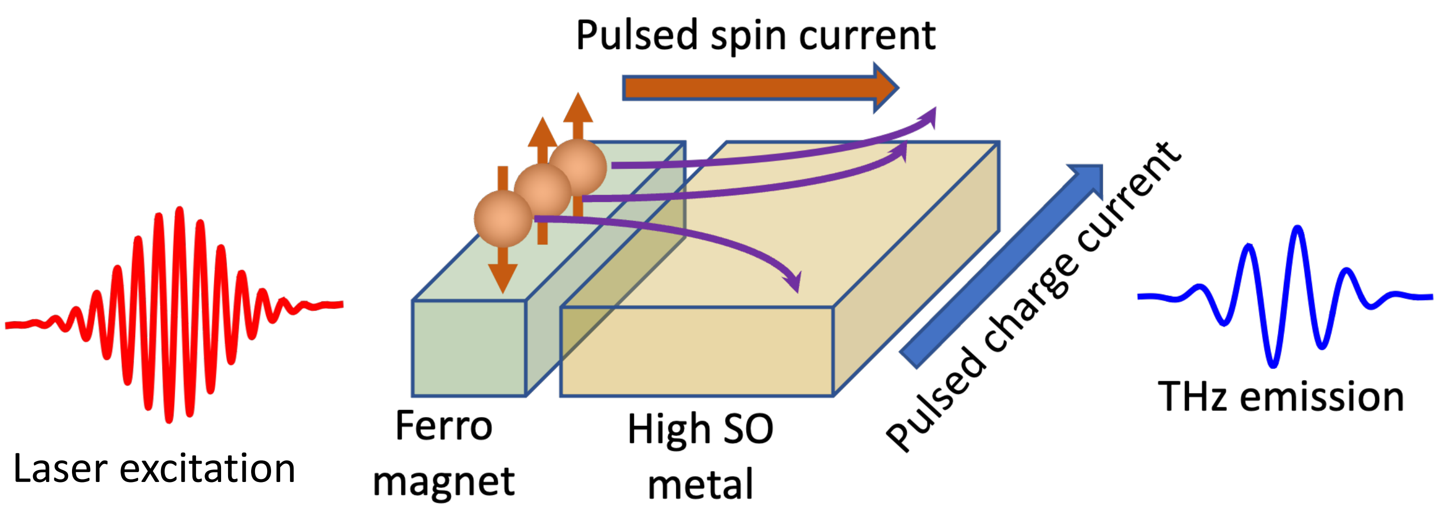
NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

Fundamentals of spin transport for THz spintronic

Marco BATTIATO

Nanyang Technological University
Singapore

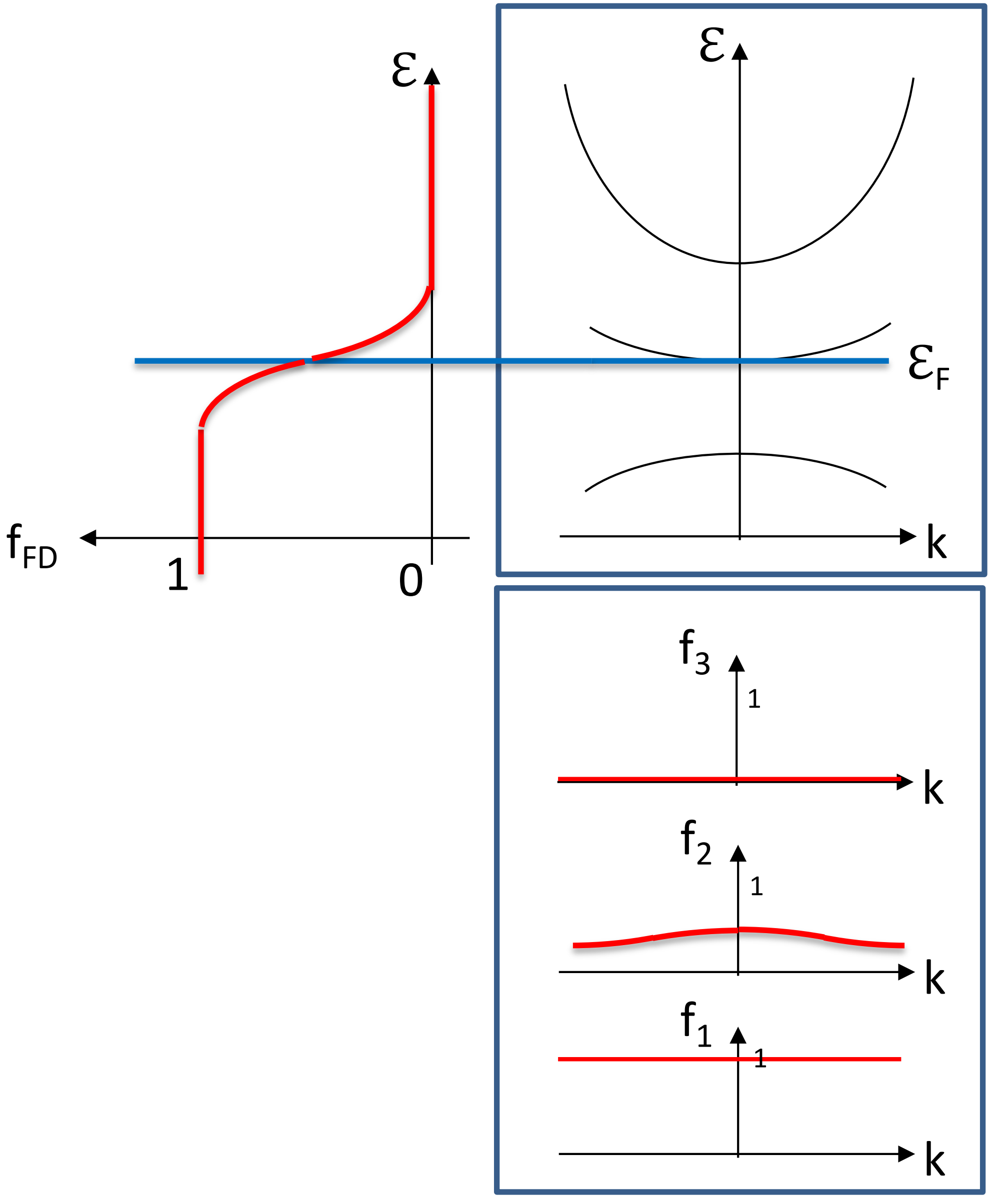
Spintronics THz emitters: step by step



- ❑ Laser excitation
- ❑ Transport during thermalization
  - ○ Thermalization of excited carriers
  - ○ Transport out of equilibrium
- ❑ Spin to charge conversion
- ❑ Production and extraction of THz radiation

Kampfrath, Battiato et al. **Nature Nanotech.** 8, 256 (2013)

Population in excited material



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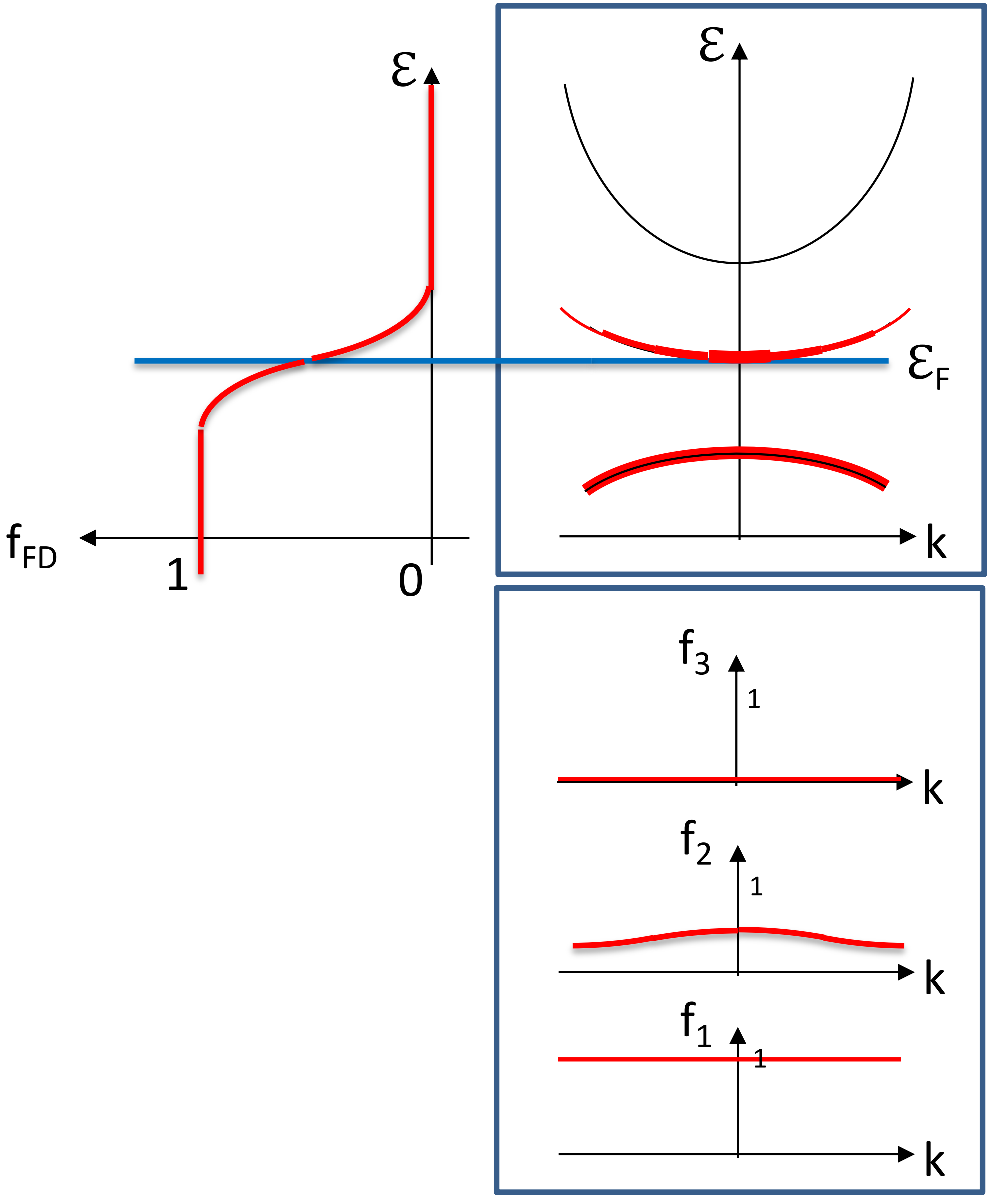
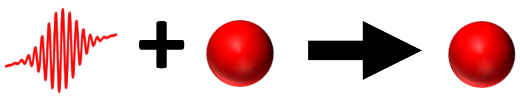
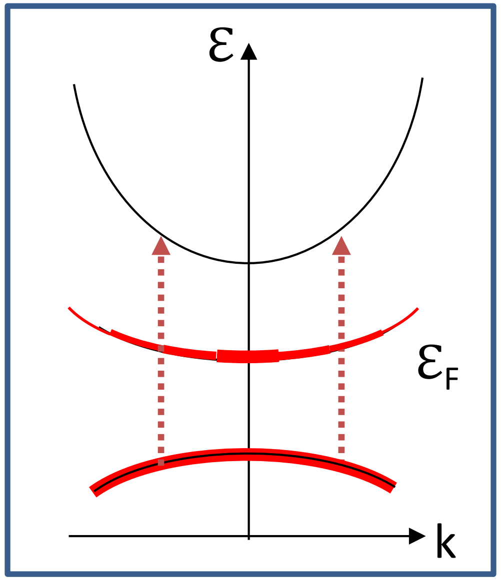


