Recoil and Cumulant Theory in Core-Level Photoemission

Simone Ritarossi- University of Roma Tre

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Graphite / Graphene case study

Energetic and mechanical view of recoil

Photoemission and recoil: energetic balance

We consider core-level photoemission from an atom of mass M, with a bound electron of binding energy E_B (in the initial state).

Energy conservation (non-relativistic nucleus): $h\nu + E_{\mathrm{init}} = E_{\mathrm{final}} + E_{\mathrm{kin}} + E_{\mathrm{R}}$

- $h\nu$ is the photon energy,
- E_{kin} is the kinetic energy of the photoelectron,
- E_{R} is the recoil energy of the ion (or lattice),
- Binding energy → $E_B = E_{\mathrm{final}} - E_{\mathrm{init}}$.

$$h\nu = E_B + E_{\mathrm{kin}} + E_{\mathrm{R}}.$$

Key point: E_{R} appears as a *binding energy shift* that grows with $h\nu$ through E_{kin}.

Two-body kinematics

To understand E_R mechanically, consider the simplest two-body problem:

- initial state: atom at rest, electron bound;
- final state: electron with momentum $\boldsymbol{p}_e$, ion with momentum $\boldsymbol{P}_R$.

Momentum conservation (XPS regime, $|\boldsymbol{p}_\gamma| \ll |\boldsymbol{p}_e|$):

$$\boldsymbol{p}_\gamma \simeq 0 \quad \Rightarrow \quad \boldsymbol{p}_e + \boldsymbol{P}_R \simeq 0 \quad \Rightarrow \quad \boldsymbol{P}_R = -\boldsymbol{p}_e. \tag{1}$$

Kinetic energies: $E_\mathrm{kin} = \frac{\boldsymbol{p}_e^2}{2m}, \quad E_\mathrm{R} = \frac{\boldsymbol{P}_R^2}{2M} = \frac{\boldsymbol{p}_e^2}{2M}$

$$\boldsymbol{p}_e^2 = 2m\,E_\mathrm{kin} \quad \Rightarrow \quad E_\mathrm{R} = \frac{1}{2M}(2m\,E_\mathrm{kin}) = \frac{m}{M}\,E_\mathrm{kin} \in (0, 0.35)eV \tag{2}$$

From atomic recoil to lattice recoil:

- the recoiling site is *bound* in a lattice;
- total momentum is shared among collective vibrational modes (phonons).

Takata's phonon recoil model and anisotropy: graphite case

Core-level photoemission with recoil: physical picture

- We consider x-ray photoemission from a core electron of a carbon atom in a crystal.
- The atom is located at lattice site

  $$\mathbf{R} = \mathbf{R}_0 + \mathbf{u},$$

  with $\mathbf{R}_0$ the equilibrium position and $\mathbf{u}$ the vibrational displacement (thermal + zero-point).
- Emission of an electron with momentum $\hbar\mathbf{k}$ implies a recoil of the lattice: the crystal absorbs the momentum through its phonon modes (This is fully analogous to the Mössbauer effect)
- Core wave function in the *adiabatic approximation*:

  $$\psi_c(\mathbf{r}) = \varphi_c(\mathbf{r} - \mathbf{R}).$$

Interaction with the x-ray field

- Interaction hamiltonian:

$$H_I = (\ a + a^\dagger\ )\, \boldsymbol{\epsilon} \cdot \mathbf{p},$$

  where:

  - $a, a^\dagger$: photon annihilation/creation operators,
  - $\boldsymbol{\epsilon}$: x-ray polarization vector,
  - $\mathbf{p}$: electron momentum operator.

- Photon momentum is neglected:

$$|\mathbf{k}_\gamma| \ll |\mathbf{k}_e|$$

  in the x-ray energy range of interest, so only the electron momentum matters for recoil.

- The nuclear mass is large, so recoil is transferred to the lattice degrees of freedom (phonons).

Initial and final states of the transition

- Initial state:

$$|i\rangle = |h\nu\rangle \otimes |c\rangle \otimes |i_{\mathrm{ph}}\rangle,$$

  with:
  - $|h\nu\rangle$: one-photon state,
  - $|c\rangle$: core-electron state (energy ϵ_c),
  - $|i_{\mathrm{ph}}\rangle$: initial phonon state.
- Final state:

$$|f\rangle = |0\rangle \otimes |\mathbf{k}\rangle \otimes |f_{\mathrm{ph}}\rangle,$$

  with:
  - $|0\rangle$: photon vacuum,
  - $|\mathbf{k}\rangle$: plane wave of the emitted electron,

$$\langle \mathbf{r}|\mathbf{k}\rangle = (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}},$$

  - $|f_{\mathrm{ph}}\rangle$: final phonon state.

