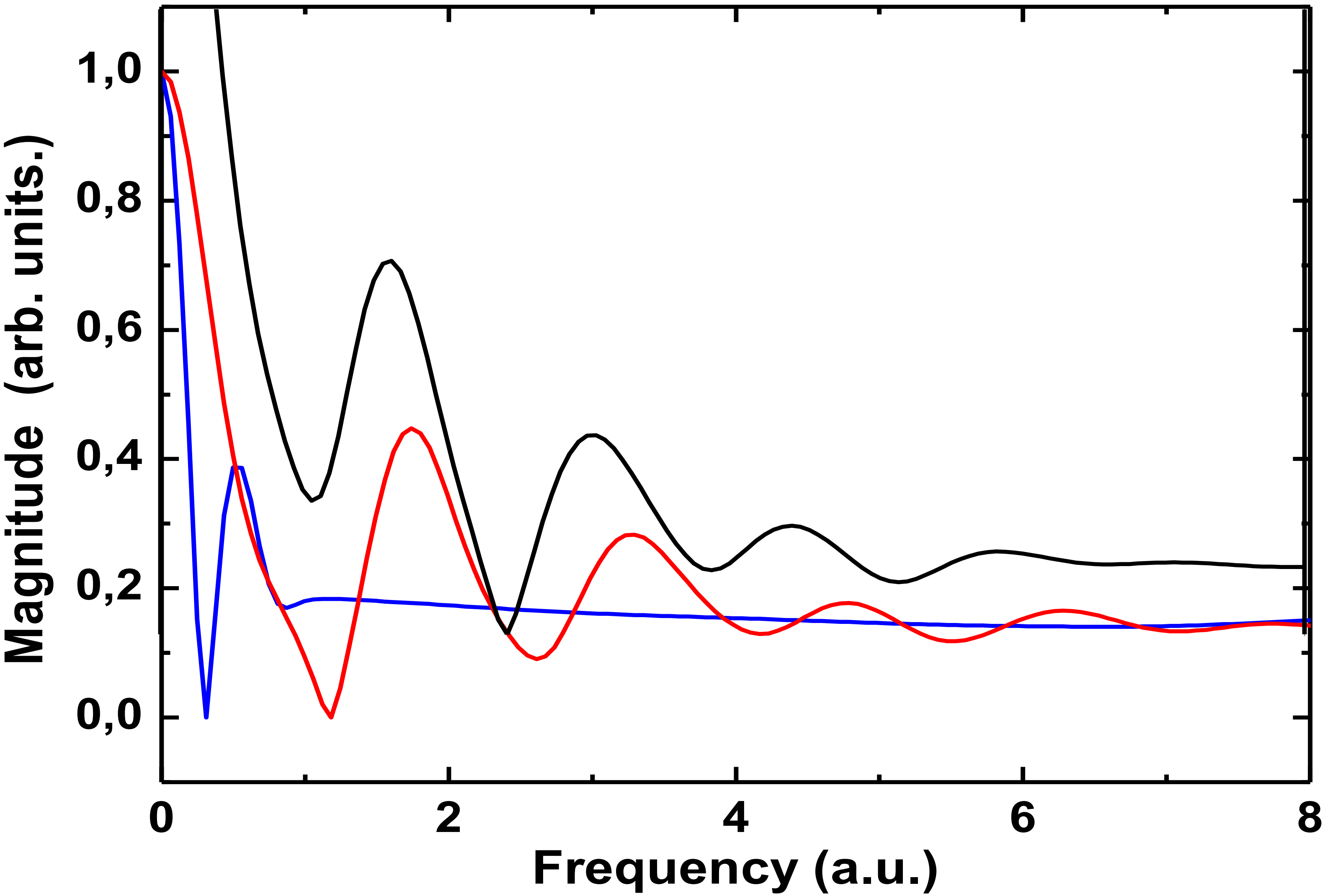


# Conclusion & Perspectives

**The key ingredient of the present work is the relative magnitude between the de Broglie’s wavelength of the ejected electrons and the molecular interatomic distance.**

## Perspectives

- Extension to full dimensions
- Triatomic systems
- Application to new materials (graphen)
- Extension to Laser-diatomic molecules
- Slow ion-atom collisions: electron transfer processes!!!!
  (via the formation of the transient molecule by the passing projectile and the atomic target)
  capture into highly excited states.
- Extension to slow ion-molecule collisions.



1,0
0,8
0,6
0,4
0,2
0,0
0
2
4
6
8
Frequency (a.u.)
Magnitude (arb. units.)