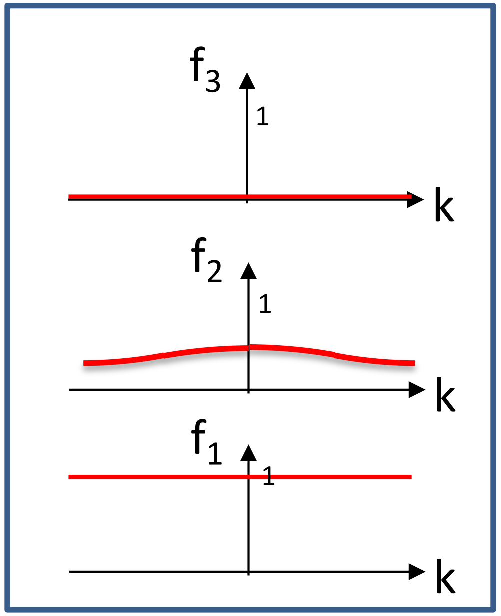
… We can do the same with phonon bands

Basics of laser excitation

Under perfectly monochromatic light







- Momentum conservation

$$k_1 + k_{h\upsilon} = k_2$$

$$k_{h\upsilon} \approx 0$$

$$k_1 \approx k_2$$ Vertical transition

- Energy conservation

$$\mathcal{E}(k_1) + h\upsilon = \mathcal{E}(k_2)$$

- Population

$$\mathrm{f}(k_1) > 0$$

$$\mathrm{f}(k_2) < 1$$ Pauli exclusion principle

- Scattering Matrix element

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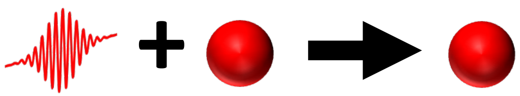

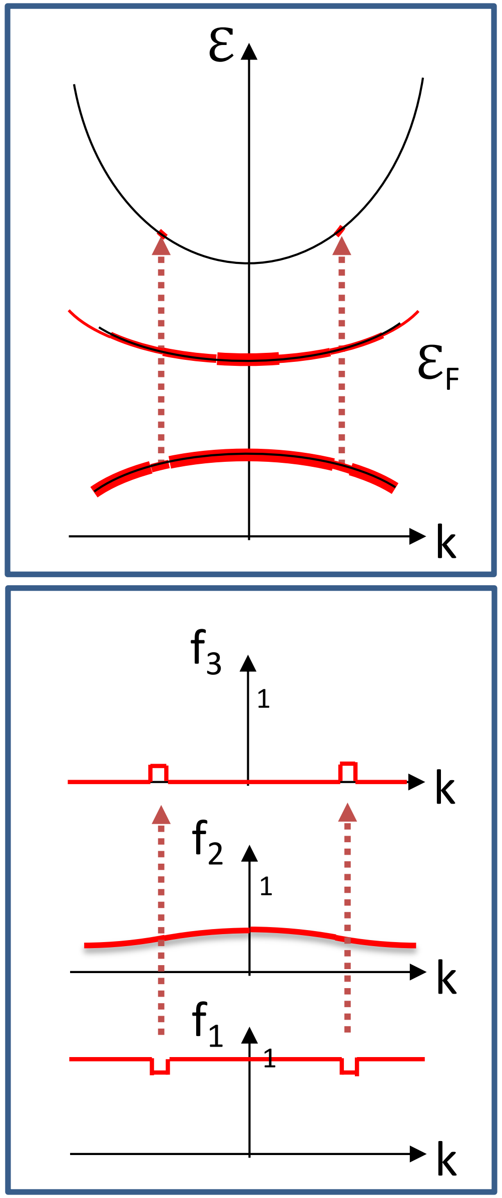

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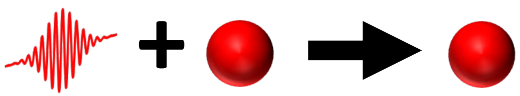

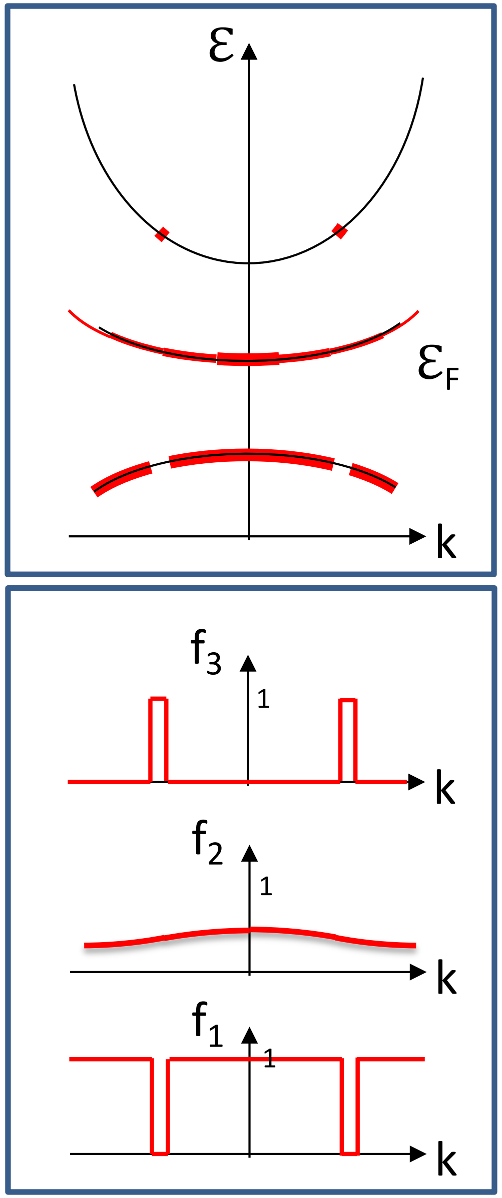

If nothing else happens photons keep being absorbed and electrons being excited
(we will see later what happens in reality)

