ポジトロニウム負イオン光脱離断面積の計算
(Calculation of the photo-detachment cross sections of Ps^-)

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概要 (outline)

1. 理論 (Theory)
   1.1　1光子及び2光子吸収により光脱離
   (One- and two-photo detachment)
   1.2　原子軌道緊密結合法
   (Atomic orbital close coupling method)

２. 結果 (Results)
   2.1 One-photon detachment cross section
   2.2 Two-photon detachment cross section

One- and two-photon detachment cross sections within the perturbation theory

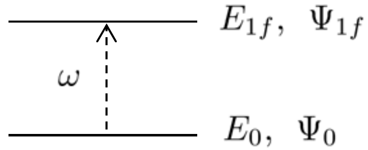
$$\sigma^{(1)} = \pi(2\pi\alpha)\omega < \Psi_{1f}|\hat{e}\cdot\mathbf{D}|\Psi_0 > |^2.$$

α: fine-structure constant. ω: photon energy.

Ψ_0: the initial bound state, E_0.

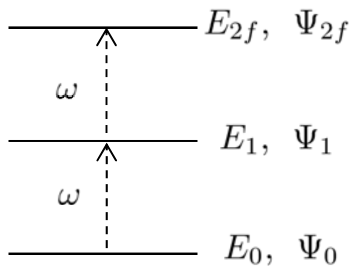
Ψ_{1f}: a final scattering state, $E_{1f} = E_0 + \omega$.

$\hat{\mathbf{e}}$: (linear) polarization, $\quad$ $\mathbf{D}$:dipole operator.



$$\sigma^{(2)} = \pi(2\pi\alpha)^2\omega^2|A^{(2)}|^2,$$

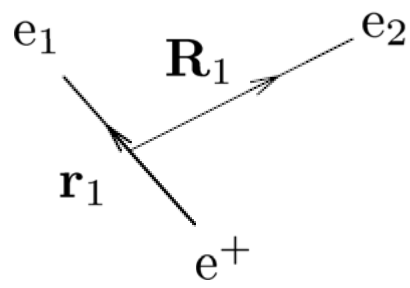
$$\begin{aligned} A^{(2)} &= \lim_{\eta\to+0} < \Psi_{2f}|\hat{\mathbf{e}}\cdot\mathbf{D}\underline{\frac{1}{E_1 - H + \mathrm{i}\eta}\hat{\mathbf{e}}\cdot\mathbf{D}|\Psi_0 >} \\ &=< \Psi_{2f}|\hat{\mathbf{e}}\cdot\mathbf{D}|\ \Psi_1 > \end{aligned}$$



$$\begin{aligned} &(E_1 - H)\Psi_1 = \hat{\mathbf{e}}\cdot\mathbf{D}\Psi_0, \quad && E_1 = E_0 + \omega \\ &(E_2 - H)\Psi_{2f} = 0\ , && E_{2f} = E_0 + 2\omega \end{aligned}$$

Ps^- system $\quad (\mathrm{e}^-, \mathrm{e}^-, \mathrm{e}^+)$

$(\mathrm{e}_1, \mathrm{e}^+) + \mathrm{e}_2$



Kinetic energy term

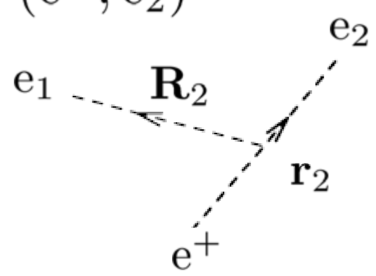
$$T = -\frac{1}{2M}\nabla^2_{R_1} - \frac{1}{2m}\nabla^2_{r_1} = -\frac{1}{2M}\nabla^2_{R_2} - \frac{1}{2m}\nabla^2_{r_2}$$

$$= -\frac{1}{2m}\nabla^2_{r_1} - \frac{1}{2m}\nabla^2_{r_2} - \frac{1}{m_+}\nabla_{r_1}\cdot\nabla_{r_2}$$

$$M = \frac{m_e(m_e+m_+)}{2m_e+m_+} = \frac{2}{3}m_e, \;\; m = \frac{m_e m_+}{m_e+m_+} = \frac{1}{2}m_e$$

m_e: electron mass, $\quad m_+$: positron mass

$\mathrm{e}_1 + (\mathrm{e}^+, \mathrm{e}_2)$



Hamiltonian $\quad H = T - \dfrac{1}{r_1} - \dfrac{1}{r_2} + \dfrac{1}{r_{12}}$

Symmetry $\Gamma = \{L, S, \Pi\}, \quad [H, \mathbf{L}^2] = [H, L_z] = [H, \mathbf{S}^2] = [H, \Pi] = 0$