Matrix element and recoil operator

- Electronic part of the matrix element:

$$\langle \mathbf{k}|\mathbf{p}|c\rangle = \int d^3r\, \psi_{\mathbf{k}}^*(\mathbf{r})\,(-i\hbar\nabla)\,\psi_c(\mathbf{r}).$$

$$\psi_{\mathbf{k}}^*(\mathbf{r}) = (2\pi)^{-3/2} e^{-i\mathbf{k}\cdot\mathbf{r}}, \quad \psi_c(\mathbf{r}) = \varphi_c(\mathbf{r}-\mathbf{R}).$$

- Def.:

$$\mathbf{s} = \mathbf{r} - \mathbf{R} \quad \Rightarrow \quad \langle \mathbf{k}|\mathbf{p}|c\rangle = e^{-i\mathbf{k}\cdot\mathbf{R}}\,\boldsymbol{\mu},$$

with

$$\boldsymbol{\mu} = (2\pi)^{-3/2} \int d^3s\, e^{-i\mathbf{k}\cdot\mathbf{s}}(-i\hbar\nabla_s)\,\varphi_c(\mathbf{s}).$$

- Full matrix element:

$$\langle f|H_I|i\rangle = \boldsymbol{\epsilon}\cdot\boldsymbol{\mu}\,\langle f_{\mathrm{ph}}|e^{-i\mathbf{k}\cdot\mathbf{R}}|i_{\mathrm{ph}}\rangle.$$

Spectrum

- The spectrum can be written as

$$I(E) = \frac{|\boldsymbol{\epsilon} \cdot \boldsymbol{\mu}|^2}{2\pi} \int_{-\infty}^{+\infty} dt\, e^{-iEt/\hbar}\, e^{-\Gamma|t|/\hbar}\, F(t),$$

where Γ is the core-hole lifetime broadening.

- The generating function (phonon factor) is

$$F(t) = \left\langle e^{i\mathbf{k}\cdot\mathbf{u}(t)} e^{-i\mathbf{k}\cdot\mathbf{u}(0)} \right\rangle,$$

with the average taken over the canonical ensemble of the harmonic crystal.

- Physically, $F(t)$ measures how the lattice responds in time to the momentum kick $\hbar\mathbf{k}$.

Displacement of the emitting atom

We consider the displacement field of the emitting atom in a harmonic crystal, expanded in phonon normal modes:

$$\boldsymbol{u}(t) = \sum_{\boldsymbol{q},\lambda} \sqrt{\frac{\hbar}{2M_{\mathrm{at}}\omega_{\boldsymbol{q}\lambda}}}\, \boldsymbol{e}_{\boldsymbol{q}\lambda} \left(\hat{b}_{\boldsymbol{q}\lambda} e^{-i\omega_{\boldsymbol{q}\lambda} t} + \hat{b}^{\dagger}_{\boldsymbol{q}\lambda} e^{+i\omega_{\boldsymbol{q}\lambda} t} \right), \tag{3}$$

where:

- $\boldsymbol{q}$: wavevector in the first Brillouin zone,
- λ: phonon branch (polarization),
- M_{at}: mass of the emitting atom,
- $\boldsymbol{e}_{\boldsymbol{q}\lambda}$: normalized polarization vector,
- $\hat{b}_{\boldsymbol{q}\lambda}$, $\hat{b}^{\dagger}_{\boldsymbol{q}\lambda}$: phonon annihilation/creation operators.

Projected displacement and recoil factor

The recoil is governed by the displacement projected along the photoelectron momentum direction $\boldsymbol{k} \to \xi(t) \equiv \boldsymbol{k} \cdot \boldsymbol{u}(t)$. The **recoil factor** is defined as

$$F(t) = \left\langle e^{i\xi(t)} e^{-i\xi(0)} \right\rangle_{\mathrm{ph}}. \tag{4}$$

Introduce $A \equiv i\xi(t) - i\xi(0)$, so that $F(t) = \langle e^{A} \rangle$.

It's easy to show (*cumulant approach*) that $\ln F(t) = G_{\mathrm{ph}}(t)$ with $G_{\mathrm{ph}}(t)$ of the familiar Takata/Fujikawa form, expressed in terms of phonon frequencies and Bose factors:

$$G_{\mathrm{ph}}(t) = \ln F(t) = \sum_{\boldsymbol{q},\lambda} \lambda_{\boldsymbol{q}\lambda}^{2} \left[(2n_{\boldsymbol{q}\lambda} + 1)(\cos \omega_{\boldsymbol{q}\lambda} t - 1) - i \sin \omega_{\boldsymbol{q}\lambda} t \right]. \tag{5}$$

$$\to G_{\mathrm{ph}}(t) = \int_0^\infty d\omega \, \frac{\beta_{\mathrm{ph}}(\omega)}{\omega^2} \left[(2n_B(\omega) + 1)(\cos \omega t - 1) - i \sin \omega t \right], \tag{6}$$

where $n_B(\omega)$ is the Bose factor at frequency ω. In Takata's case, β_{ph} is chosen to encode both the recoil scale and the anisotropic graphite DOS.

