ICD - The Decay Widths I

1^{st} order theory and general characteristics

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ICD Summer School

Bad Honnef
September 1^{st} – 5^{th}

1. Wigner-Weisskopf theory
   - Evolution of the state vector
   - ICD – the mechanism
   - Asymptotic behavior of the decay width
2. ICD widths – examples
   - Short-range and asymptotic behavior
   - Polarization dependence
3. Summary

Resonant scattering – Siegert states

- Regular solution of Schrödinger equation [$l = 0,\ V(r \to 0) = 0$]

$$\Psi_E(r) = Ae^{ikr} + Be^{-ikr}, \qquad E = \frac{k^2}{2}$$

  - bound states: $k = i\kappa,\ \kappa > 0 \ \Rightarrow\ E < 0,\ \Psi_E(r) \in L^2$

Kukulin, Krasnopol'sky and Horáček, Theory of Resonances, Kluwer (1989)

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  - resonance states: $k = \alpha - i\beta,\ \alpha > 0,\ \beta > 0$
    $\Rightarrow\ E = E_{\mathrm{R}} - i\Gamma/2$, $\Psi_E(r)$ divergent (Siegert state)
    $\Rightarrow$ **cannot be represented in an L^2 basis**

Kukulin, Krasnopol'sky and Horáček, Theory of Resonances, Kluwer (1989)

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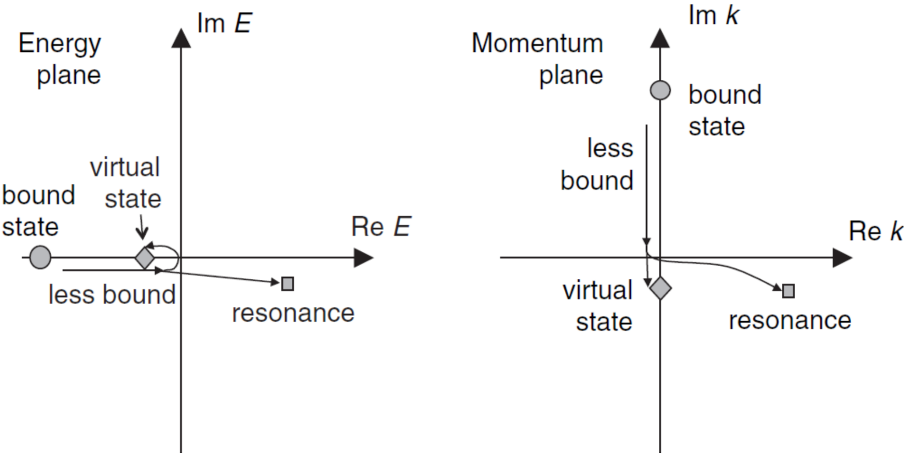
  - virtual states: $k = -i\beta,\ \beta > 0\ \Rightarrow\ E < 0, \Psi_E(r)$ divergent

Kukulin, Krasnopol'sky and Horáček, Theory of Resonances, Kluwer (1989)

Complex energy plane



F. Nunes, PHY982 course, NSCL (http://www.nscl.msu.edu/ nunes/phy982/phy982prog2014.htm)

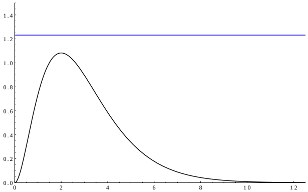
Example – potential scattering

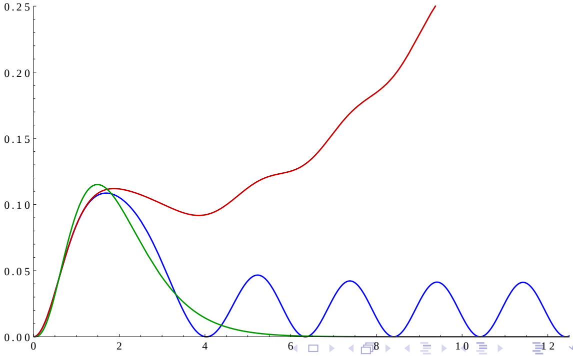
$$V(r) = 2r^2 e^{-r} \qquad E_{\text{res}} = 1.2318 - \frac{i}{2}0.3299$$