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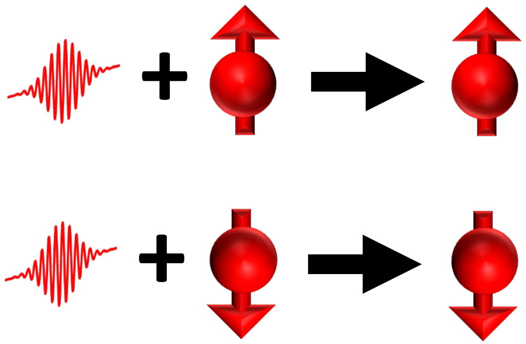
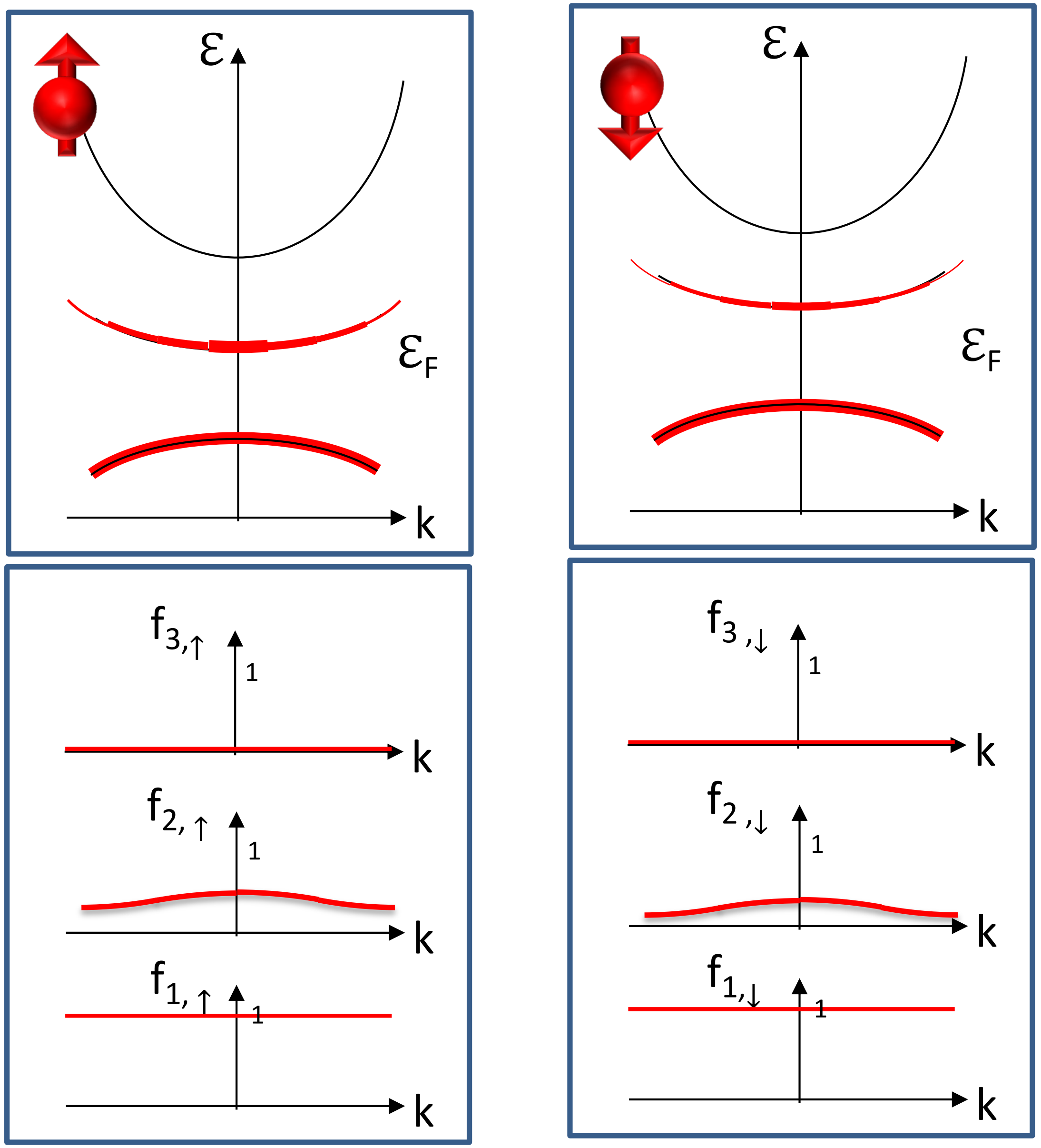
Laser excitation (with a spin)

In the absence of spin-orbit coupling





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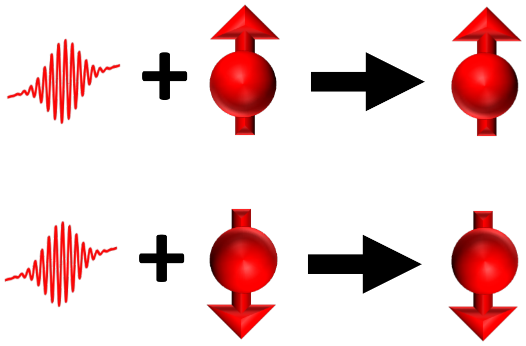