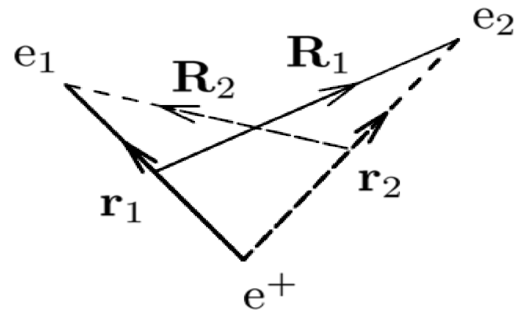
Angular momentum $\mathbf{L} = \mathbf{l}_{r_1} + \mathbf{l}_{r_2} = \mathbf{l}_{R_c} + \mathbf{l}_{r_c}$

Spin $\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2$,

Parity, $\quad \Pi\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(-\mathbf{r}_1, -\mathbf{r}_2)$

Atomi orbital (AO) basis

$$\phi^{\Gamma}_{n\ell l}(\mathbf{r},\hat{\mathbf{R}}) = \frac{u_{n\ell}(r)}{r}(Y_\ell(\hat{\mathbf{r}}) \otimes Y_l(\hat{\mathbf{R}}))_{LM_M}$$



AO expansion,

$$\Psi^{\Gamma} = \sum_{\mu=1}^{N}\left(\frac{f_\mu(R_1)}{R_1}\phi^{\Gamma}_{\mu}(\mathbf{r}_1,\hat{R}_1) + (-1)^S\frac{f_\mu(R_2)}{R_2}\phi^{\Gamma}_{\mu}(\mathbf{r}_2,\hat{R}_2)\right)$$

f_μ: unknown function

From $\int d\hat{\mathbf{R}}_1 \int d\mathbf{r}_1 \phi^{\Gamma *}_{\mu}(\mathbf{r}_1,\hat{\mathbf{R}}_1)(H-E)\Psi^{\Gamma} = 0$,

$$-\frac{1}{2M}\left[\frac{d^2}{dR_1^2} - \frac{l_\mu(l_\mu+1)}{R_1^2} - k_\mu^2\right] f_\mu(R_1) + \sum_{\nu=1}^{N}\left(V^D_{\mu\nu} + (-1)^S V^X_{\mu\nu}\right) f_\nu(R_1) = 0$$

coupled integro-differential equations

$$f_\mu(R) = \sum_{i=1}^{N_B} C_{\mu i}\ B_i(R), \quad 0 \le R \le R_{max}, \quad C_{\mu i}\text{: coefficient}$$

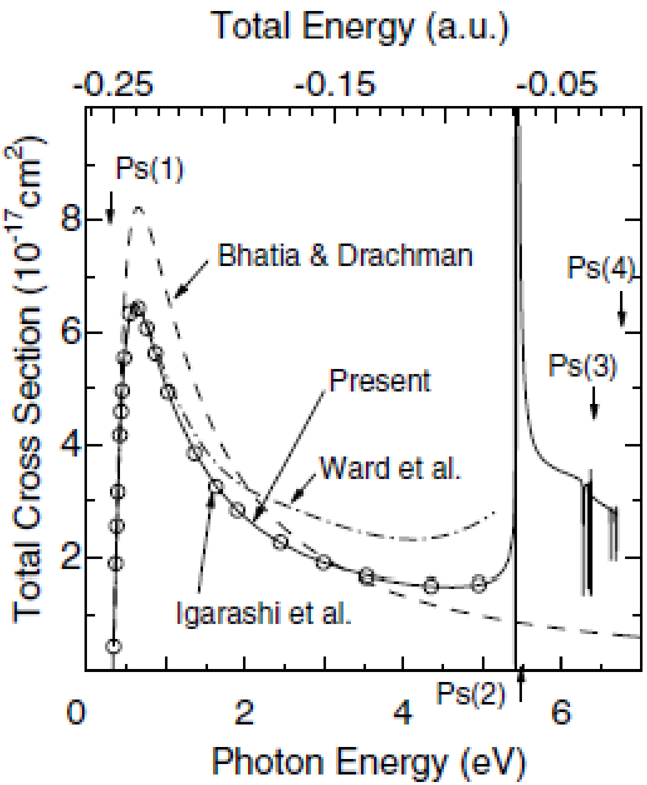
$$\Psi^{\Gamma} = \sum_{i=1}^{N_B}\sum_{\mu=1}^{N} C_i^{\mu}\underline{\left(B_i(R_1)\phi_\mu(\mathbf{r}_1,\hat{R}_1) + (-1)^S B_i(R_2)\phi_\mu(\mathbf{r}_2,\hat{R}_2)\right)} \equiv \sum_{i=1}^{N_B}\sum_{\mu=1}^{N} C_i^{\mu}\mathcal{B}_{i\mu}$$

