Time-dependent theory of laser-assisted Auger decay induced by ultra-short pulses

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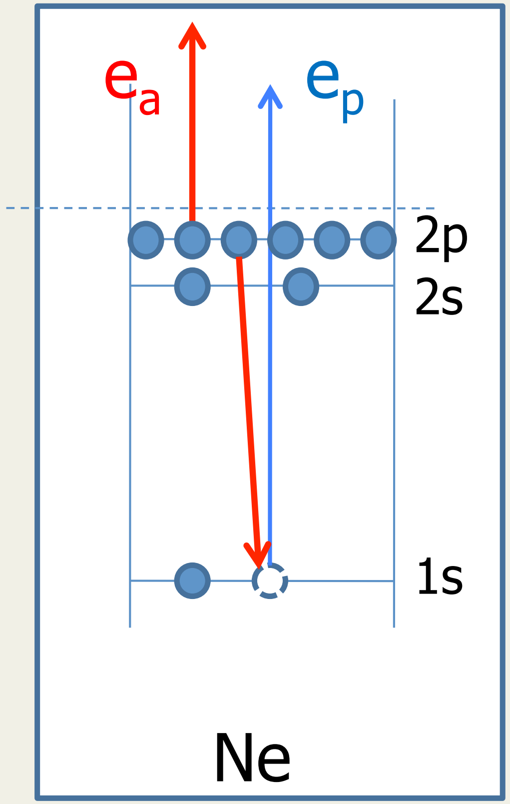
Inner-shell photoionization and Auger decay



$$KL_{23}L_{23}$$

Discovery: Lise Meitner 1923 and Pierre Auger 1925

$$\gamma + A(J_0\pi_0) \rightarrow A^{+}(J_i\pi_i) + e_{ph}$$

$$\hookrightarrow A^{2+}(J_f\pi_f) + e_A$$

Resonant photo double ionization

Energy conservation:

$$\hbar\omega + E_0 = \epsilon_p + \epsilon_A + E_f^{(2+)}$$

⬇

$$\hbar\omega + E_0 = E_i^{(+)} + \epsilon_p \quad \text{and} \quad E_i^{(+)} = E_f^{(2+)} + \epsilon_A$$

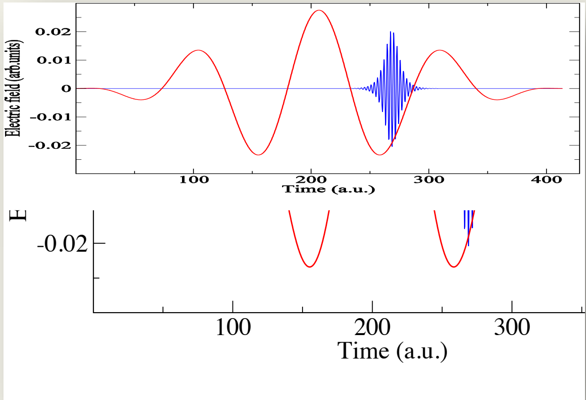
Auger spectroscopy

Time-resolved study of Auger decay

First experiment: M. Drescher et al. Nature 419, 803, 2002

Attosecond XUV pulse

ω= 70 – 130 eV



Infrared (IR) laser pulse:

$I = 10^{12} – 10^{14}$ W/cm^2

ω= 1.66 eV (800 nm),
T_L = 2.5 fs

The main parameters: τ_L - duration of the IR pulse

T_L - period of the IR pulse

τ_{XUV} - duration of the XUV pulse

τ_A - Auger life-time

Suppose:

$$\tau_{XUV} \ll T_L$$

Two limiting cases:

$\tau_A \ll T_L$ Streaking

$\tau_A \gg T_L$ Sidebands

Time-dependent description of the Auger process in a strong laser field

A. Auger decay without laser field

A.K. Kazansky, N.M. Kabachnik PRA 73, 062712 (2006)

$$i\frac{\partial \phi_d(\vec{r},t)}{\partial t} = \left(\hat{H}_1(\vec{r}) - i\frac{\Gamma}{2}\right)\phi_d(\vec{r},t) - \frac{1}{2} z \mathcal{E}_X(t)\phi_0(\vec{r}) \exp(-iE_{exc}t)\,,$$

$$i\frac{\partial \phi_\epsilon(\vec{r},t)}{\partial t} = (\hat{H}_2(\vec{r}) + \epsilon)\phi_\epsilon(\vec{r},t) + \hat{V}_\epsilon^* \phi_d(\vec{r},t)\,. \qquad E_{exc} = \omega_0 - |\epsilon_0| \qquad \epsilon = E_A - E_{A0}$$

No direct interaction between photo and Auger electrons

Expanding the wave functions in partial waves, we solve the system for partial wave functions and calculate the amplitudes:

$$\mathcal{A}_\ell(\epsilon, E) = \exp[i\eta_\ell(E)] \int_0^\infty dr u_\epsilon^{(\ell)}(r, t \to +\infty)\chi_-^{(\ell)*}(E; r)$$

and the TDCS

$$\frac{d^3\sigma(\epsilon, E, \Omega)}{d\epsilon dE d\Omega} = \frac{2\pi\omega_0}{cK}\left|\sum_\ell \mathcal{A}_\ell(\epsilon, E) Y_{\ell 0}(\theta)\right|^2$$

B. Auger decay in a strong laser field

A.K. Kazansky et al, J. Phys. B 42, 245601 (2009)