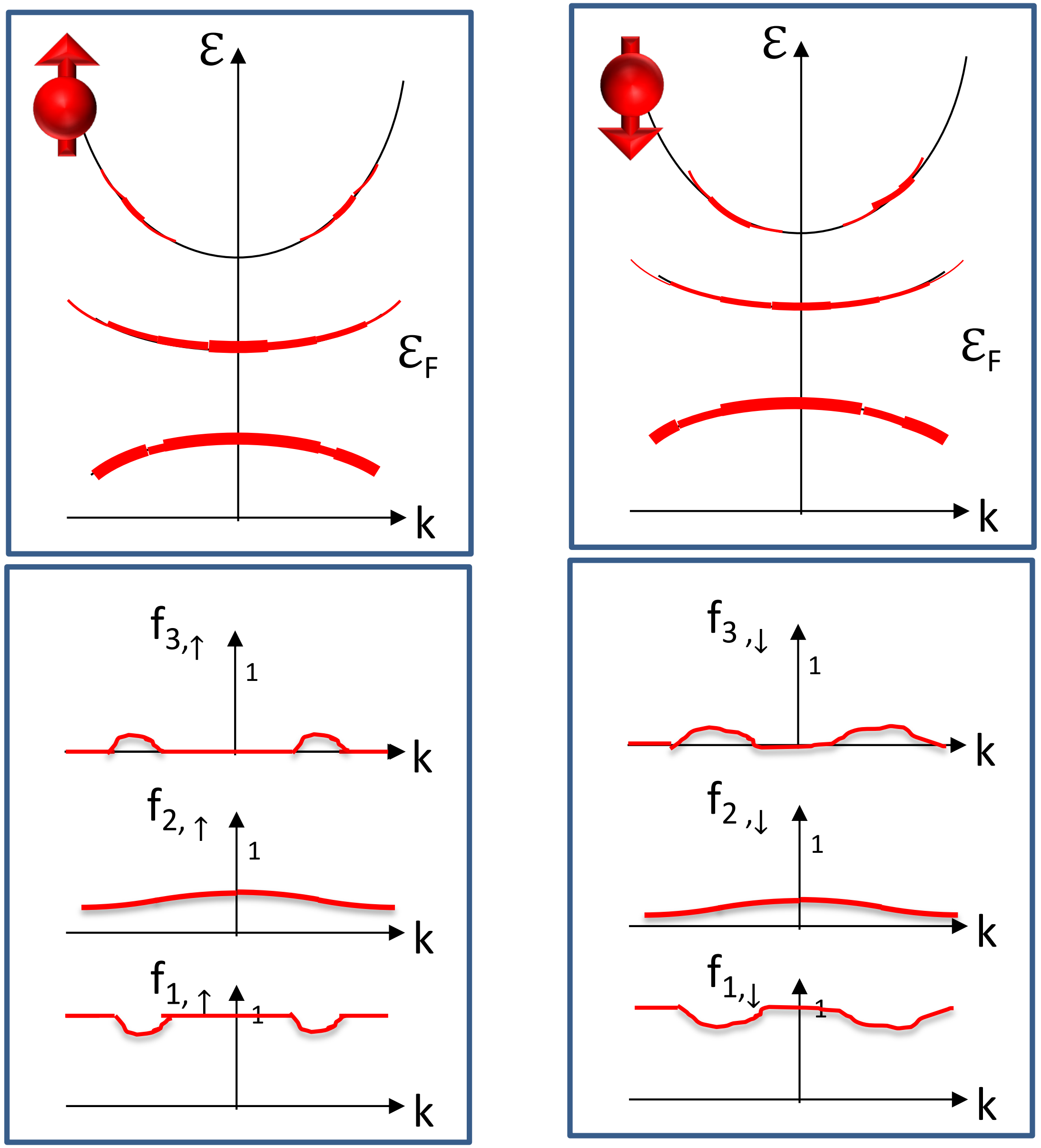

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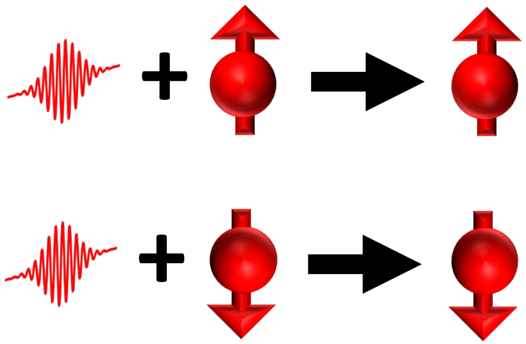
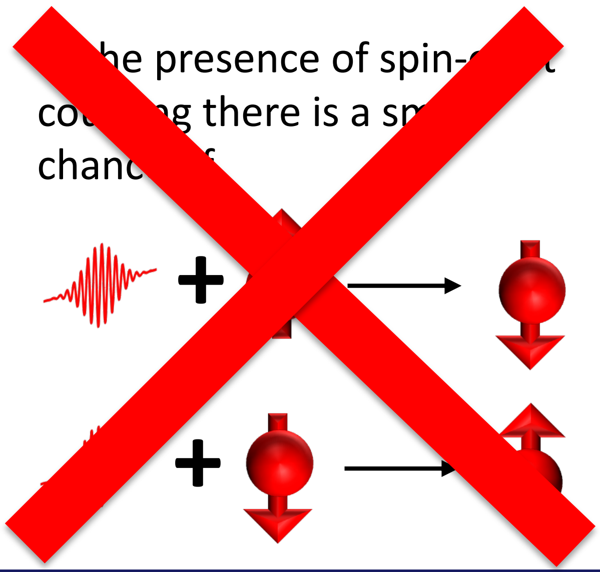
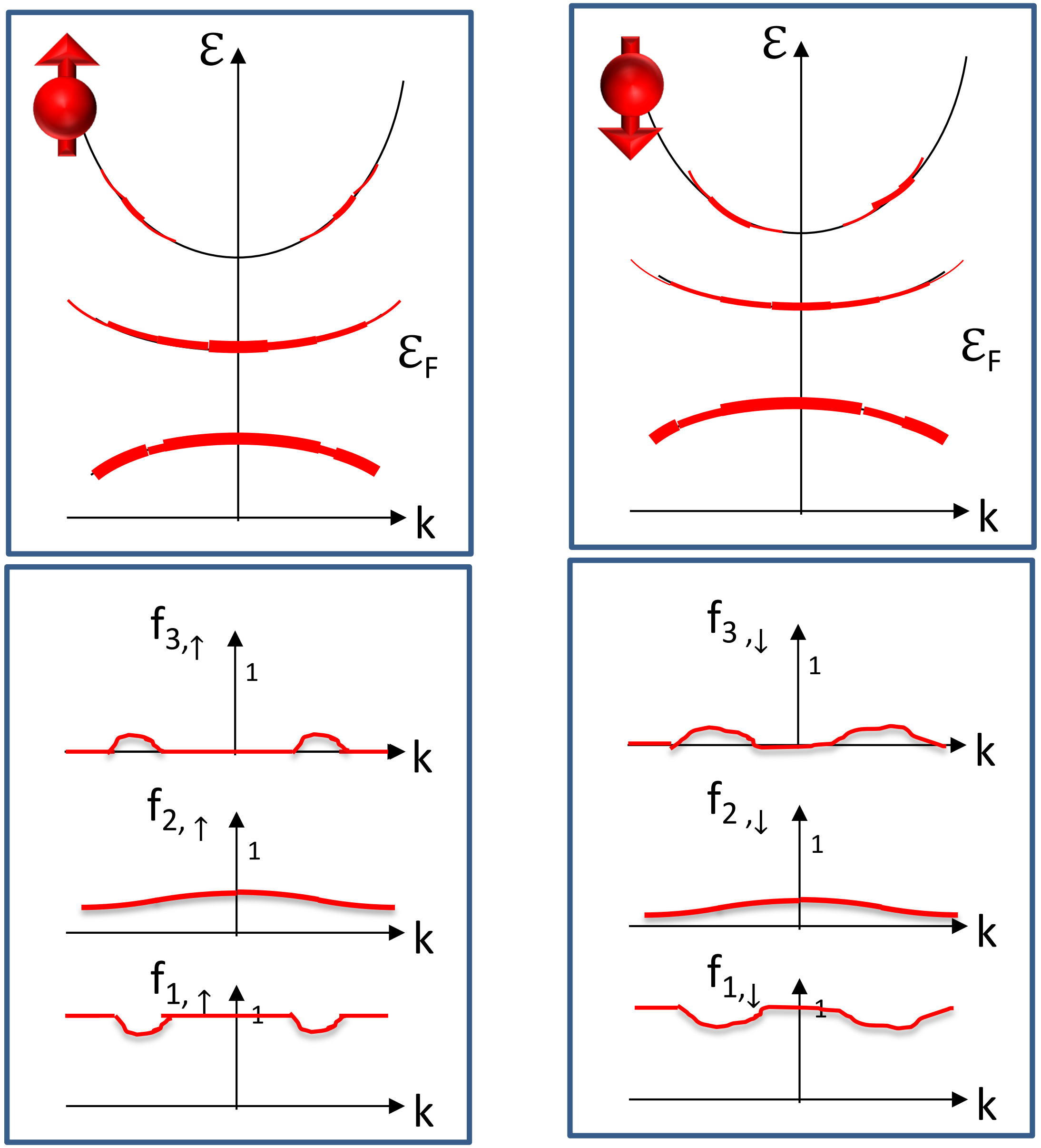
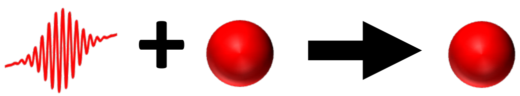


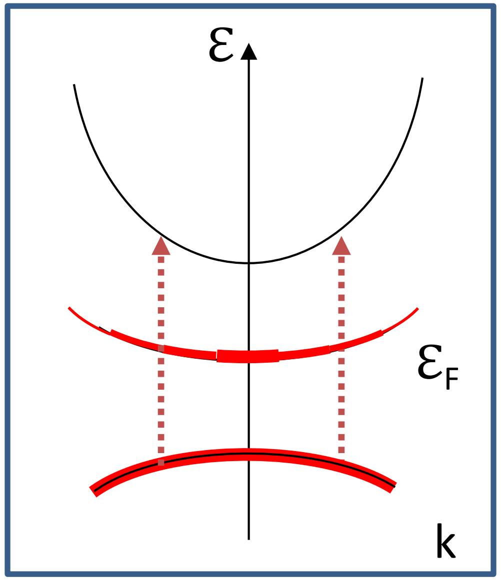




Laser excitation: absorption spectrum

Under perfectly monochromatic light





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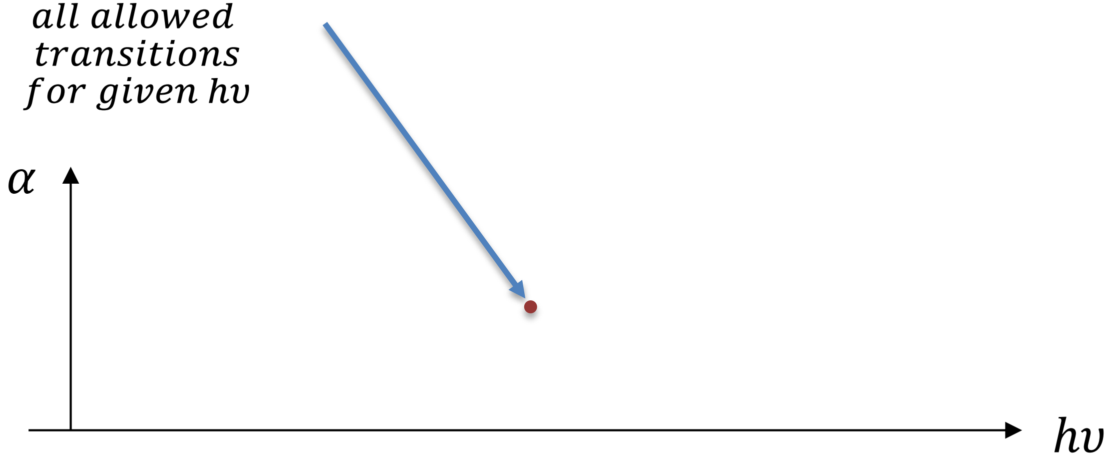
$$\sum_{\substack{all\ allowed\\ transitions\\ for\ given\ h\nu}} W_{n_1,n_2}(k_1,k_2)\, f_{n_1}(k_1)\left(1 - f_{n_2}(k_2)\right)$$



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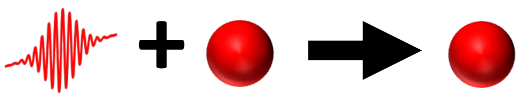
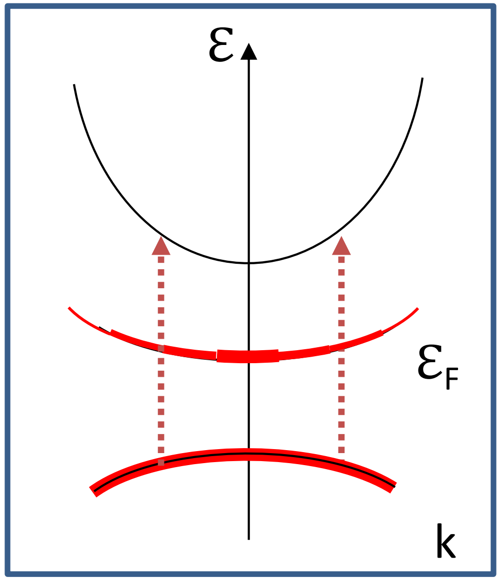
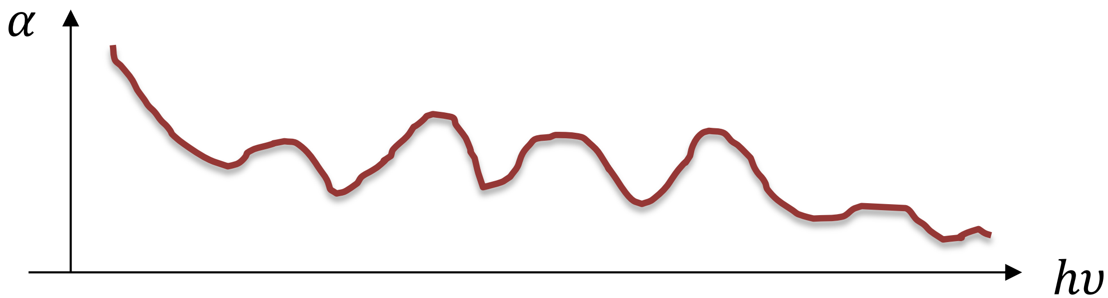




$$\sum_{\substack{all\ allowed\\ transitions\\ for\ given\ h\upsilon}} W_{n_1,n_2}(k_1,k_2)\, f_{n_1}(k_1)\left(1 - f_{n_2}(k_2)\right)$$



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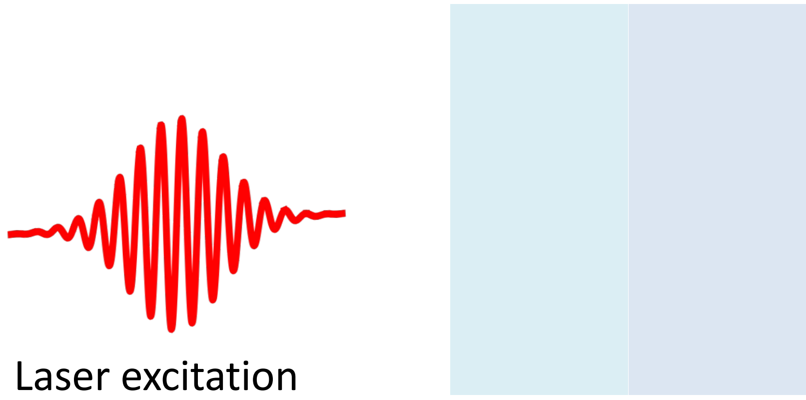
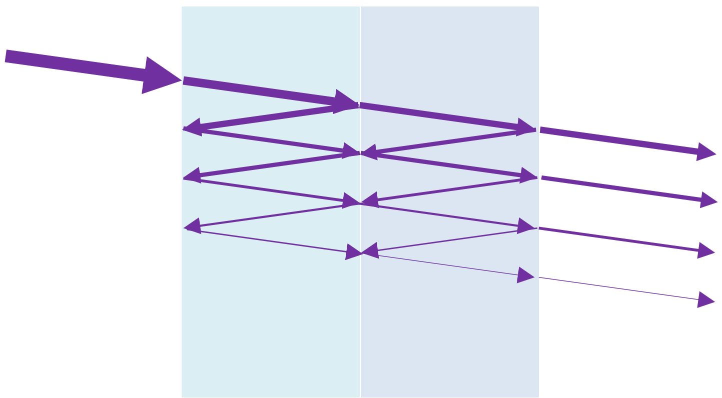
Laser excitation: multilayer