Anisotropy in graphite: directional DOS

For graphite/graphene, phonons are strongly anisotropic. Takata (graphite) separates *in-plane* stretching (s) and *out-of-plane* bending (b) acoustic branches, and defines an effective directional DOS:

$$D_{\hat{\boldsymbol{k}}}(\omega;\vartheta) = \cos^2\vartheta\, D_s(\omega) + \sin^2\vartheta\, D_b(\omega), \tag{7}$$

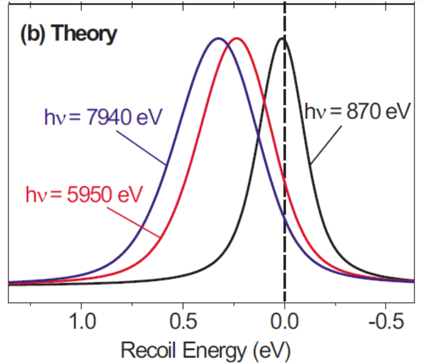
where:

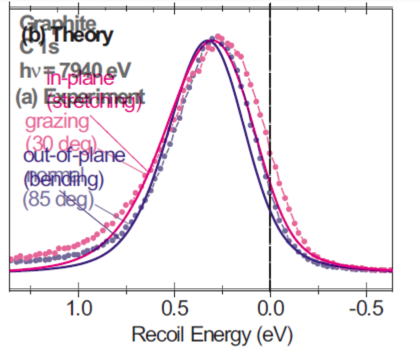
- ϑ is the angle between $\hat{\boldsymbol{k}}$ and the basal plane,
- $D_s(\omega)$ is the in-plane (stretching) DOS,
- $D_b(\omega)$ is the out-of-plane (bending) DOS.

Photoelectron spectrum

$$I_{\mathrm{ph}}(E; h\nu, \vartheta) \propto \mathrm{Re} \int_0^{\infty} dt\, e^{iEt}\, e^{G_{\mathrm{ph}}(t; h\nu, \vartheta)}\, e^{-\Gamma t}.$$

The position of the main phonon peak shifts approximately by $E_{\mathrm{ph}}(h\nu) \simeq \delta E(h\nu)$.





Beyond phonons: explicit electronic contributions

We want to add $\beta_{\mathrm{el}}(\omega)$:

$$\beta(\omega) = \beta_{\mathrm{ph}}(\omega; h\nu, \vartheta) + \beta_{\mathrm{el}}(\omega) + \cdots \, . \tag{8}$$

The total cumulant is then

$$C(t; h\nu, \vartheta) = C_{\mathrm{ph}}(t; h\nu, \vartheta) + C_{\mathrm{el}}(t) + \cdots \, , \tag{9}$$

with each contribution computed from its own spectral density.

Takata's model corresponds to keeping only C_{ph};. In general, we can specify $\beta_{\mathrm{el}}(\omega)$ to generate Doniach–Šunjić-like tails and discuss the unified phonon+electronic recoil lineshape.

$$I_{\mathrm{ph}}(E; h\nu, \vartheta) \propto \mathrm{Re} \int_0^{\infty} dt \, e^{iEt} \, e^{G_{\mathrm{ph}}(t; h\nu, \vartheta)} \, e^{C_{\mathrm{el}}}(t) \, e^{-\Gamma t}.$$

From cumulant factorization to convolution

The photoemission spectrum can be written as

$$I(E; h\nu, \vartheta) \propto \mathrm{Re} \int_0^\infty dt\, e^{iEt}\, e^{C_{\mathrm{ph}}(t; h\nu, \vartheta)}\, e^{C_{\mathrm{el}}(t)}\, e^{-\Gamma t}. \tag{10}$$

Define the well-known functions:

$$F_{\mathrm{ph}}(t; h\nu, \vartheta) = e^{C_{\mathrm{ph}}(t; h\nu, \vartheta)}, \qquad F_{\mathrm{el}}(t) = e^{C_{\mathrm{el}}(t)}.$$

Let I_{ph} and I_{el} be their Fourier transforms. Then, by the convolution theorem,

$$I(E; h\nu, \vartheta) = \left[\, I_{\mathrm{ph}}(\cdot; h\nu, \vartheta) * I_{\mathrm{el}}(\cdot) * L_\Gamma(\cdot) \right](E), \tag{11}$$

i.e. the **cumulant factorization is exactly equivalent** to a **convolution** of a phonon spectrum and an electronic spectrum.