- Solution of SE at real and complex energy

$$(H - E)|\Psi_E\rangle = 0 \qquad E \in \mathbb{R}/\mathbb{C}$$

- Discrete state – L^2, not Hamiltonian eigenstate





Wigner-Weisskopf theory – Introduction

- First order time-dependent perturbation theory
- Semiquantitative, but offers useful qualitative insights
- Applicable for metastable states well described in single-particle picture:

$$|\Phi_I^{(N-1)}\rangle = c_{\mathrm{iv}}|\Phi_0^N\rangle$$

- Detailed derivation – Santra and Cederbaum, Phys. Rep. **368** (2002)

Weisskopf and Wigner, Z. Phys. **63**, 54 (1930)

Sakurai, Modern Quantum Mechanics, Addison-Wesley, 1994

Wigner-Weisskopf – The Goal

- Prepare system in the metastable state

$$|\Psi^{(N-1)}(t=0)\rangle = |\Phi_I^{(N-1)}\rangle = c_{\mathrm{iv}}|\Phi_0^N\rangle$$

- Solve TDSE for $|\Psi^{(N-1)}(t)\rangle$

- Evaluate the survival probability amplitude

$$C_I(t) = \langle\Phi_I^{(N-1)}|\Psi^{(N-1)}(t)\rangle$$

- Show that the survival probability decreases exponentially

$$P_I(t) = P_I(0)e^{-\frac{t}{\tau_I}} \qquad \tau_I = \frac{\hbar}{\Gamma_I}$$

Outline

Wigner-Weisskopf theory – Hamiltonian

$$\hat{H}^{(N-1)} = \hat{H}_0^{(N-1)} + \hat{H}_I^{(N-1)}$$

$$\hat{H}_0^{(N-1)} = \sum_J \langle \Phi_J^{(N-1)} | \hat{H} | \Phi_J^{(N-1)} \rangle | \Phi_J^{(N-1)} \rangle \langle \Phi_J^{(N-1)} |$$

$$\hat{H}_I^{(N-1)} = \sum_J \sum_{K \neq J} \langle \Phi_J^{(N-1)} | \hat{H} | \Phi_K^{(N-1)} \rangle | \Phi_J^{(N-1)} \rangle \langle \Phi_K^{(N-1)} |$$

- Unperturbed part $\hat{H}_0^{(N-1)}$ – diagonal in the chosen basis
- Initial metastable state $|\Phi_I^{(N-1)}\rangle$ – discrete eigenvector of $\hat{H}_0^{(N-1)}$
- Decay of $|\Phi_I^{(N-1)}\rangle$ is induced by the off-diagonal part $\hat{H}_I^{(N-1)}$

Wigner-Weisskopf theory – TDSE

- Time-dependent Hamiltonian

$$\hat{H}^{(N-1)}(t) \equiv \hat{H}_0^{(N-1)} + e^{\eta t} \hat{H}_I^{(N-1)}, \quad \eta > 0$$

  - $\eta \to 0^+$ gives physical $\hat{H}$
  - $t \to -\infty$ gives unperturbed $\hat{H}_0$

- TDSE in interaction picture

$$i\hbar \frac{\partial}{\partial t} |\Psi^{(N-1)}(t)\rangle_{\mathrm{int}} = \hat{V}_{\mathrm{int}}(t) |\Psi^{(N-1)}(t)\rangle_{\mathrm{int}}$$

$$|\Psi^{(N-1)}(t)\rangle_{\mathrm{int}} = e^{i\hat{H}_0^{(N-1)} t/\hbar} |\Psi^{(N-1)}(t)\rangle$$

$$\hat{V}_{\mathrm{int}}(t) \equiv e^{\eta t} e^{i\hat{H}_0^{(N-1)} t/\hbar} \hat{H}_I^{(N-1)} e^{-i\hat{H}_0^{(N-1)} t/\hbar}$$