What we said above is in the case of spatially uniform photon density in a single material. What happens when there is a multilayer



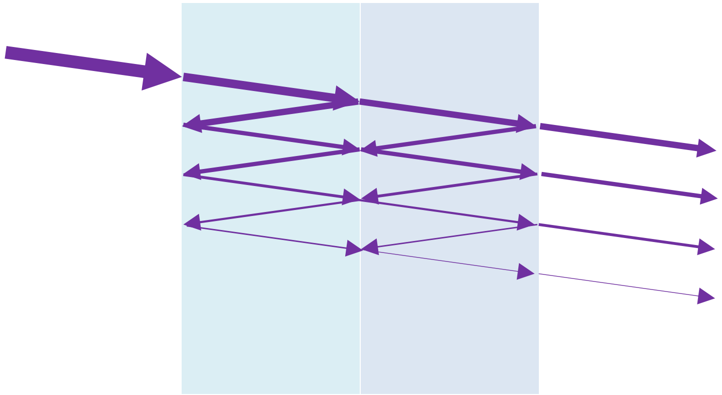
The photons, while being absorbed, will move throughout the sample, following Maxwell's equations



Laser excitation: multilayer

To treat this we can use the well-known Transfer Matrix Method

Transfer Matrix Method (TMM)



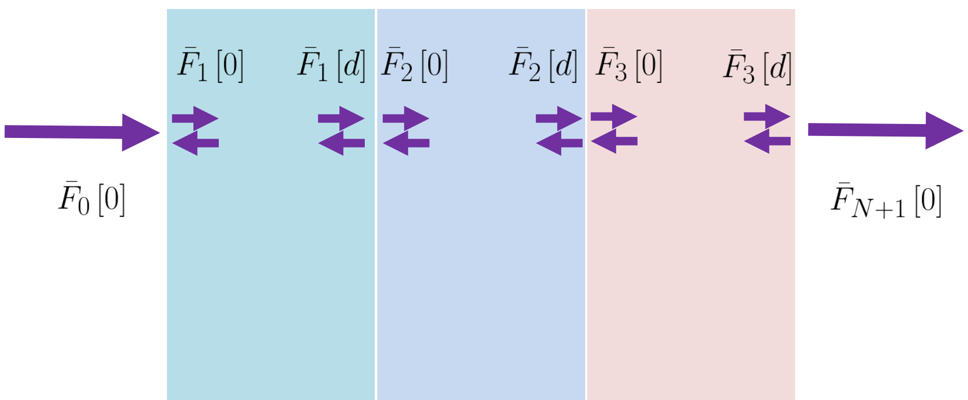
$$\partial_z E\,[z,t] = \mu\,\partial_t H\,[z,t]$$

$$\partial_z H\,[z,t] = \epsilon\,\partial_t E\,[z,t]$$

Maxwell's equations

$$E[z,t] = f^{>}[t]e^{ikz} + f^{<}[t]e^{-ikz}$$

$$H[z,t] = \sqrt{\frac{\epsilon}{\mu}} f^{>}[t]e^{ikz} - \sqrt{\frac{\epsilon}{\mu}} f^{<}[t]e^{-ikz}$$



$$\bar{F}\,[\omega, z] = a[\omega, z]\bar{f}\,[\omega]$$

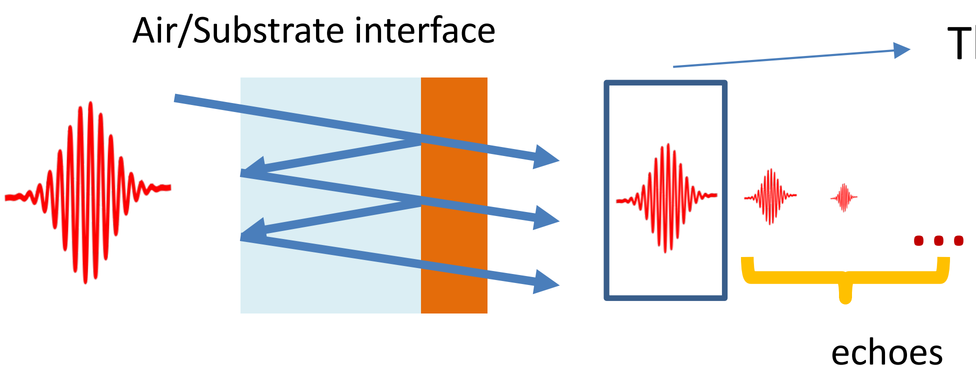
$$\bar{f}_{N+1} = (a_{N+1}[0])^{-1}\left(\prod_{j=N}^{1} M_j[d_j]\right) a_0[0]\bar{f}_0 = T_{[0,N+1]}\bar{f}_0$$

$$\begin{bmatrix} f^{>}_{N+1} \\ 0 \end{bmatrix} = T_{[0,N+1]} \begin{bmatrix} f^{>}_0 \\ f^{<}_0 \end{bmatrix}$$

It is then possible to reconstruct the photon density and therefore the spatial profile of electron excitations

Laser excitation: echo

Using TMM naively for the laser excitation leads to an overestimation of the excitation



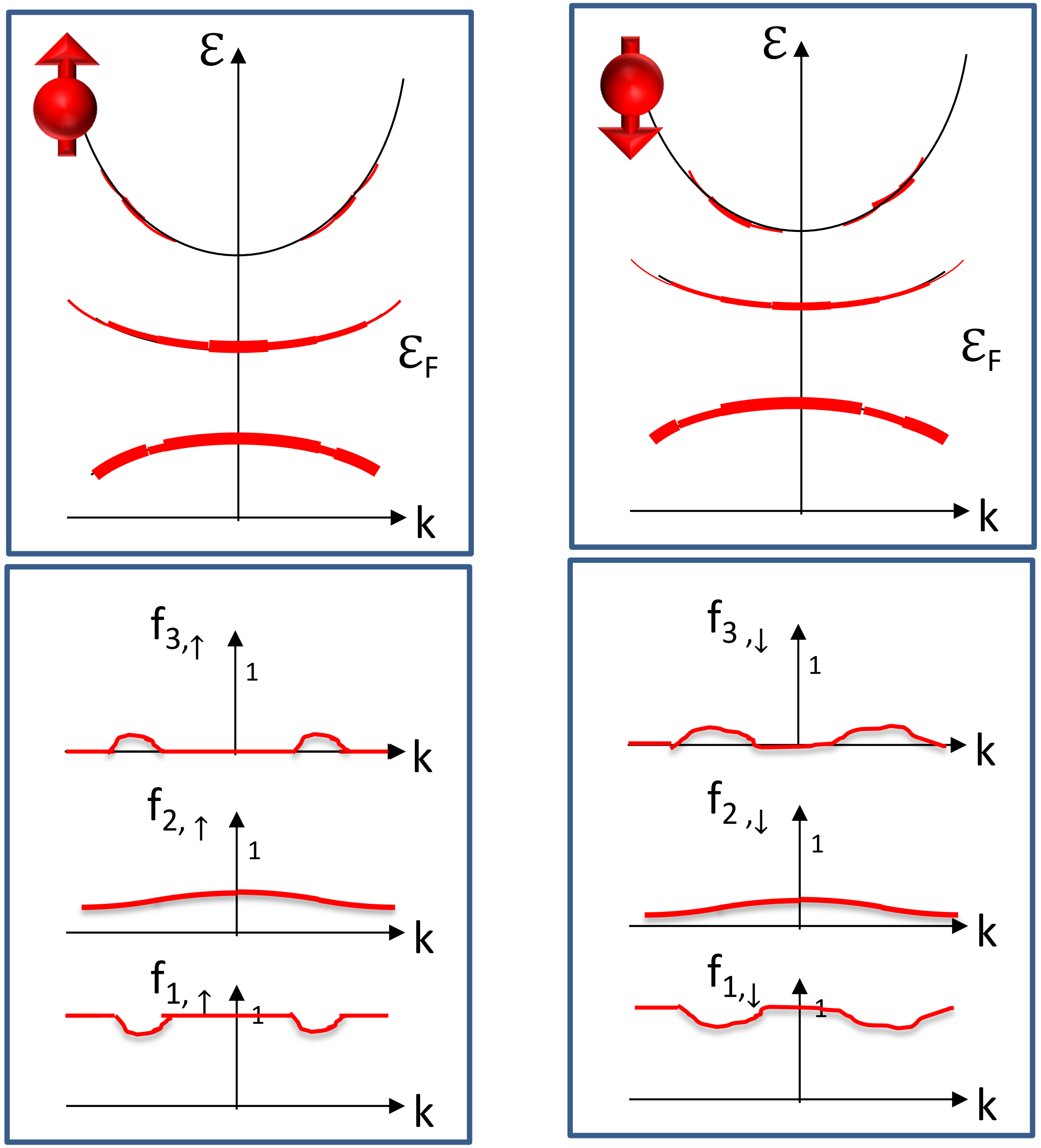
$$\begin{bmatrix} f_{N+1}^{>\text{no echo}} \\ 0 \end{bmatrix} = T_{[S,N+1]} \begin{bmatrix} f_S^{>*} \\ f_S^{<*} \end{bmatrix} = T_{[S,N+1]} \begin{bmatrix} t_{[0,S]} f_0^{>} \\ f_S^{<*} \end{bmatrix}$$

$$f_S^{>*} = t_{[0,S]} f_0^{>} \qquad f_{N+1}^{>\text{no echo}} = t_{[0,S]} t_{[S,N+1]} f_0^{>} .$$