Example: KLL Auger transition in Ne
E_e= 13.6 eV, E_A = 800 eV

$$i\frac{\partial\phi_d(\vec{r},t)}{\partial t} = \left(\hat{H}_1(\vec{r}) - i\frac{\Gamma}{2} - z\mathcal{E}_L(t)\right)\phi_d(\vec{r},t) - \frac{1}{2}z\mathcal{E}_X(t)\phi_0(\vec{r})\exp(-iE_{exc}t)\,,$$

$$i\frac{\partial\bar{\phi}_\epsilon(\vec{r},t)}{\partial t} = \left(\hat{H}_2(\vec{r}) + \frac{1}{2}[\vec{k} - \vec{A}_L(t)]^2 - E_{A0} - z\mathcal{E}_L(t)\right)\bar{\phi}_\epsilon(\vec{r},t) + \hat{V}_\epsilon^*\phi_d(\vec{r},t)\,.$$

$$\bar{\phi}_\epsilon(\vec{r},t) = \phi_\epsilon(\vec{r},t)\exp(-\Phi_V(k,t))$$

$$\Phi_V(\vec{k},t) = \frac{1}{2}\int_{-\infty}^{t}(\vec{k} - \vec{A}_L(t'))^2 dt'$$

Main approximations:
1. SFA for the Auger electron
2. All inner electrons are not effected by the laser field
3. No direct interaction between photo and Auger electrons

Advantages: Interaction of slow photoelectron with the ion is taken into account – Near threshold phenomena (PCI), rescattering in the strong field, population of Rydberg states etc.

Calculations for Ne KLL Auger transitions

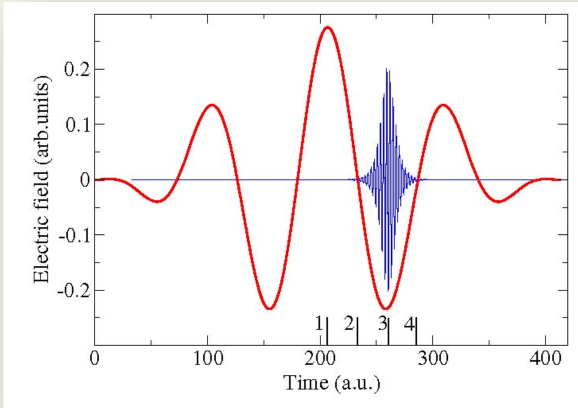
A. Spectra and angular distributions of photoelectrons

Basic parameters:

Ne (1s) E_b = 870.1 eV

τ_A - 2.4 fs, E_A = 804.3 eV

X-ray pulse: τ_X - 330 as

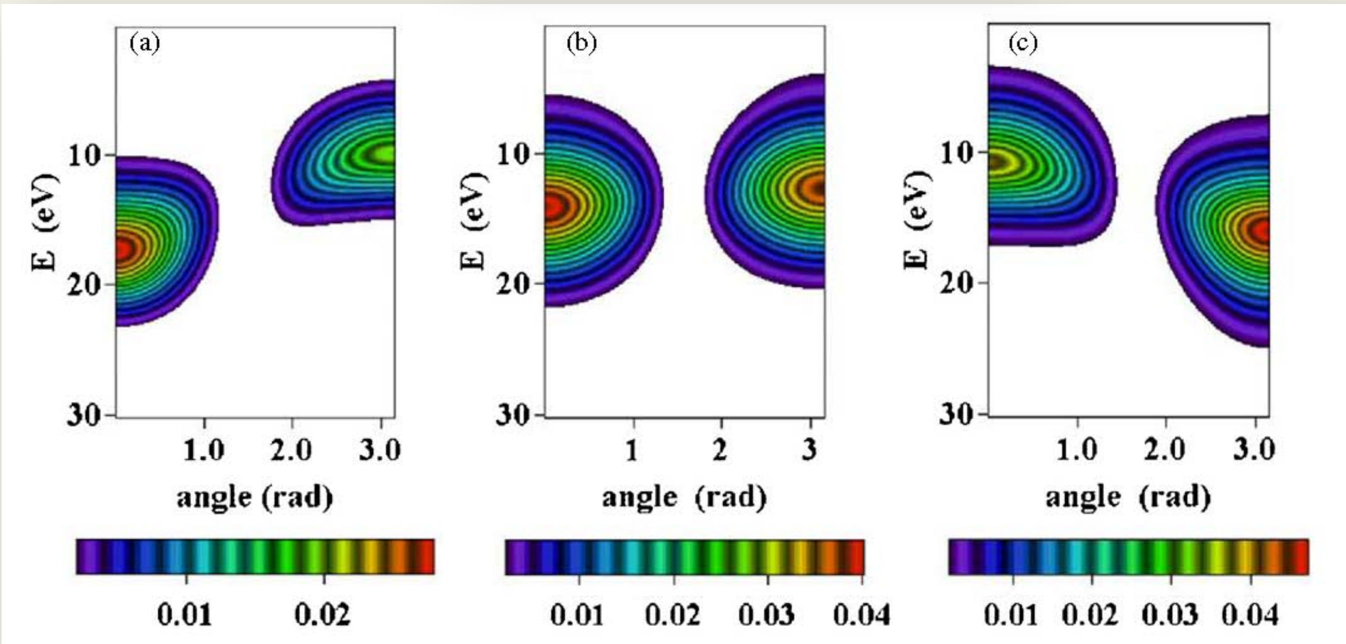


IR pulse: 800 nm

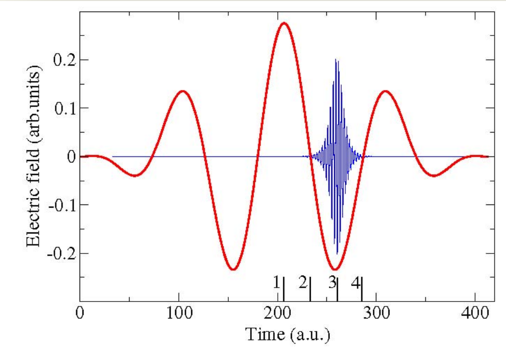
τ_L - 5 fs T_L = 2.5 fs

I = 10^{12} W/cm^2

$$\frac{d^2\sigma(E_e,\theta_e)}{dE_e d\theta_e}$$



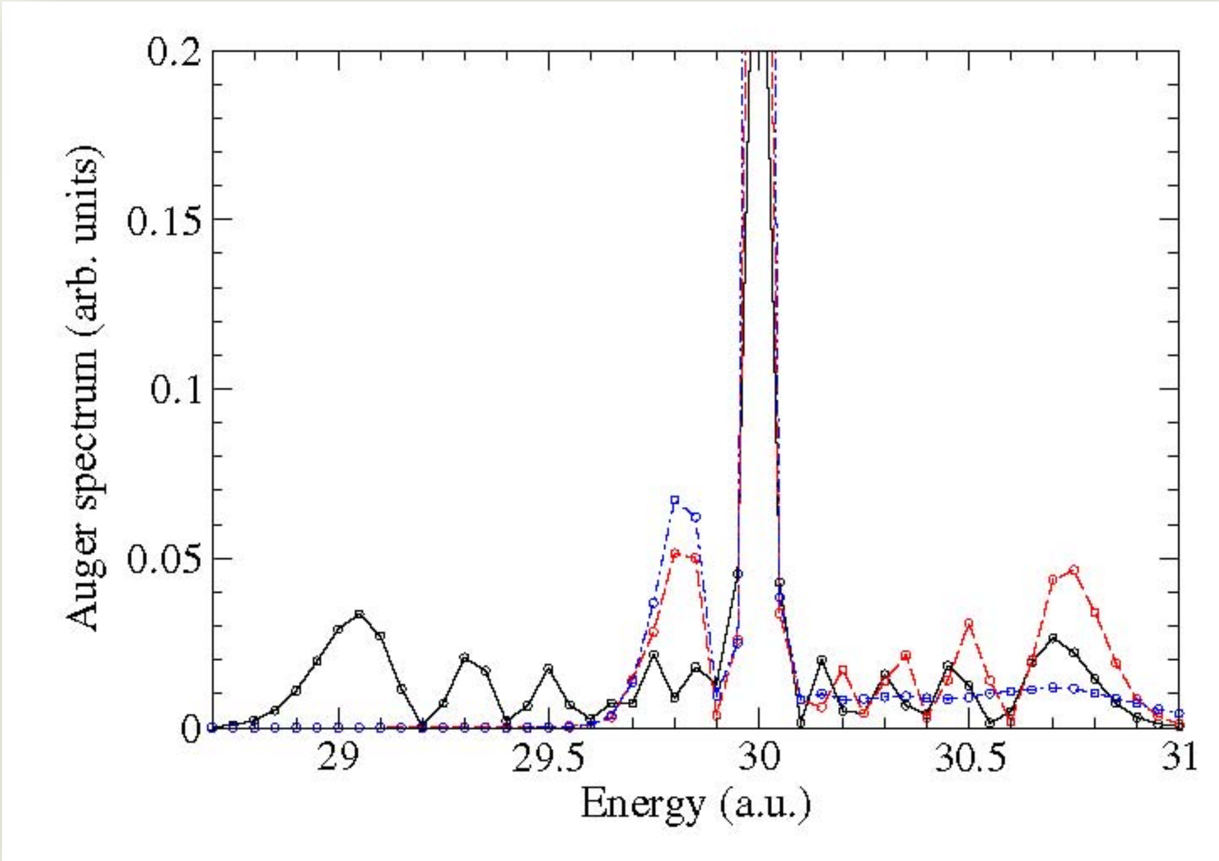
B. Spectra of Auger electrons



E_A = 804.3 eV (30 a.u.)

τ_A - 2.4 fs, T_L = 2.5 fs

Θ_A = 0



C. Angular distributions of Auger electrons

Ne KLL Auger spectra at different emission angles

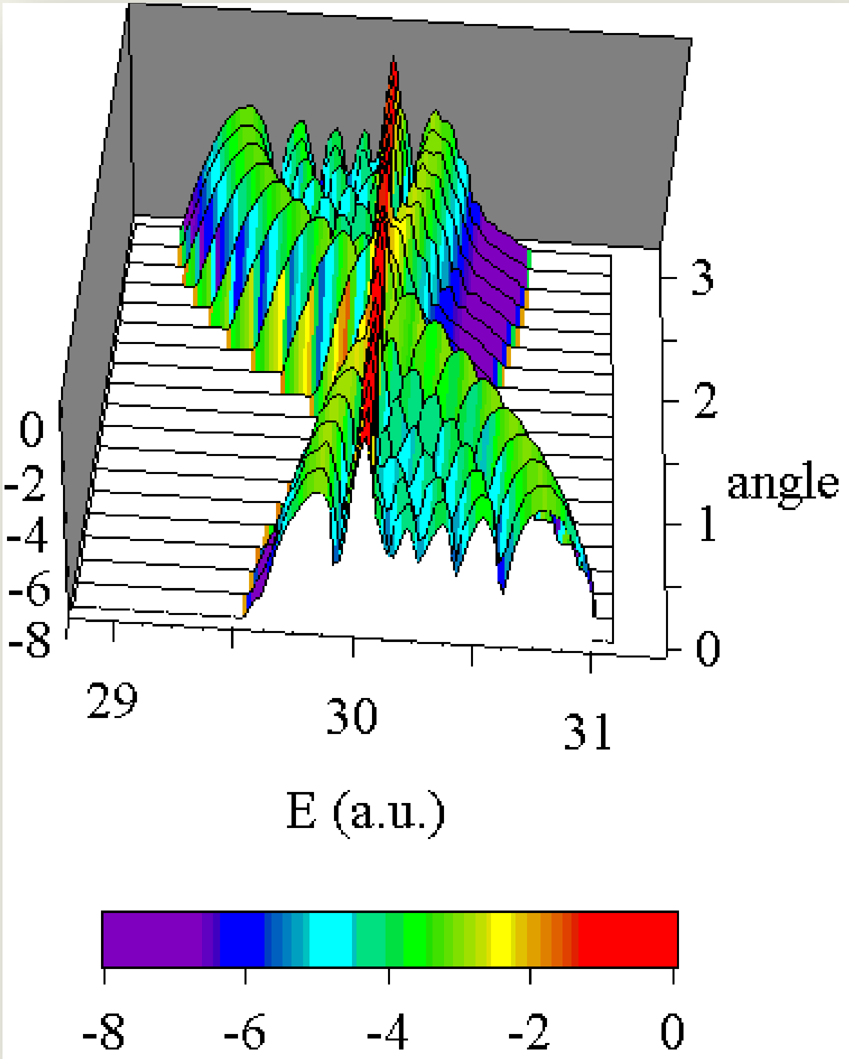
Parameters:

$E_A = 30 a.u.$

$\tau_A = 2.4$ fs

$\tau_X = 330$ as

$\tau_L = 5$ fs



Sideband structure for Auger electrons

A. Kazansky and N. Kabachnik J. Phys. B 43, 035601 (2010)

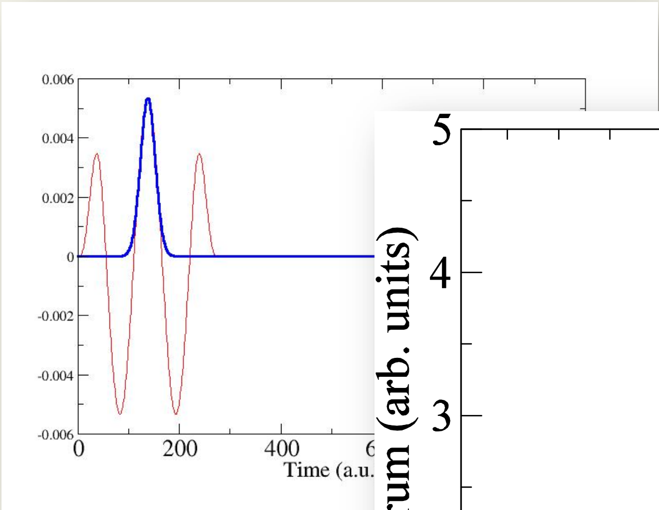
Ne (1s), KLL

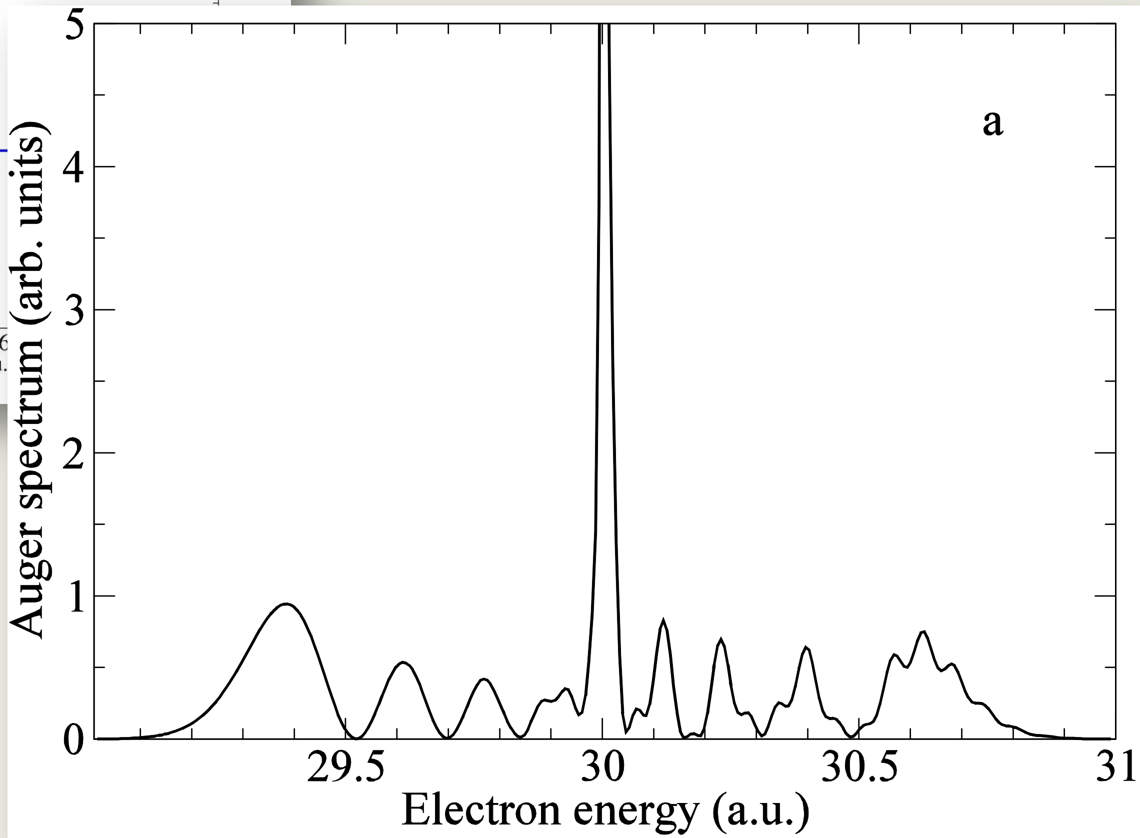
X-ray: τ_X = 1 fs

E_A = 800 eV (30 a.u.)