Solution of TDSE

- Initial condition

$$|\Psi^{(N-1)}(t)\rangle = |\Phi_I^{(N-1)}\rangle$$

- Formal integration of TDSE yields

$$|\Psi^{(N-1)}(t)\rangle_{\text{int}} = |\Phi_I^{(N-1)}\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} \hat{V}_{\text{int}}(t')|\Psi^{(N-1)}(t')\rangle_{\text{int}}\, dt'$$

- Perturbation expansion

$$|\Psi^{(N-1)}(t)\rangle_{\text{int}} = |\Phi_I^{(N-1)}\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \hat{V}_{\text{int}}(t')|\Phi_I^{(N-1)}\rangle - \frac{1}{\hbar^2}\int_{-\infty}^{t} dt'\, \hat{V}_{\text{int}}(t') \int_{-\infty}^{t'} dt''\, \hat{V}_{\text{int}}(t')|\Phi_I^{(N-1)}\rangle + \ldots$$

Decay of the initial state

- Exploiting
  - simple time-dependence of $\hat{V}_{\mathrm{int}}(t)$
  - the off-diagonal character of $\hat{H}_I$

  yields the probability amplitude

$$C_I(t) = 1 - \frac{1}{\hbar^2} \sum_{F \neq I} |\langle \Phi_F^{(N-1)} | \hat{H}^{(N-1)} | \Phi_I^{(N-1)} \rangle|^2 \frac{e^{2\eta t}}{2\eta[\eta + i(\omega_F - \omega_I)]}$$

- Derivative of the probability amplitude

$$\dot{C}_I(t) = -\frac{1}{\hbar^2} \sum_{F \neq I} |\langle \Phi_F^{(N-1)} | \hat{H}^{(N-1)} | \Phi_I^{(N-1)} \rangle|^2 \frac{e^{2\eta t}}{\eta + i(\omega_F - \omega_I)}$$

Decay of the initial state

- Ratio $\dot{C}_I(t)/C_I(t)$ through lowest order in interaction

$$\frac{\dot{C}_I(t)}{C_I(t)} = -\frac{i}{\hbar} e^{2\eta t/\hbar} \sum_{F \neq I} \frac{|\langle \Phi_F^{(N-1)} | \hat{H}^{(N-1)} | \Phi_I^{(N-1)} \rangle|^2}{\hbar(\omega_I - \omega_F) + i\eta}$$

- Limit $\eta \to 0^+$ now possible with the aid of

$$\lim_{\eta \to 0^+} \frac{1}{x + i\eta} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)$$

$$\frac{\dot{C}_I(t)}{C_I(t)} = -\mathcal{P}\frac{i}{\hbar} \sum_{F \neq I} \frac{|\langle \Phi_F^{(N-1)} | \hat{H}^{(N-1)} | \Phi_I^{(N-1)} \rangle|^2}{\hbar(\omega_I - \omega_F)} + \frac{\pi}{\hbar} \sum_{F \neq I} |\langle \Phi_F^{(N-1)} | \hat{H}^{(N-1)} | \Phi_I^{(N-1)} \rangle|^2 \delta(\hbar[\omega_I - \omega_F])$$

$$\equiv -\frac{i}{\hbar}\left(\Delta_I - \frac{i}{2}\Gamma_I\right)$$

Probability amplitude in Schrödinger picture

- Integration of the above differential equation

$$C_l(t) = C_l(0)e^{-i(\Delta_l - i\Gamma_l/2)t/\hbar}$$

- Probability amplitude in Schrödinger picture

$$\langle\Phi_l^{(N-1)}|\Psi^{(N-1)}(t)\rangle = \langle\Phi_l^{(N-1)}|e^{-i\hat{H}_0 t/\hbar}|\Psi^{(N-1)}(t)\rangle_{\mathrm{int}}$$
$$= C_l(0)e^{-i(\hbar\omega_l + \Delta_l - i\Gamma_l/2)t/\hbar} \equiv C_l(0)e^{-iE_{\mathrm{res}}t/\hbar}$$