Clean graphene: convolutive recoil model

Clean graphene

We now specialise to **clean graphene**:

- single C 1s chemical environment (no C–O, no H, no defects),
- recoil described by an **anisotropic phonon cumulant** of Takata-type,
- electronic many-body effects encoded in an **effective mixing kernel** K_{mix} fitted once at a reference photon energy and then reused,
- instrumental resolution described by a Gaussian G_{inst}.

Convolution chain for clean graphene

Convolution chain:

$$I_{\mathrm{model}}(E;\theta) = \big(I_{\mathrm{ph}}[\theta] \otimes K_{\mathrm{mix}} \otimes G_{\mathrm{inst}}\big)(E), \tag{12}$$

$$K_{\mathrm{mix}}(E) = \sum_{j=1}^{K_{\mathrm{tot}}} w_j\, K_j\big(E;\mathrm{parameters}_j\big), \qquad \sum_{j=1}^{K_{\mathrm{tot}}} w_j = 1, \quad w_j \geq 0. \tag{13}$$

Electronic components:

$$K_j \in \begin{cases} \mathrm{DS}\big(E;\, s_j, \Gamma_j, \alpha_j\big) & \text{(edge-like electronic channels)}, \\ \mathcal{N}\big(E;\, s_j, \mathrm{FWHM}_j\big) & \text{(plasmon-like Gaussian satellites)}, \end{cases} \qquad G_{\mathrm{inst}}(E) = \mathcal{N}\big(E;\, \mathrm{FWHM}_{\mathrm{inst}}\big).$$

- Better choice: five K_j components (from exp.)
- All electronic parameters at the *reference* photon energy (e.g. $h\nu_{\mathrm{ref}} = 0.8\ \mathrm{keV}$), so $\{w_j, s_j, \Gamma_j, \alpha_j, \mathrm{FWHM}_j\}_{j=1}^{K_{\mathrm{tot}}}$ are then *reused* to predict higher photon energies.

Graphene phonon DOS used in the model

For clean graphene we adopt an **anisotropic acoustic DOS** of Takata/graphite type, specialised to 2D graphene:

Acoustic stretching (in-plane, LA+TA):

$$D_s^{(}\omega) = \frac{2}{\left(\omega_D^{(s)}\right)^2}\,\omega\,1_{(0,\omega_D^{(s)}]}(\omega),$$

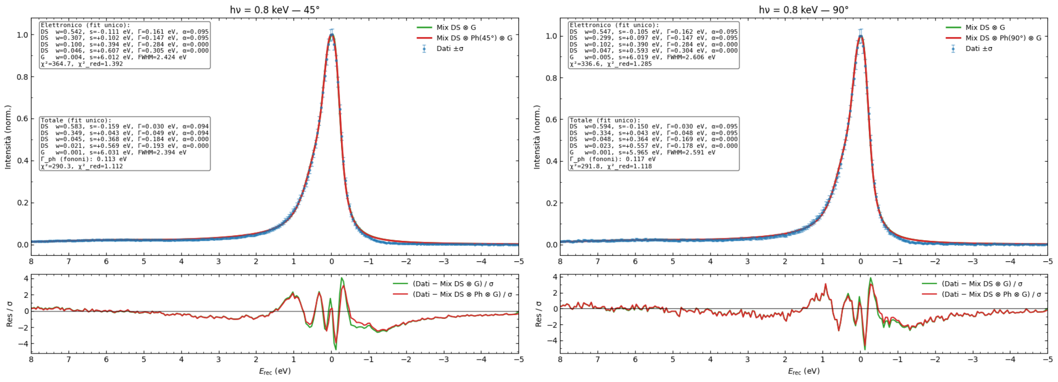
a 2D Debye-like DOS (linear in ω) up to a cutoff $\omega_D^{(s)}$.