IR: τ_L = 4.0 fs

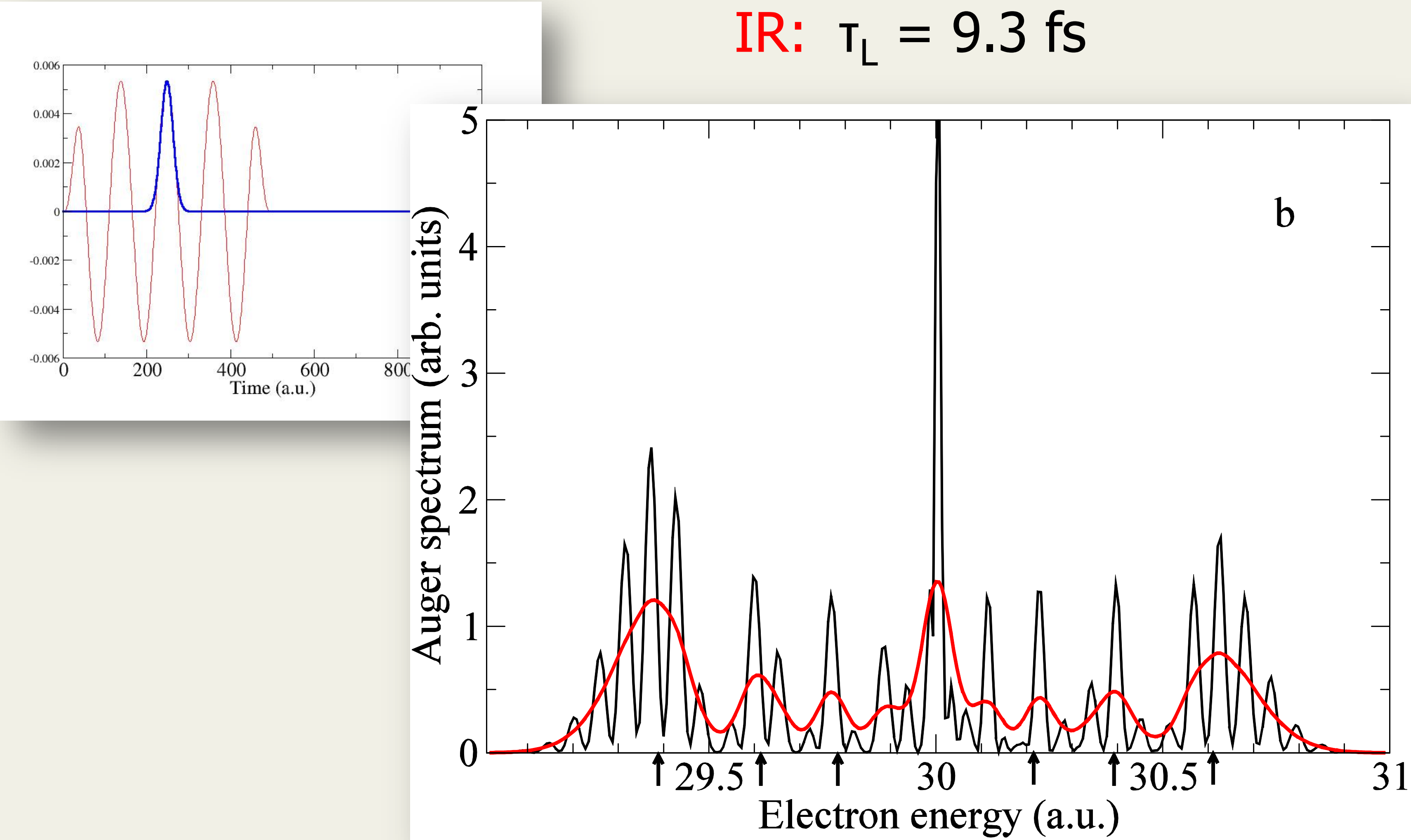
τ_A = 2.4 fs (100 a.u.)