We will see how echo has a way more serious effect on the THz frequency range

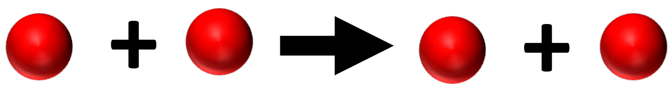
Y Yang, S Dal Forno, M Battiato, J Infr Millim, 42 1142 (2021)

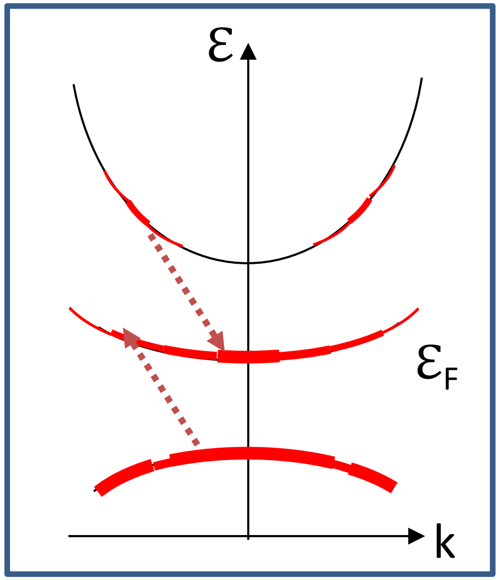
Laser excitation

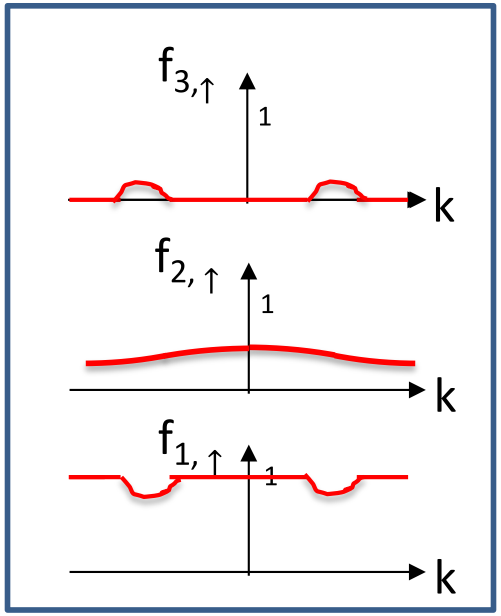


Thermalisation

Excited electrons can scatter







- ❑ Momentum conservation

$$k_1 + k_2 = k_3 + k_4$$

In reality there is the possibility of umklapp and the correct equation is

$$k_1 + k_2 = k_3 + k_4 + G$$

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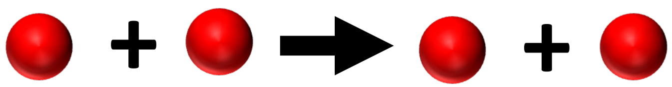

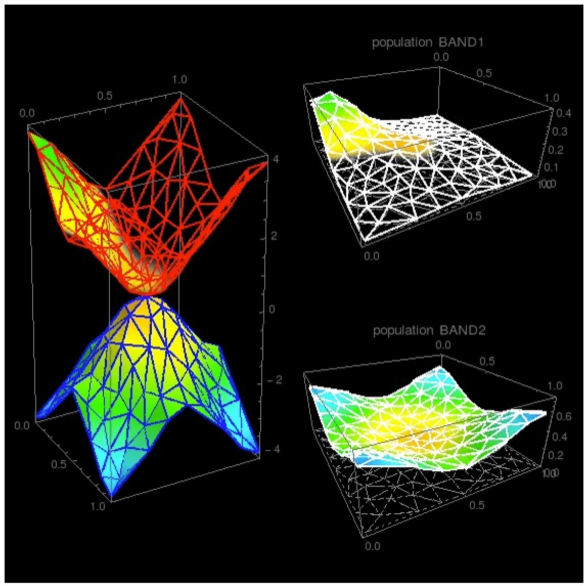

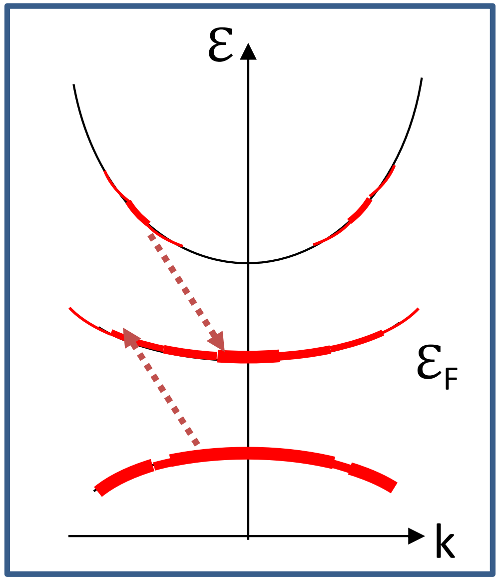

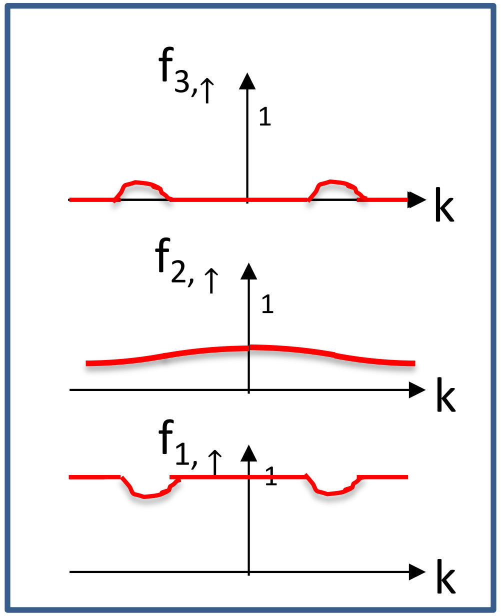

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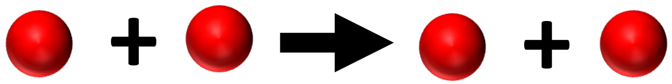
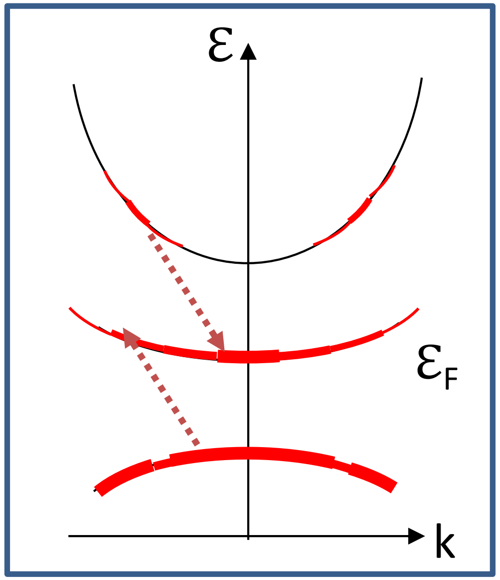
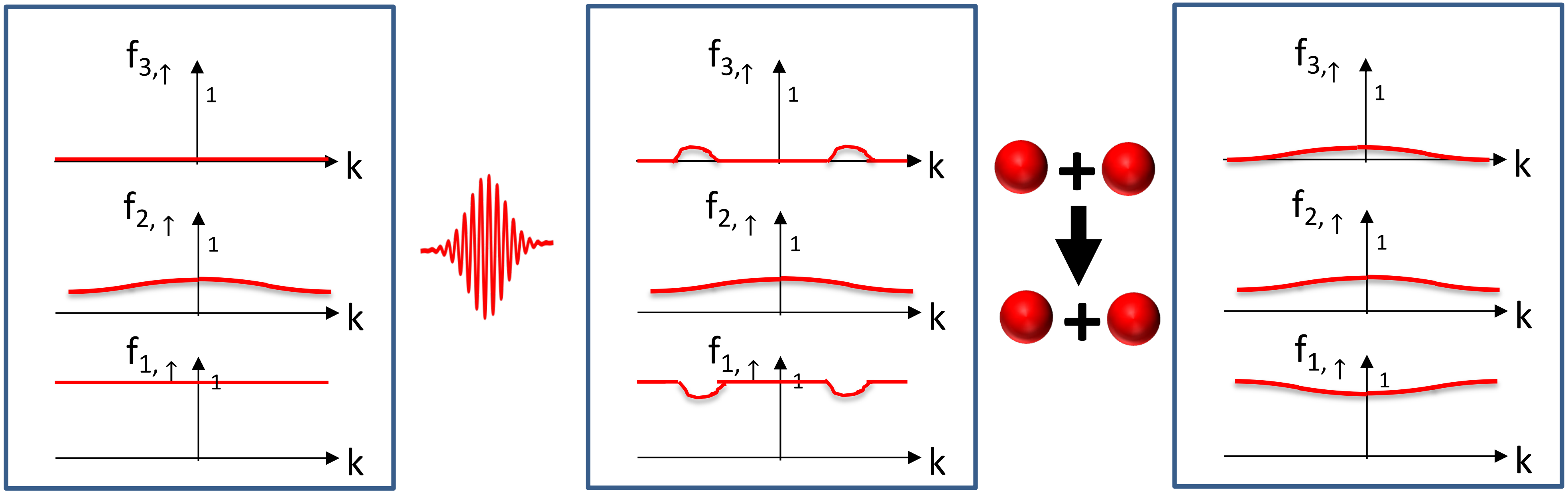
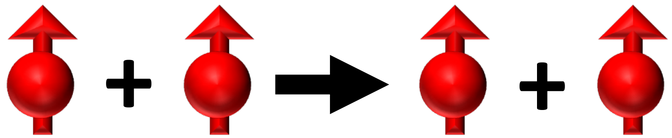




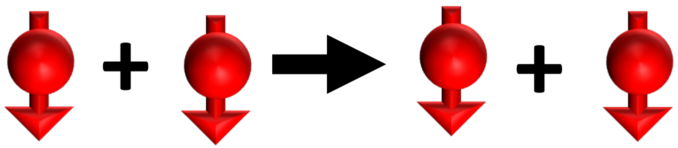
Higher temperature!!!