Acoustic bending (out-of-plane, ZA):

$$D_b(\omega) = \frac{1}{\omega_D^{(b)}}\,1_{(0,\,\omega_D^{(b)}]}(\omega),$$

Clean graphene: fits, components and recoil

$h\nu = 0.8$ **keV**



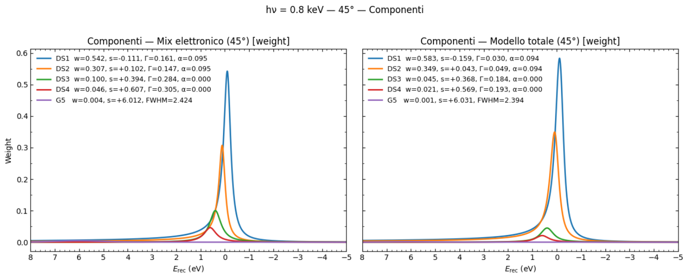
```
Elettronico (fit unico):
DS  w=0.542, s=-0.111 eV, Γ=0.161 eV, α=0.095
DS  w=0.307, s=+0.102 eV, Γ=0.147 eV, α=0.095
DS  w=0.100, s=+0.394 eV, Γ=0.284 eV, α=0.000
DS  w=0.046, s=+0.607 eV, Γ=0.305 eV, α=0.000
G   w=0.004, s=+6.012 eV, FWHM=2.424 eV
χ²=364.7, χ²_red=1.392
```

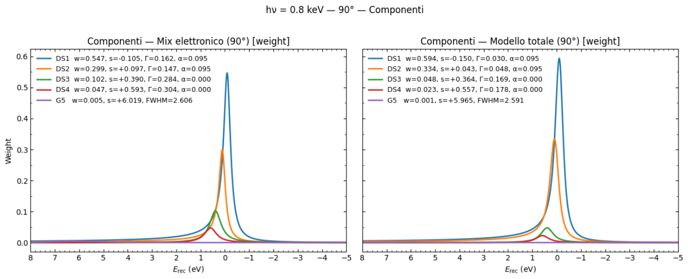
```
Totale (fit unico):
DS  w=0.583, s=-0.159 eV, Γ=0.030 eV, α=0.094
DS  w=0.349, s=+0.043 eV, Γ=0.049 eV, α=0.094
DS  w=0.045, s=+0.368 eV, Γ=0.184 eV, α=0.000
DS  w=0.021, s=+0.569 eV, Γ=0.193 eV, α=0.000
G   w=0.001, s=+6.031 eV, FWHM=2.394 eV
Γ_ph (fononi): 0.113 eV
χ²=290.3, χ²_red=1.112
```

```
Elettronico (fit unico):
DS  w=0.547, s=-0.105 eV, Γ=0.162 eV, α=0.095
DS  w=0.299, s=+0.097 eV, Γ=0.147 eV, α=0.095
DS  w=0.102, s=+0.390 eV, Γ=0.284 eV, α=0.000
DS  w=0.047, s=+0.593 eV, Γ=0.304 eV, α=0.000
G   w=0.005, s=+6.019 eV, FWHM=2.606 eV
χ²=336.6, χ²_red=1.285
```

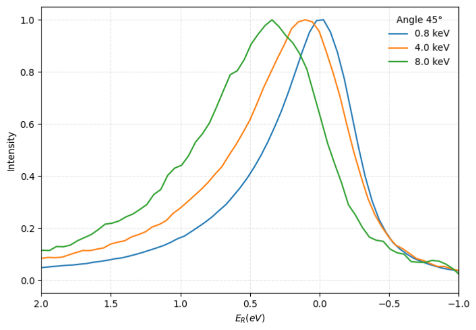
```
Totale (fit unico):
DS  w=0.594, s=-0.150 eV, Γ=0.030 eV, α=0.095
DS  w=0.334, s=+0.043 eV, Γ=0.048 eV, α=0.095
DS  w=0.048, s=+0.364 eV, Γ=0.169 eV, α=0.000
DS  w=0.023, s=+0.557 eV, Γ=0.178 eV, α=0.000
G   w=0.001, s=+5.965 eV, FWHM=2.591 eV
Γ_ph (fononi): 0.117 eV
χ²=291.8, χ²_red=1.118
```