- Interaction with continuum – resonance energy shifted from $\hbar\omega_l$ by
  - Δ_l – level shift (real)
  - Γ_l – decay width (imaginary)

- Probability of finding system in the initial state $|\Phi_l(N-1)\rangle$

$$P_l(t) = |C_l(t)|^2 = P_l(0)e^{-\frac{t}{\tau_l}} \qquad \tau_l = \frac{\hbar}{\Gamma_l}$$

Fourier decomposition – resonance profile

- Fourier transformation

$$e^{-i(\hbar\omega_I+\Delta_I-i\Gamma_I/2)t/\hbar} = \int f(\omega)e^{-i\omega t}d\omega$$

gives

$$|f(\omega)|^2 \propto \frac{1}{(\hbar\omega - \hbar\omega_I - \Delta_I)^2 + \Gamma_I{}^2/4}$$

- $f(\omega)$ – "distribution" of the discrete state over the continuum of eigenstates of full Hamiltonian (cf. Fano theory tomorrow)

- Γ_I has the meaning of "**full width at half maximum**" of the resonance profile

Sakurai, Modern Quantum Mechanics, Addison-Wesley, 1994

Outline

ICD – decay of an inner-valence vacancy

- Initial state – inner-valence vacancy

$$|\Phi_I^{(N-1)}\rangle = c_{\mathrm{iv}}|\Phi_0^N\rangle$$

- "Golden-rule" formula for the decay width

$$\Gamma_I = 2\pi \sum_{F \neq I} \left| \langle \Phi_F^{(N-1)} | \hat{H} | \Phi_I^{(N-1)} \rangle \right|^2 \delta(E_F - E_I)$$

- Hamiltonian in HF quasi-particle picture:

$$\hat{H} = \sum_p \varepsilon_p c_p^\dagger c_p - \sum_{pqi} V_{pi[qi]} c_p^\dagger c_q + \frac{1}{2} \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_s c_r$$

$$V_{pqrs} = \iint \varphi_p^\dagger(\mathbf{x}_1)\varphi_r(\mathbf{x}_1) \frac{e^2}{|\mathbf{x}_1 - \mathbf{x}_2|} \varphi_q^\dagger(\mathbf{x}_2)\varphi_s(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2$$

Decay mechanism – NeAr example

- **Initial state**: $\mathrm{Ne}^+(2s^{-1})$ $\quad |\Phi_I^{(N-1)}\rangle = c_{\mathrm{Ne}(2s)\downarrow}|\Phi_0^N\rangle$
- **Final state**: $\mathrm{Ne}^+(2p^{-1}) + \mathrm{Ar}^+(3p^{-1}) + e^-$

$$|\Phi_F^{(N-1)}\rangle = \frac{1}{\sqrt{2}}\left(c^\dagger_{\mathbf{k}\uparrow} c_{\mathrm{Ne}(2p)\downarrow} c_{\mathrm{Ar}(3p)\uparrow} - c^\dagger_{\mathbf{k}\uparrow} c_{\mathrm{Ne}(2p)\uparrow} c_{\mathrm{Ar}(3p)\downarrow}\right)|\Phi_0^N\rangle$$

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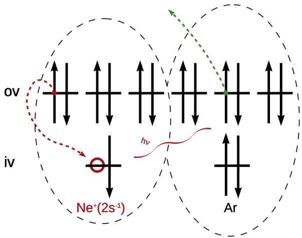
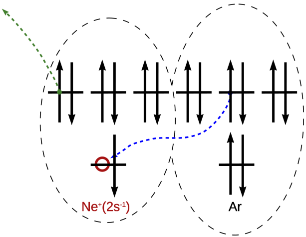
$$\langle\Phi_F^{(N-1)}|\hat{H}|\Phi_I^{(N-1)}\rangle = \iint \varphi_{2s}^{\mathrm{Ne}}(\mathbf{x}_1)\varphi_{2p'}^{\mathrm{Ne}}(\mathbf{x}_1)\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\varphi_{3p}^{\mathrm{Ar}}(\mathbf{x}_2)\varphi_{\mathbf{k}}(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2$$