Thermalisation with spin



Spin preserving



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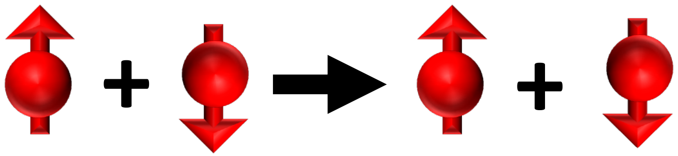
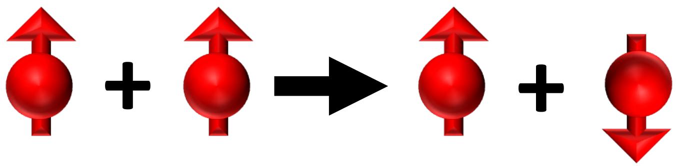


Spin preserving

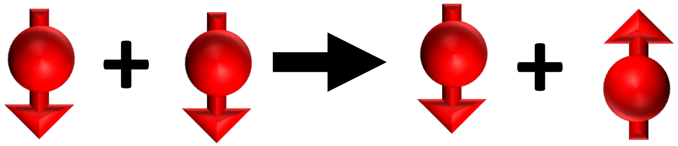
This is important to properly understand how energy is deposited

Eschenlor, Battiato et al, **Nature Mater** 12, 332 (2013).

In the presence of spin orbit coupling, with lower probability there can be

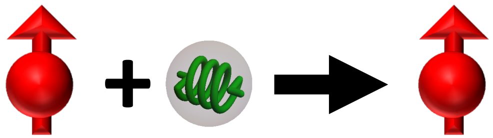


Spin flipped



Spin flipped

Cooling down with phonons



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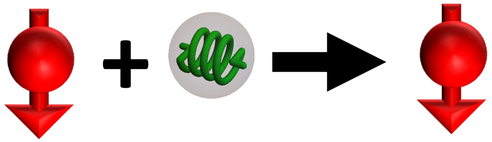

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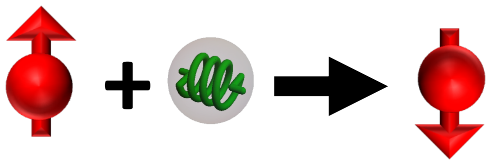
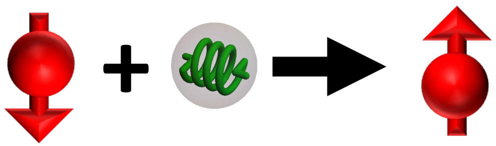


Spin flipped (Elliot-Yafet)



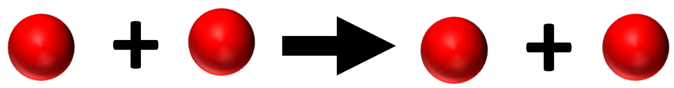
Spin flipped (Elliot-Yafet)

Usually slower than electron-electron scatterings (… well it's a bit more complicated than that)

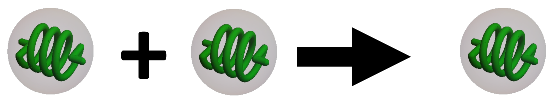
Cooling down with phonons

What is the effect?
In general, it can be complicated and complex phenomena can arise, like phonon bottlenecks

Let us make some approximations just to get an intuitive understanding



Fast



Fast

Slow

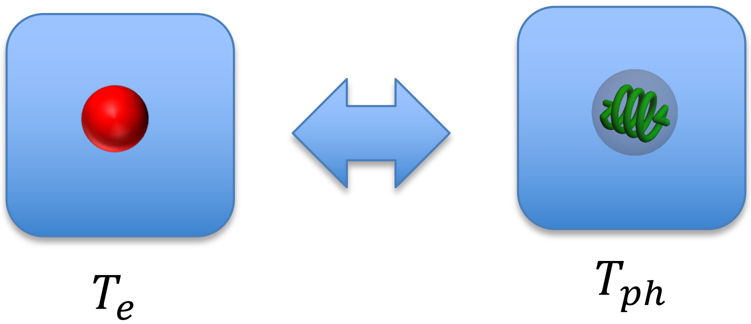
Notice that this is not always a good approximation

Cooling down with phonons

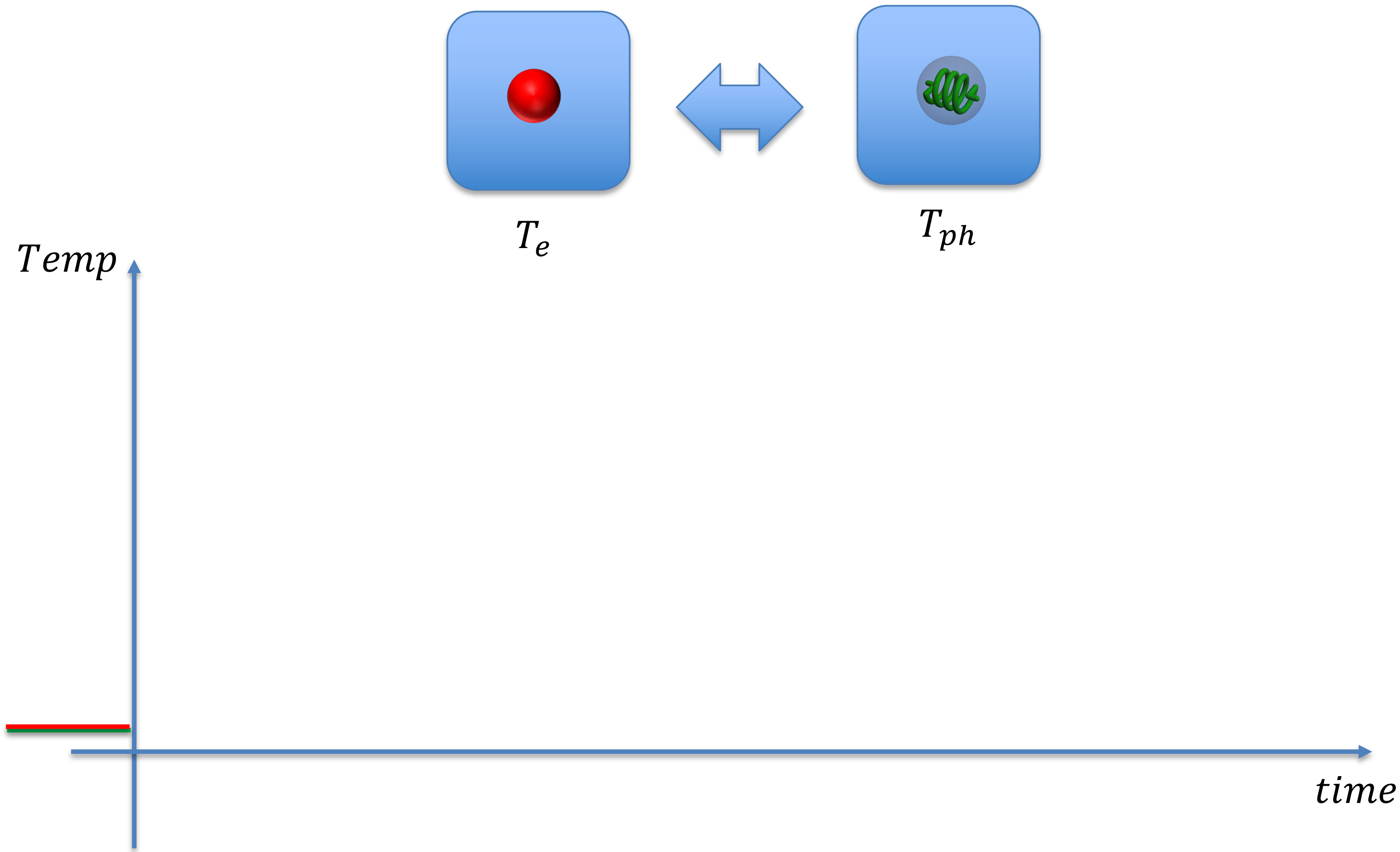
In that case, the electrons and the phonons can be described as two systems