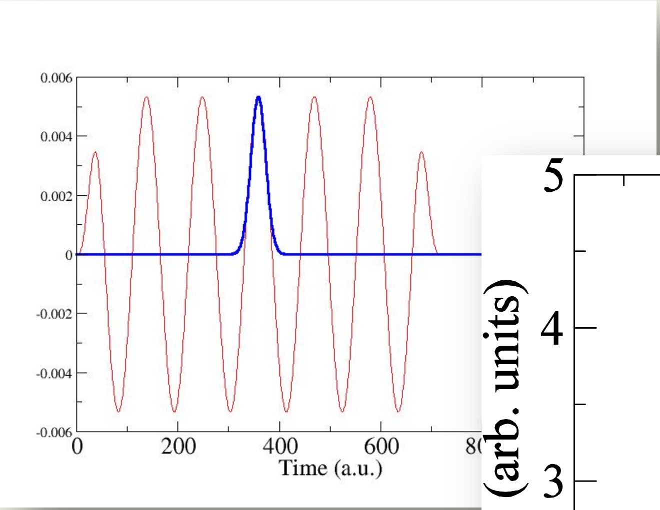


Sideband structure for Ne KLL Auger transition

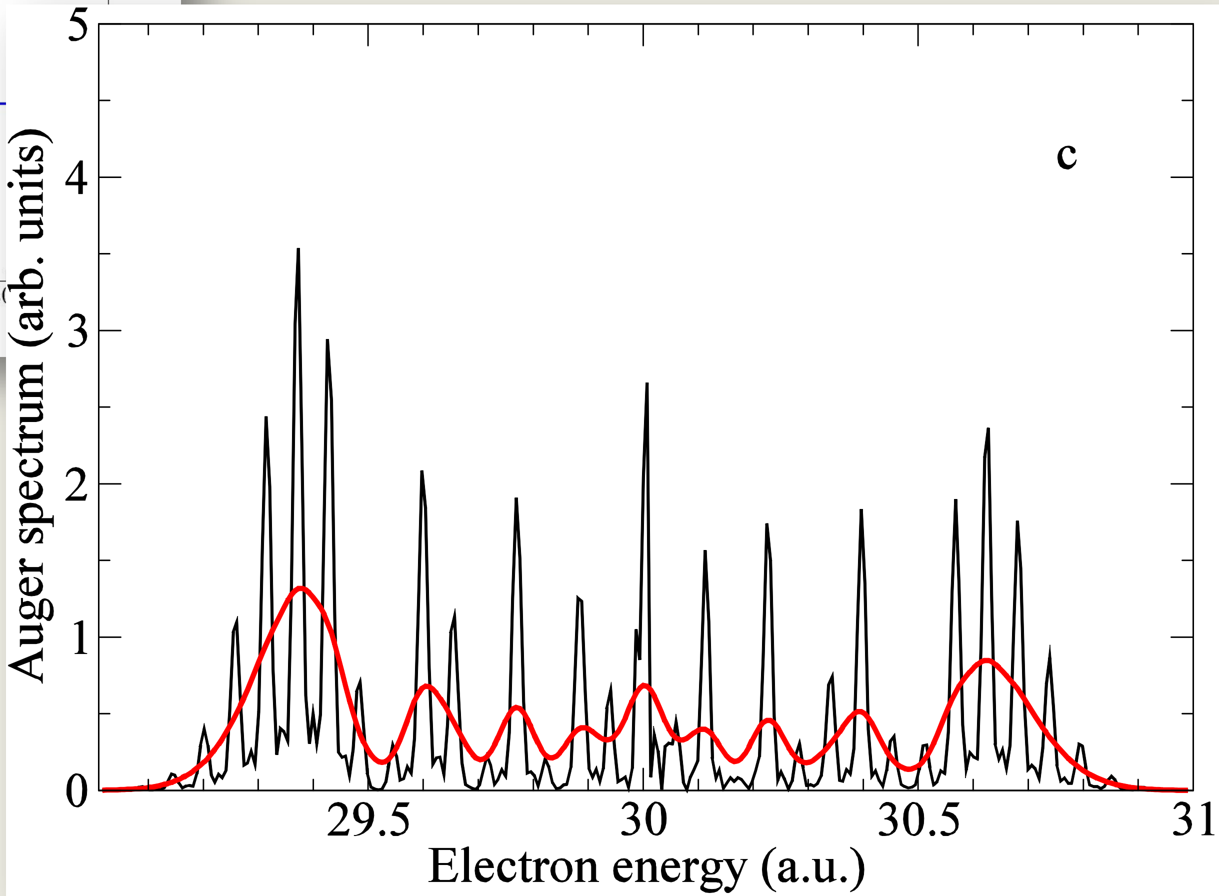
IR: $\tau_L = 9.3$ fs



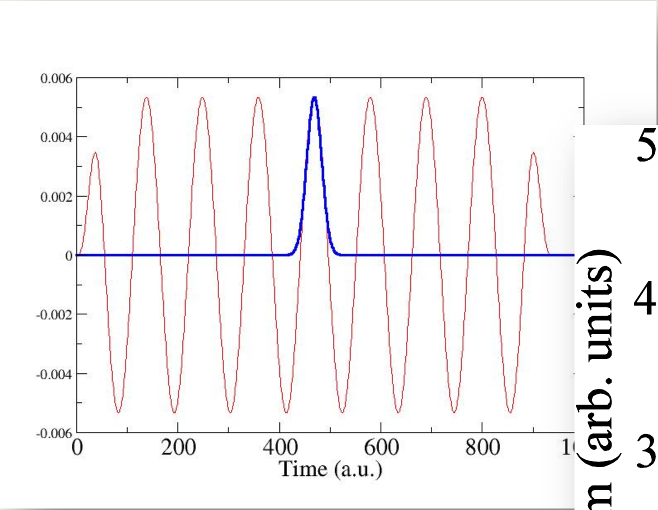
Sideband structure for Ne KLL Auger transition