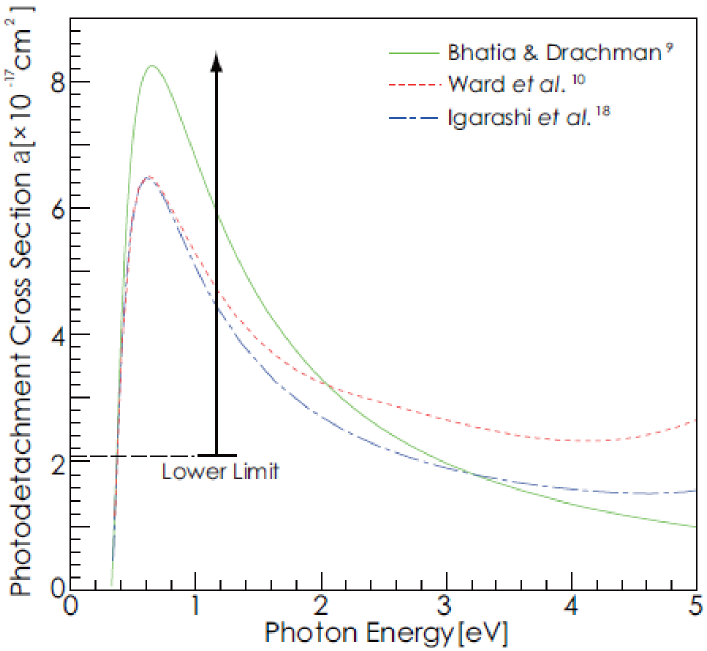
$$\int_0^{R_{max}} d\mathbf{R}_1 \int d\mathbf{r}_1 \mathcal{B}^*_{i\mu}(H-E)\Psi^{\Gamma} = 0 \to \quad \sum_{j=1}^{N_B}\sum_{\nu=1}^{N}\left(\int_0^{R_{max}} d\mathbf{R}_1 \int d\mathbf{r}_1 \mathcal{B}^*_{i\mu}(H-E)\mathcal{B}_{j\nu}\right) C_j^{\nu} = 0$$

coupled integro-differential equations $\Rightarrow$ algebraic equations

One-photon detachment cross sections of Ps^-

$$\hbar\omega + \mathrm{Ps}^- \to \mathrm{e}^- + \mathrm{Ps}(n)$$



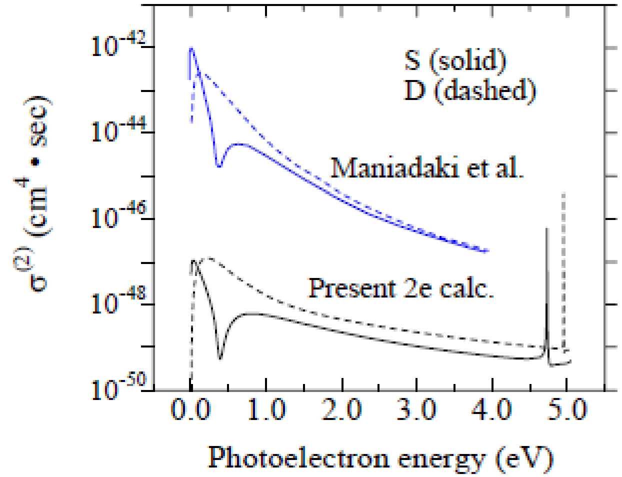


Igarashi, Shimamura, Toshima
N. J. Phys. **2** 17 (2000)

Michishio et al.
Phys. Rev. Lett. **106**, 153401 (2011)