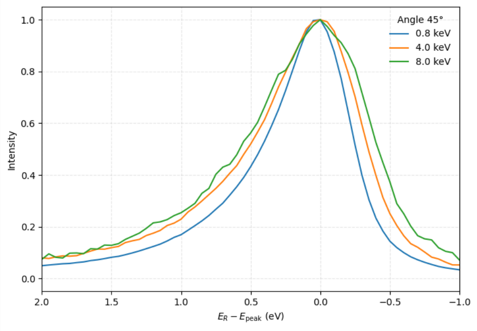
K_{mix}


hν = 0.8 keV — 45° — Componenti
Componenti — Mix elettronico (45°) [weight]
DS1 w=0.542, s=-0.111, Γ=0.161, α=0.095
DS2 w=0.307, s=+0.102, Γ=0.147, α=0.095
DS3 w=0.100, s=+0.394, Γ=0.284, α=0.000
DS4 w=0.046, s=+0.607, Γ=0.305, α=0.000
G5 w=0.004, s=+6.012, FWHM=2.424
Weight
0.6
0.5
0.4
0.3
0.2
0.1
0.0
8 7 6 5 4 3 2 1 0 −1 −2 −3 −4 −5
E_{rec} (eV)
Componenti — Modello totale (45°) [weight]
DS1 w=0.583, s=-0.159, Γ=0.030, α=0.094
DS2 w=0.349, s=+0.043, Γ=0.049, α=0.094
DS3 w=0.045, s=+0.368, Γ=0.184, α=0.000
DS4 w=0.021, s=+0.569, Γ=0.193, α=0.000
G5 w=0.001, s=+6.031, FWHM=2.394
8 7 6 5 4 3 2 1 0 −1 −2 −3 −4 −5
E_{rec} (eV)

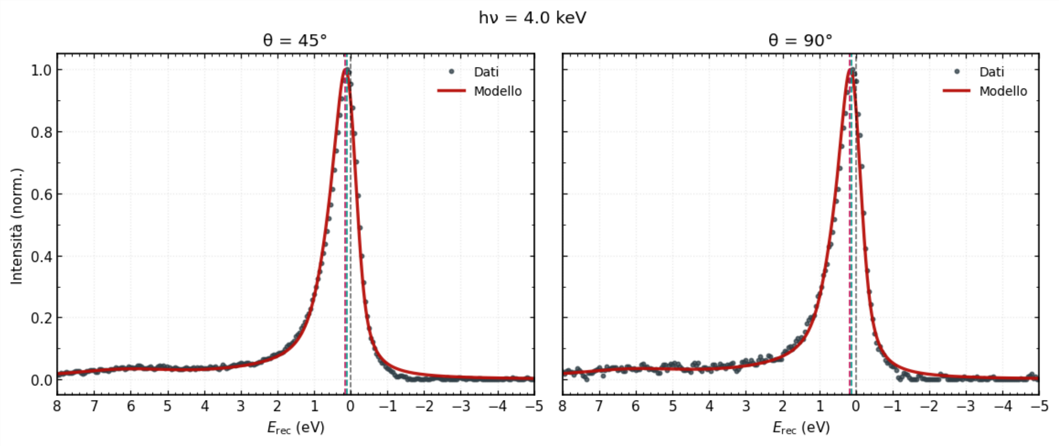

hν = 0.8 keV — 90° — Componenti
Componenti — Mix elettronico (90°) [weight]
DS1 w=0.547, s=-0.105, Γ=0.162, α=0.095
DS2 w=0.299, s=+0.097, Γ=0.147, α=0.095
DS3 w=0.102, s=+0.390, Γ=0.284, α=0.000
DS4 w=0.047, s=+0.593, Γ=0.304, α=0.000
G5 w=0.005, s=+6.019, FWHM=2.606
Weight
0.6
0.5
0.4
0.3
0.2
0.1
0.0
8 7 6 5 4 3 2 1 0 −1 −2 −3 −4 −5
E_{rec} (eV)
Componenti — Modello totale (90°) [weight]
DS1 w=0.594, s=-0.150, Γ=0.030, α=0.095
DS2 w=0.334, s=+0.043, Γ=0.048, α=0.095
DS3 w=0.048, s=+0.364, Γ=0.169, α=0.000
DS4 w=0.023, s=+0.557, Γ=0.178, α=0.000
G5 w=0.001, s=+5.965, FWHM=2.591
8 7 6 5 4 3 2 1 0 −1 −2 −3 −4 −5
E_{rec} (eV)