$$+\iint \varphi_{2s}^{\mathrm{Ne}}(\mathbf{x}_1)\varphi_{3p}^{\mathrm{Ar}}(\mathbf{x}_1)\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\varphi_{2p'}^{\mathrm{Ne}}(\mathbf{x}_2)\varphi_{\mathbf{k}}(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2$$



energy transfer

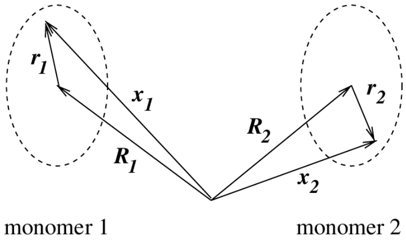


electron transfer

Outline

Asymptotic dependence on intermolecular distance

$$\frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} = \frac{1}{R} - \frac{\mathbf{u}_R \cdot (\mathbf{r}_1 - \mathbf{r}_2)}{R^2} + \frac{3(\mathbf{u}_R \cdot (\mathbf{r}_1 - \mathbf{r}_2))^2 - (\mathbf{r}_1 - \mathbf{r}_2)^2}{2R^3} + O\left(\frac{1}{R^4}\right)$$



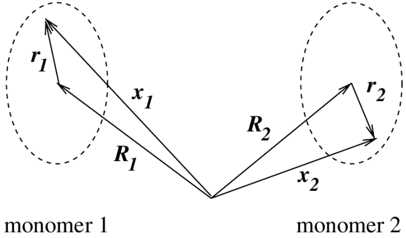
$$\langle \varphi_{\mathrm{ov}_1} | \varphi_{\mathrm{iv}_1} \rangle = 0$$

$$\langle \varphi_{\mathrm{ov}_2} | \varphi_{\mathbf{k}} \rangle = 0$$

Santra and Cederbaum, Phys. Rep. **368**, 1 (2002)

Asymptotic dependence on intermolecular distance

$$\frac{1}{|\mathbf{x}_1-\mathbf{x}_2|}=\frac{1}{R}-\frac{\mathbf{u}_R\cdot(\mathbf{r}_1-\mathbf{r}_2)}{R^2}+\frac{3(\mathbf{u}_R\cdot(\mathbf{r}_1-\mathbf{r}_2))^2-(\mathbf{r}_1-\mathbf{r}_2)^2}{2R^3}+O\left(\frac{1}{R^4}\right)$$



$$\langle\varphi_{\mathrm{ov}_1}|\varphi_{\mathrm{iv}_1}\rangle=0$$

$$\langle\varphi_{\mathrm{ov}_2}|\varphi_{\mathbf{k}}\rangle=0$$

$$V_{\mathrm{ov}_1,\mathrm{ov}_2,\mathrm{iv}_1,\mathbf{k}}=\iint\varphi_{\mathrm{iv}_1}(\mathbf{x}_1)\varphi_{\mathrm{ov}_1}(\mathbf{x}_1)\frac{e^2}{|\mathbf{x}_1-\mathbf{x}_2|}\varphi_{\mathrm{ov}_2}(\mathbf{x}_2)\varphi_{\mathbf{k}}(\mathbf{x}_2)d\mathbf{x}_1d\mathbf{x}_2$$

$$\approx\frac{e^2}{R^3}\langle\varphi_{\mathrm{ov}_1}|\mathbf{r}_1|\varphi_{\mathrm{iv}_1}\rangle\langle\varphi_{\mathrm{ov}_2}|\mathbf{r}_2|\varphi_{\mathbf{k}}\rangle-\frac{3e^2}{R^3}\langle\varphi_{\mathrm{ov}_1}|\mathbf{r}_1\cdot\mathbf{u}_R|\varphi_{\mathrm{iv}_1}\rangle\langle\varphi_{\mathrm{ov}_2}|\mathbf{r}_2\cdot\mathbf{u}_R|\varphi_{\mathbf{k}}\rangle$$