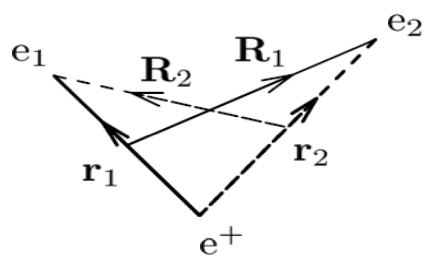
Two-photon detachment cross sections of Ps^-

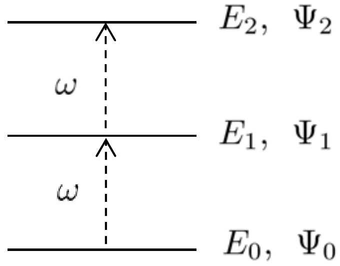
$$2\hbar\omega + \mathrm{Ps}^- \rightarrow \mathrm{e}^- + \mathrm{Ps(1s)}$$

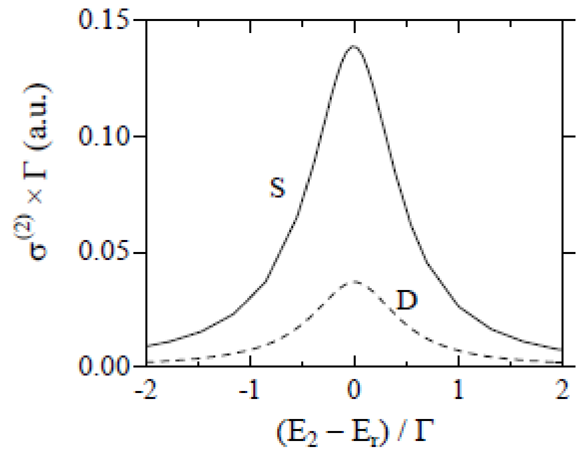


Selection rule

$$\Psi_0(^1\mathrm{S}^e) \rightarrow \Psi_1(^1\mathrm{P}^o) \rightarrow \Psi_2(^1\mathrm{S}^e,\ ^1\mathrm{D}^e)$$







Resonance parameter

	E_r (eV)	Γ (meV)	
$^1\mathrm{S}^e$	4.7340	1.2	present
	4.7340	1.2	CR
$^1\mathrm{D}^e$	4.9550	0.050	present
	4.9549	0.049	CR

E_r in photoelectron energy

- For photon energy above the one-photon detachment, one- and two photondetachments occur simultaneously.
- The best way to distinguish them is to meaure the momentum of ejected electrons. But it may be diffucult for Ps^- system.

Rates for one- and two-photon detachment of Ps^-

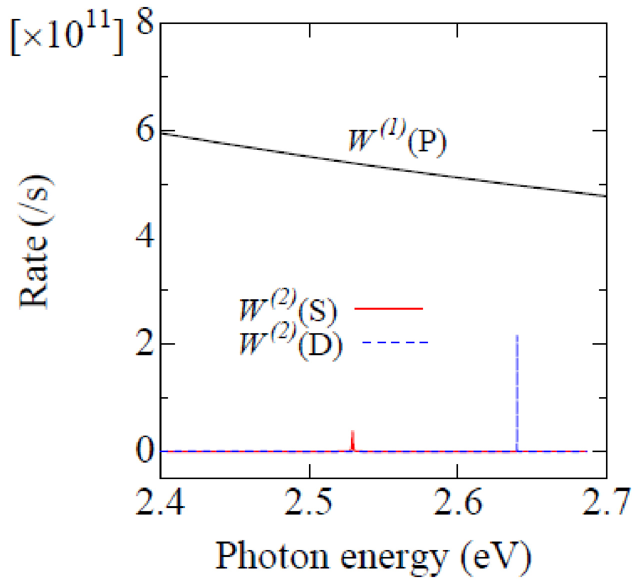
Laser intensity I ($\mathrm{W/cm^2}$)
$I = \hbar\omega F$,
photon flux F (photons/($\mathrm{cm^2}$ s))

Rate (/s)

$W^{(1)} = \sigma^{(1)}\ F$

$W^{(2)} = \sigma^{(2)}\ F^2$

Laser intensity $I = 1.0 \times 10^{10}\ \mathrm{W/cm^2}$



Summary

- Two-photon detachment cross sections ($\sigma^{(2)}$) of Ps^- are calculated with the coupled channel calculations.
- The lowest $^1S^e$ and $^1D^e$ resonances below the Ps(n=2) threshold are clearly seen.
- To observe the resonances without measuring the ejected electron kinetic energy, the laser intensity $\sim 1.0 \times 10^{10}$ W/cm^2 is required.