Data: recoil shift and broadening

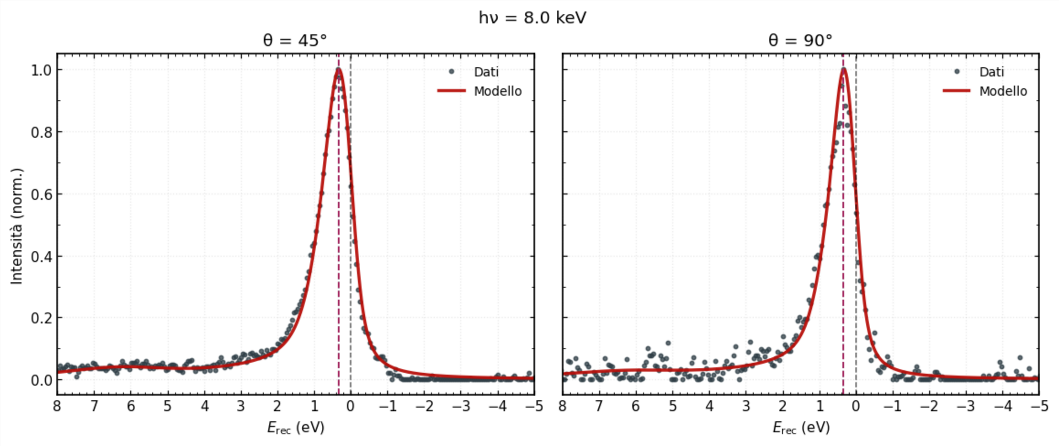




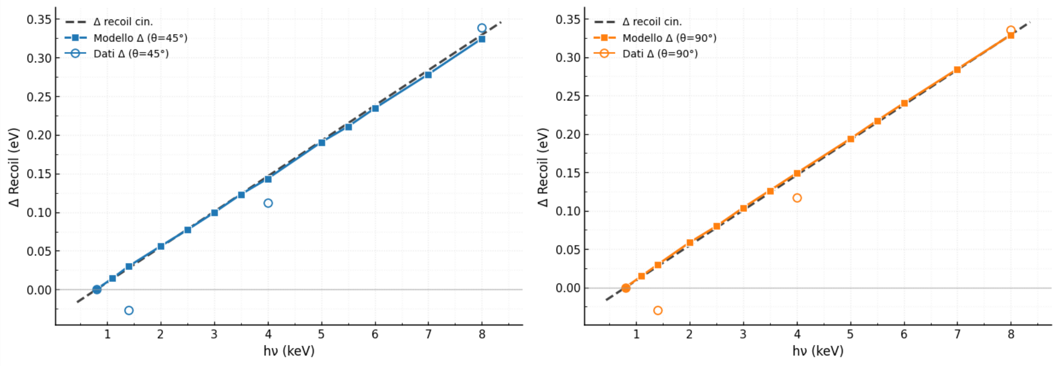
$h\nu = 4.0$ **keV**


hν = 4.0 keV
θ = 45°
θ = 90°
Dati
Modello
Intensità (norm.)
1.0
0.8
0.6
0.4
0.2
0.0
8
7
6
5
4
3
2
1
0
−1
−2
−3
−4
−5
E_{rec} (eV)

$h\nu = 8.0$ **keV**


hν = 8.0 keV
θ = 45°
θ = 90°
Dati
Modello
Intensità (norm.)
1.0
0.8
0.6
0.4
0.2
0.0
8
7
6
5
4
3
2
1
0
−1
−2
−3
−4
−5
$E_{\rm rec}$ (eV)

ΔE_{rec} vs $h\nu$



Conclusions

Recoil physics

- Recoil in core-level photoemission is the energy/momentum transfer from the photoelectron to the lattice: $E_{\mathrm{R}} \simeq \frac{m_e}{M_{\mathrm{C}}} E_{\mathrm{kin}}(h\nu)$.
- In a crystal the recoil is almost entirely stored in phonons (internal DOF).

Takata & cumulant framework

- Takata's model is a phonon-only independent-boson cumulant with anisotropic DOS: $D_{\hat{\boldsymbol{k}}}(\omega, \vartheta) = \cos^2\vartheta\, D_{\boldsymbol{s}}(\omega) + \sin^2\vartheta\, D_{\boldsymbol{b}}(\omega)$.
- The phonon spectral density $\beta_{\mathrm{ph}}(\omega; h\nu, \vartheta)$ is fixed so that $\int d\omega\, \beta_{\mathrm{ph}}(\omega)/\omega = \delta E(h\nu)$ (kinematic recoil).
- Adding an electronic spectral density $\beta_{\mathrm{el}}(\omega)$ yields a total cumulant $C = C_{\mathrm{ph}} + C_{\mathrm{el}}$ with DS-like tails.

Conclusions

Clean graphene model

- Working model: $I_{\mathrm{model}} = I_{\mathrm{ph}} \otimes K_{\mathrm{mix}} \otimes G_{\mathrm{inst}}$, with $K_{\mathrm{mix}} = \sum_j w_j K_j$ (DS + plasmon).
- Electronic parameters $\{w_j, s_j, \Gamma_j, \alpha_j\}$ are fitted once at $h\nu = 0.8$ keV and reused at higher $h\nu$; only I_{ph} and G_{inst} change.
- The model reproduces both the lineshapes and the $\Delta E_{\mathrm{rec}}(h\nu, \theta)$ trend, closely following the kinematic recoil line.