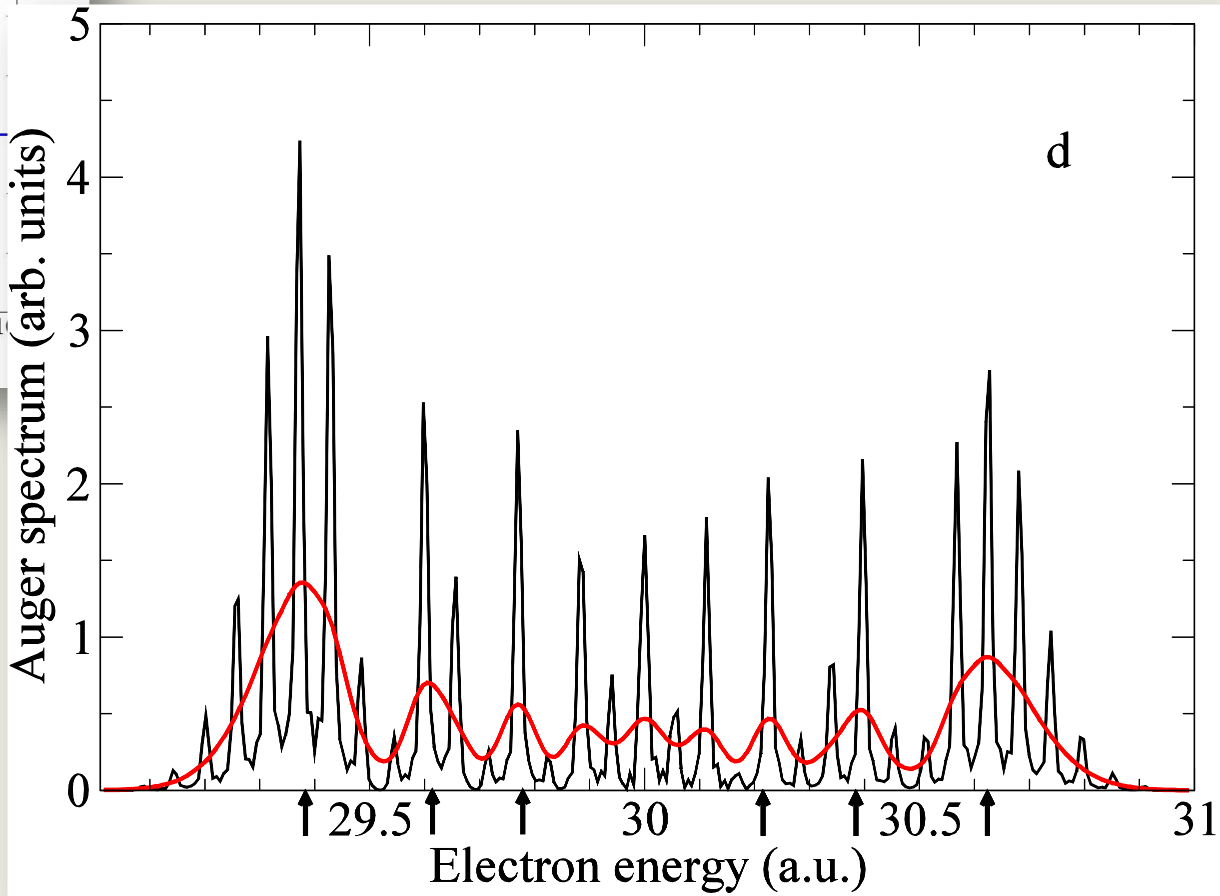
IR: τ_L = 14.7 fs



Sideband structure for Ne KLL Auger transition

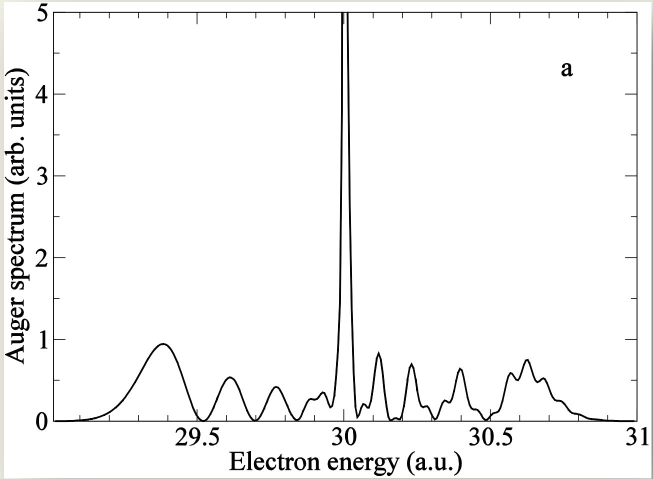


IR: τ_L = 20 fs

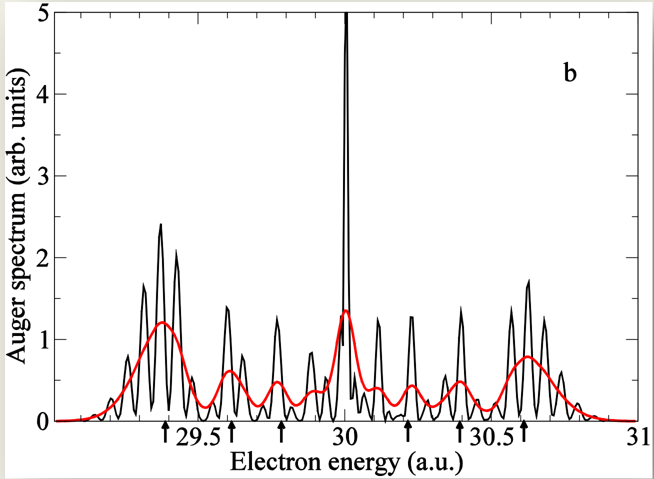


Sideband structure for Ne KLL Auger transition

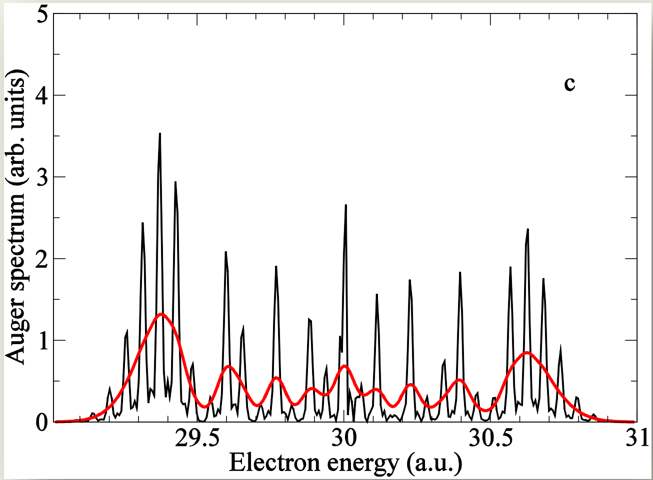
τ_L = 4.0 fs



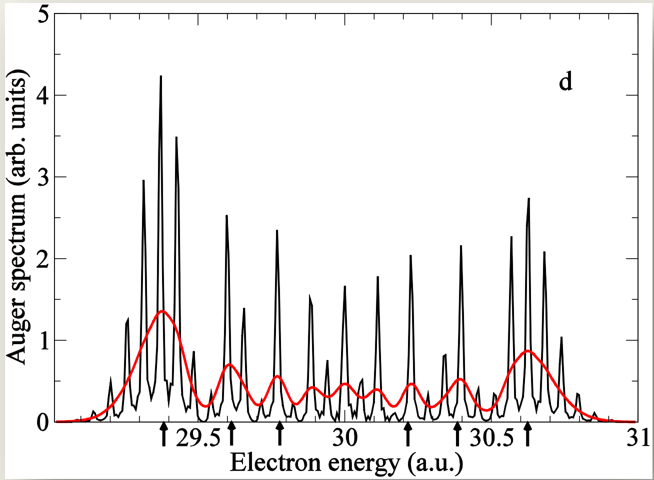
τ_L = 9.3 fs



τ_L = 14.7 fs



τ_L = 20 fs



Description of the gross structure

$$W(k) = |\mathcal{F}(k)|^2$$

$$E = k^2/2$$

$$\mathcal{F}(k) \approx \tilde{E}(k) \frac{1 - [J(k)\exp(-\Gamma T_L/2)]^N}{1 - J(k)\exp(-\Gamma T_L/2)}$$

$$\tilde{E}(k) = \int_0^{T_L} dt e^{iQ(t)}$$ where $$Q(t) = \int_0^t dt' \left(\frac{1}{2}[k - A_L(t')]^2 - E_A\right)$$