Santra and Cederbaum, Phys. Rep. **368**, 1 (2002)

$\Gamma(R)$ – Asymptotic behavior

- Asymptotic behavior of the decay width

$$\langle F|\hat{V}|I\rangle \propto \frac{1}{R^3}\left(1 + P(R)e^{-\alpha R}\right) \Longrightarrow \lim_{R\to\infty}\Gamma(R) \propto \frac{1}{R^6}$$

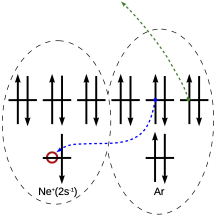
- Leading term – dipole-dipole interaction
  - virtual photon transfer model

$$\Gamma = \frac{3\hbar}{4\pi}\left(\frac{c}{\omega}\right)^4 \frac{\tau_{\mathrm{rad}}^{-1}\sigma}{R^6}$$

  - τ_{rad} – **radiative lifetime** of the inner-valence vacancy state
  - σ – **total photoionization cross section** of the neigbor at the virtual photon energy $\hbar\omega$

Matthew and Komninos, Surf. Sci. **53**, 716 (1975)
Averkukh, Müller and Cederbaum, PRL **93**, 263002 (2004)
Averbukh and Cederbaum, JCP **125**, 094107 (2006)

$\Gamma(R)$ – Deviations from the R^{-6} rule



- ETMD – electron transfer process
  - dominated by orbital overlap, $e^{-\alpha R}$ dependence
- Dipole forbidden recombination transition
  - example: Zn(3*d*) vacancy in BaZn dimer – quadrupole-dipole interaction

$$\Gamma_{0,\pm 1} = \frac{1323\hbar}{28\pi} \left(\frac{c}{\omega}\right)^6 \frac{\tau_{\mathrm{Zn}}^{-1}\sigma_{\mathrm{Ba}}}{R^8}$$

- ICD in He dimer: $\mathrm{He}^+(2s^1)\mathrm{He} \longrightarrow \mathrm{He}^+ + \mathrm{He}^+ + e^-$
  - $2s \rightarrow 1s$ single-photon recombination forbidden
  - $e^{-\alpha R}$ dominates at small distances
  - R^{-8} asymptotics – 3^{rd} order decay pathway

Averkukh, Müller and Cederbaum, PRL **93**, 263002 (2004)

Kolorenč *et al.*, PRA **82**, 013422 (2010)

Outline

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   - Evolution of the state vector
   - ICD – the mechanism
   - Asymptotic behavior of the decay width
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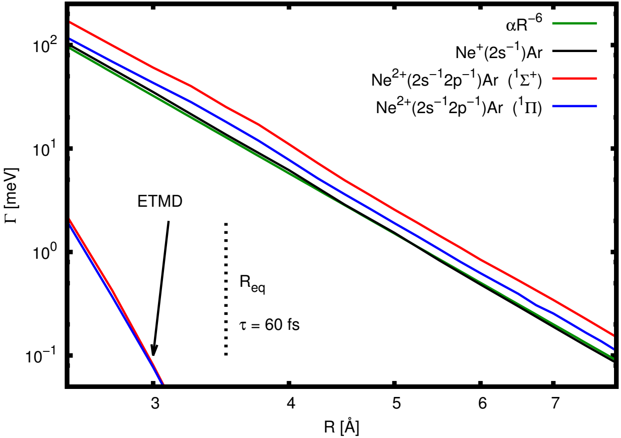
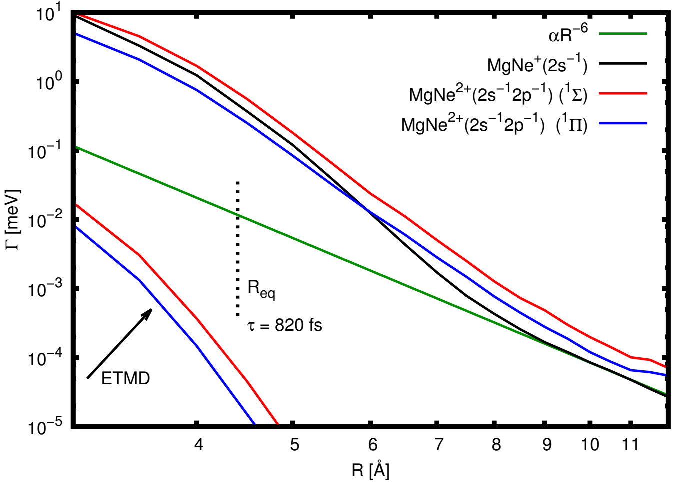
ICD & ETMD widths in NeAr