Next: hydrogenated graphene

Choosing the spectral density $\beta(\omega)$

β_{el}: exponential model

A simple and physically motivated choice for the electronic spectral density is

$$\beta_{\mathrm{el}}(\omega) = \alpha_{\mathrm{el}}\,\omega\,e^{-\omega/\omega_c}, \qquad \omega > 0, \tag{14}$$

Low- and high-frequency limits:

$$\beta_{\mathrm{el}}(\omega) \propto \omega \quad (\omega \ll \omega_c), \qquad \beta_{\mathrm{el}}(\omega) \to 0 \quad (\omega \gg \omega_c).$$

The electronic contribution to the average energy shift is

$$\Delta E_{\mathrm{el}} = \int_0^\infty d\omega\,\frac{\beta_{\mathrm{el}}(\omega)}{\omega}. \tag{15}$$

For the exponential model, $\beta_{\mathrm{el}}(\omega) = \alpha_{\mathrm{el}}\omega e^{-\omega/\omega_c}$, one finds

$$\Delta E_{\mathrm{el}} = \alpha_{\mathrm{el}}\omega_c.$$

Electronic cumulant $C_{\mathrm{el}}(t)$: closed form

We start from the exponential model

$$C_{\mathrm{el}}(t) = \alpha_{\mathrm{el}} \int_0^{\infty} d\omega\, e^{-\omega/\omega_c}\, \frac{(\cos\omega t - 1) - i\sin\omega t}{\omega},$$

We can obtain directly the closed form

$$C_{\mathrm{el}}(t) = -\frac{\alpha_{\mathrm{el}}}{2} \ln\left(1 + \omega_c^2 t^2\right) \; - \; i\,\alpha_{\mathrm{el}} \arctan(\omega_c t),$$

up to a t-independent constant (irrelevant for the normalized spectrum).

Summary:

- $\mathrm{Re}\, C_{\mathrm{el}}(t) = -\frac{\alpha_{\mathrm{el}}}{2} \ln\left(1 + \omega_c^2 t^2\right)$ controls the decay of the amplitude;
- $\mathrm{Im}\, C_{\mathrm{el}}(t) = -\alpha_{\mathrm{el}} \arctan(\omega_c t)$ encodes an additional phase/energy shift.

Short-time and long-time regimes of $C_{\rm el}(t)$

Short times $t \ll \omega_c^{-1}$: $\quad \ln\big(1+\omega_c^2 t^2\big) \simeq \omega_c^2 t^2, \qquad \arctan(\omega_c t) \simeq \omega_c t,$

$$C_{\rm el}(t) \approx -\frac{\alpha_{\rm el}}{2}\,\omega_c^2 t^2 \;-\; i\,\alpha_{\rm el}\omega_c t.$$

- Re $C_{\rm el}(t)$ is quadratic in t (Gaussian-like initial decay),
- Im $C_{\rm el}(t)$ is linear in t (energy shift contribution).

Long times $t \gg \omega_c^{-1}$: $\quad \ln\big(1+\omega_c^2 t^2\big) \simeq 2\ln(\omega_c t), \qquad \arctan(\omega_c t) \to \frac{\pi}{2}\,\mathrm{sgn}(t),$

$$C_{\rm el}(t) \approx -\alpha_{\rm el}\ln(\omega_c t) \;-\; i\,\alpha_{\rm el}\frac{\pi}{2}.$$

- Re $C_{\rm el}(t) \sim -\alpha_{\rm el}\ln t$: power-law tail in energy (DS-like behaviour),
- Im $C_{\rm el}(t)$ tends to a constant phase $\sim -\alpha_{\rm el}\pi/2$.

Original model vs new model (graphite)

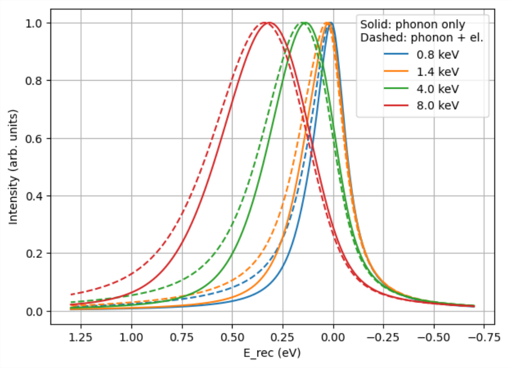


Figure 1: Stretching (30°)

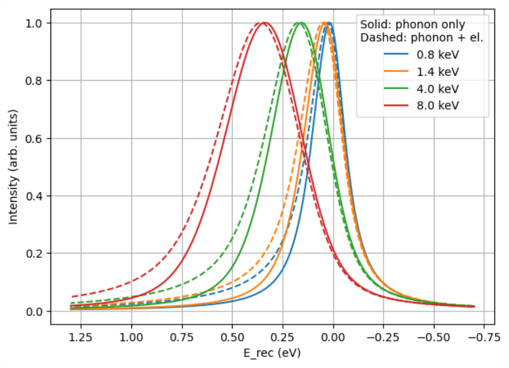


Figure 2: Bending (85°)