Suppose for simplicity that $A_L(t) = A_0 \sin \omega_L t + \alpha$

Stationary phase approximation $[k - A_L(t_s)]^2 = 2E_A$

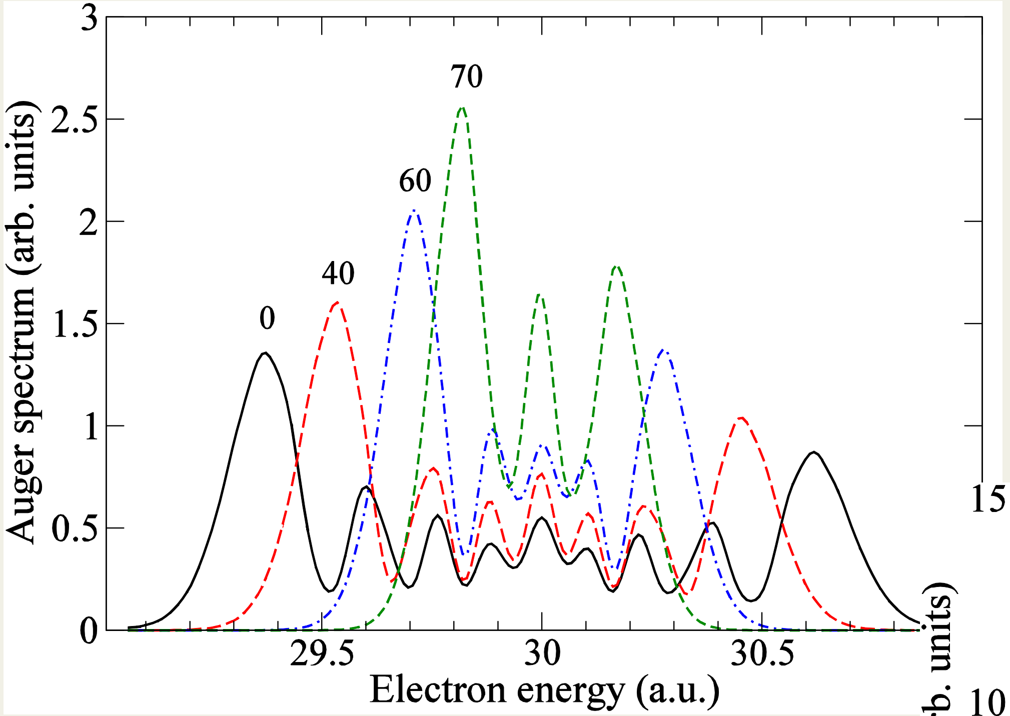
Result:

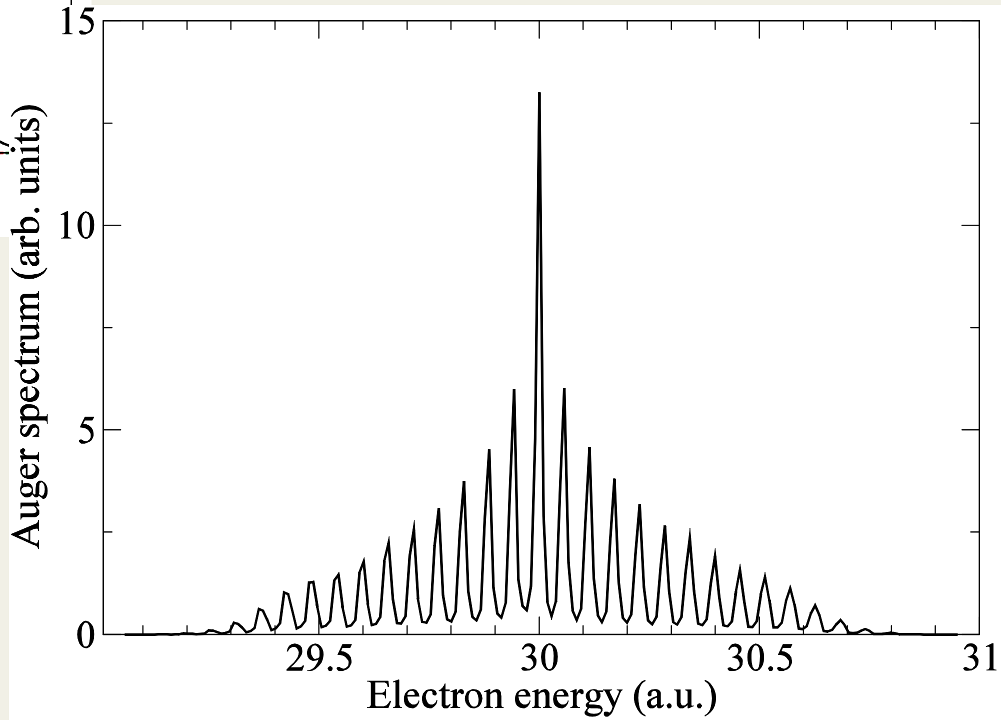
$$\tilde{E}(k) \sim Ai(S) \qquad \tilde{E}(k) \sim Ai(\bar{S})$$

$$k > \alpha + \sqrt{2E_A} \qquad k < \alpha + \sqrt{2E_A}$$

$$S = \frac{\left[(k - \alpha - A_0)^2 - k_0^2\right]}{[4A_0\omega_L^2(k - \alpha - A_0)]^{1/3}} \qquad \bar{S} = \frac{\left[(k - \alpha + A_0)^2 - k_0^2\right]}{[-4A_0\omega_L^2(k - \alpha + A_0)]^{1/3}}$$

Angular dependence of the gross structure





SUMMARY

- A quantum mechanical theory of the laser assisted Auger process in atoms excited by ultra-short XUV or X-ray pulses has been developed. It is applicable to the case of slow photo and fast Auger electrons.
- The theory describes spectra and angular distributions of photo and Auger electrons.
- Appearance of the sidebands has been investigated for short laser pulses.
- For large energy of Auger electrons the sidebands reveal the gross structure, i.e. the modulation of the intensity of the sideband lines. The gross structure is well described by the Airy function.

The END

Thank you for your attention !