$$\text{ICD}: \quad Ne^{+}(2s^{-1})Ar \longrightarrow Ne^{+}(2p^{-1}) + Ar^{+}(3p^{-1}) + e^{-}$$

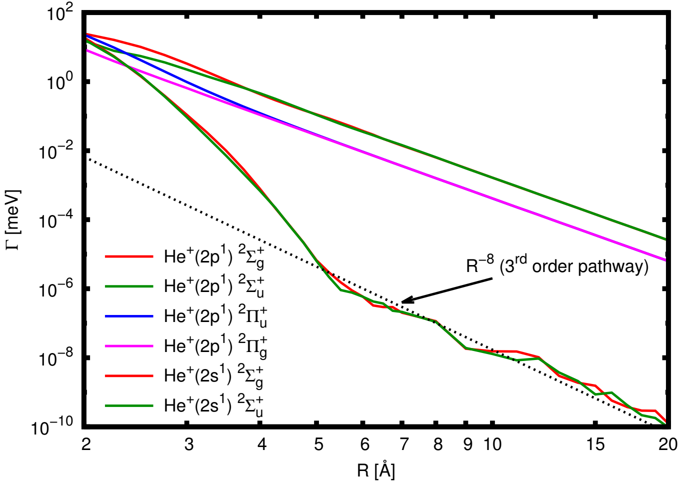
$$\text{ETMD}: \quad Ne^{+}(2s^{-1})Ar \longrightarrow NeAr^{2+}(3p^{-2}) + e^{-}$$

ICD & ETMD widths in MgNe



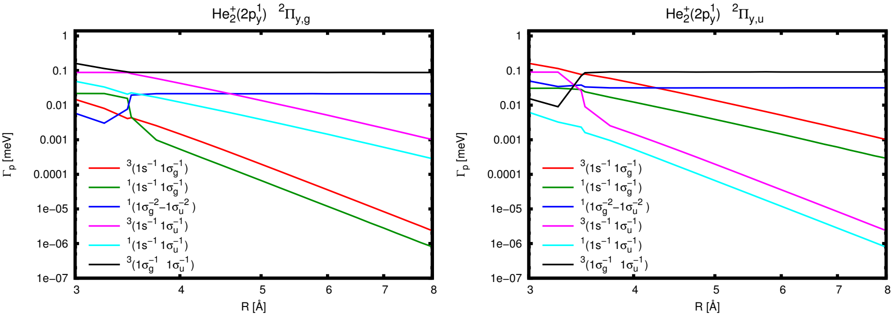
$$Ne^+(2s^{-1})Mg \rightarrow Ne^+(2p^{-1}) + Mg^+(3s^{-1}) + e^-$$

ICD in $(He_2^+)^*$



$$(He^+)^*He \longrightarrow He^+ + He^+ + e^-$$

ICD in He_3 – selection rules on the emssion site



- $\Gamma \propto \mathbf{R}^{-6}$: symmetry of ICD e^- match the polarization of the virtual photon

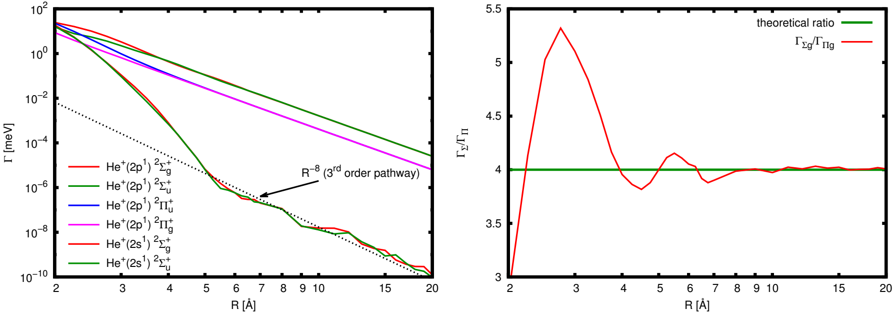
$$^2\Pi_{y,g}: \quad (\mathrm{He}_2^+)^*(2p_y^1) - \mathrm{He} \quad \longrightarrow \quad \mathrm{He}_2^+(1\sigma_u^{-1}) + \mathrm{He}^+(1s) + e^-(p_y)$$

- $\Gamma \propto \mathbf{R}^{-8}$: other channels:

$$^2\Pi_{y,g}: \quad (\mathrm{He}_2^+)^*(2p_y^1) - \mathrm{He} \quad \longrightarrow \quad \mathrm{He}_2^+(1\sigma_g^{-1}) + \mathrm{He}^+(1s) + e^-(d)$$

Outline

Symmetry dependence of the ICD width



- interaction energy between two classical dipoles

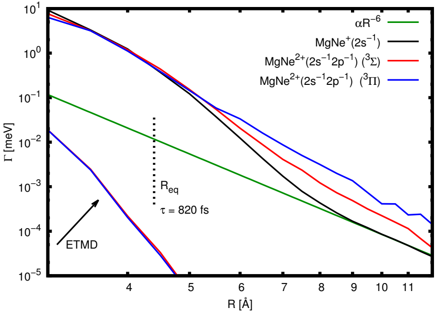
$$W = \frac{\mathbf{p}_1 \cdot \mathbf{p}_2 - 3(\mathbf{n}\cdot\mathbf{p}_1)(\mathbf{n}\cdot\mathbf{p}_2)}{|\mathbf{x}_1 - \mathbf{x}_2|^3}$$

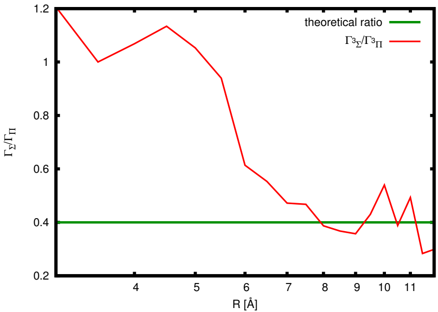
- dipoles parallel vs. perpendicular to molecular axis

$$W_{\|}/W_{\perp} = 2 \longrightarrow \Gamma_{^2\Sigma}/\Gamma_{^2\Pi} = 4$$

Gokhberg *et al.*, PRA **81**, 013417 (2010)

Symmetry dependence of the ICD width





- ICD after Auger in MgNe, triplet metastable states – more complicated case
- summation over all partial rates gives asymptotic ratio

$$\frac{\Gamma_{^3\Sigma}}{\Gamma_{^3\Pi}} = \frac{2}{5}$$

Gokhberg *et al.*, PRA **81**, 013417 (2010)

Summary

- Survival probability of finding system in the initial state

$$P_I(t) = P_I(0)\exp\left(-\frac{\Gamma_I}{\hbar}t\right)$$

- Wigner-Weisskopf "golden-rule" formula for decay width

$$\Gamma_I = 2\pi\sum_{F\neq I}\left|\langle\Phi_F^{(N-1)}|\hat{H}|\Phi_I^{(N-1)}\rangle\right|^2\delta(E_F - E_I)$$

- Typical ICD mechanism – dipole-dipole interaction, virtual photon transfer

$$\Gamma \propto R^{-6} \quad R\to\infty$$

- Deviations from the R^{-6} rule
  - electron transfer or orbital overlap contribution (at short distances)
  - dipole-forbidden transitions
- Beyond 1[st] order – CAP, complex scaling, Fano-Feshbach, ...