1. Always very close to the thermalized state
2. Exchanging energy

Thermodynamics tells us that they will equilibrate to the same temperature



Summary so far



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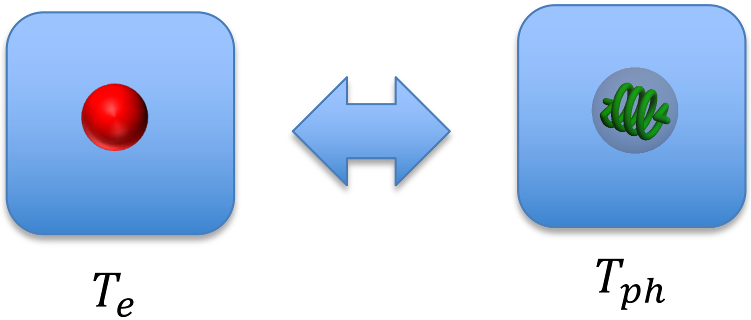
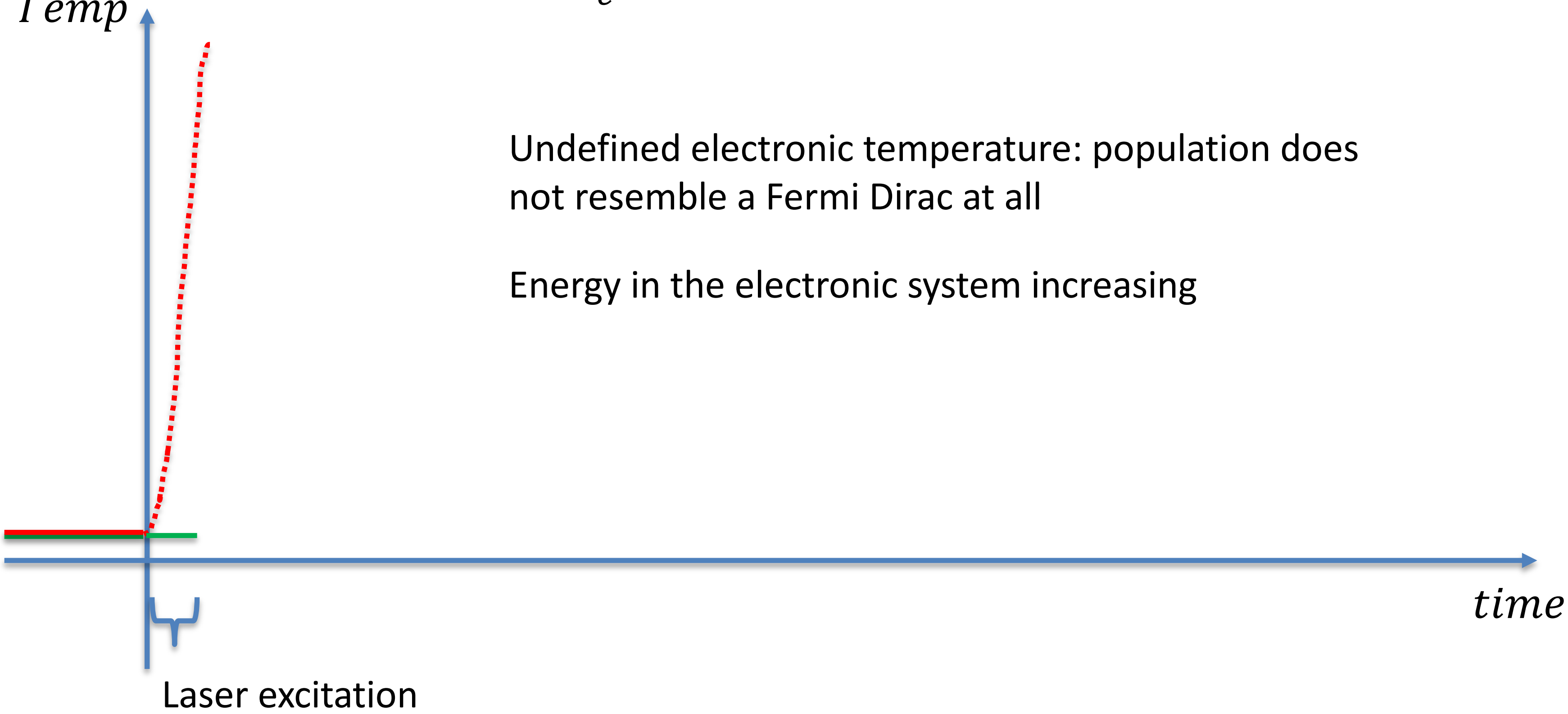
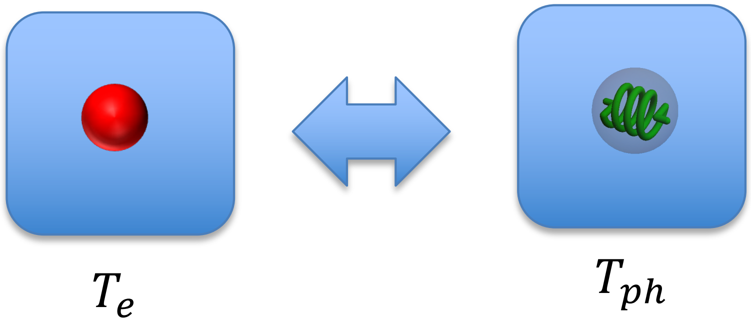




Undefined electronic temperature: population does not resemble a Fermi Dirac at all

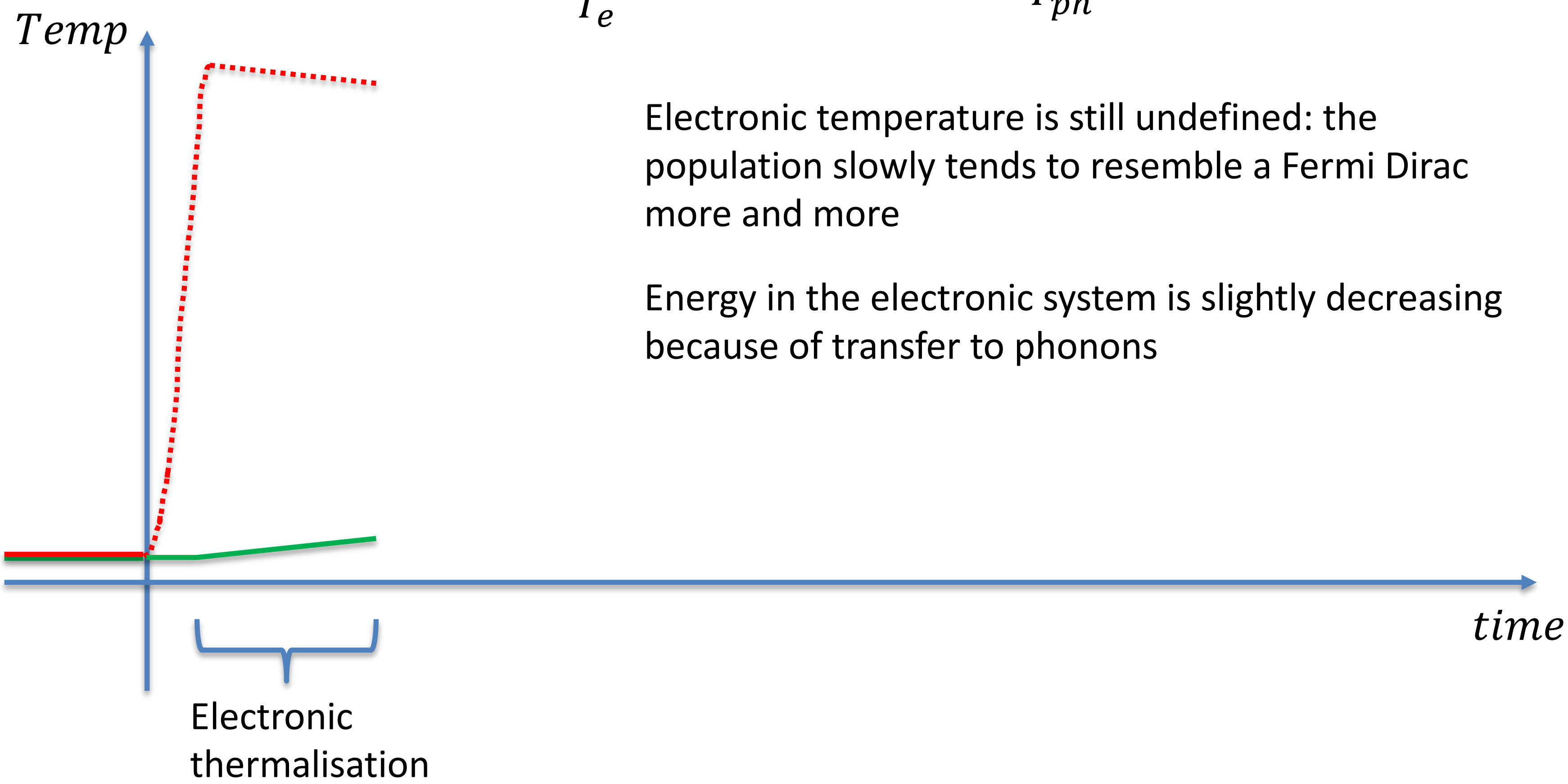
Energy in the electronic system increasing

Summary so far

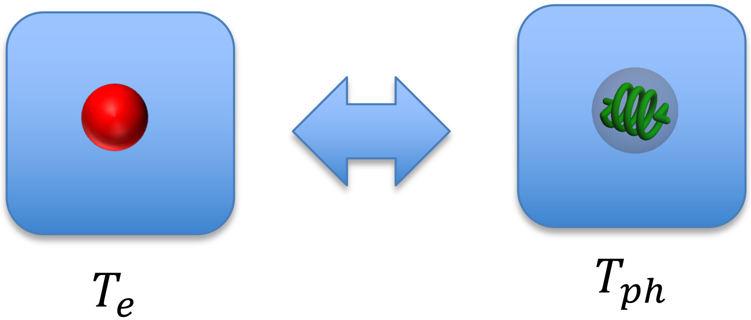


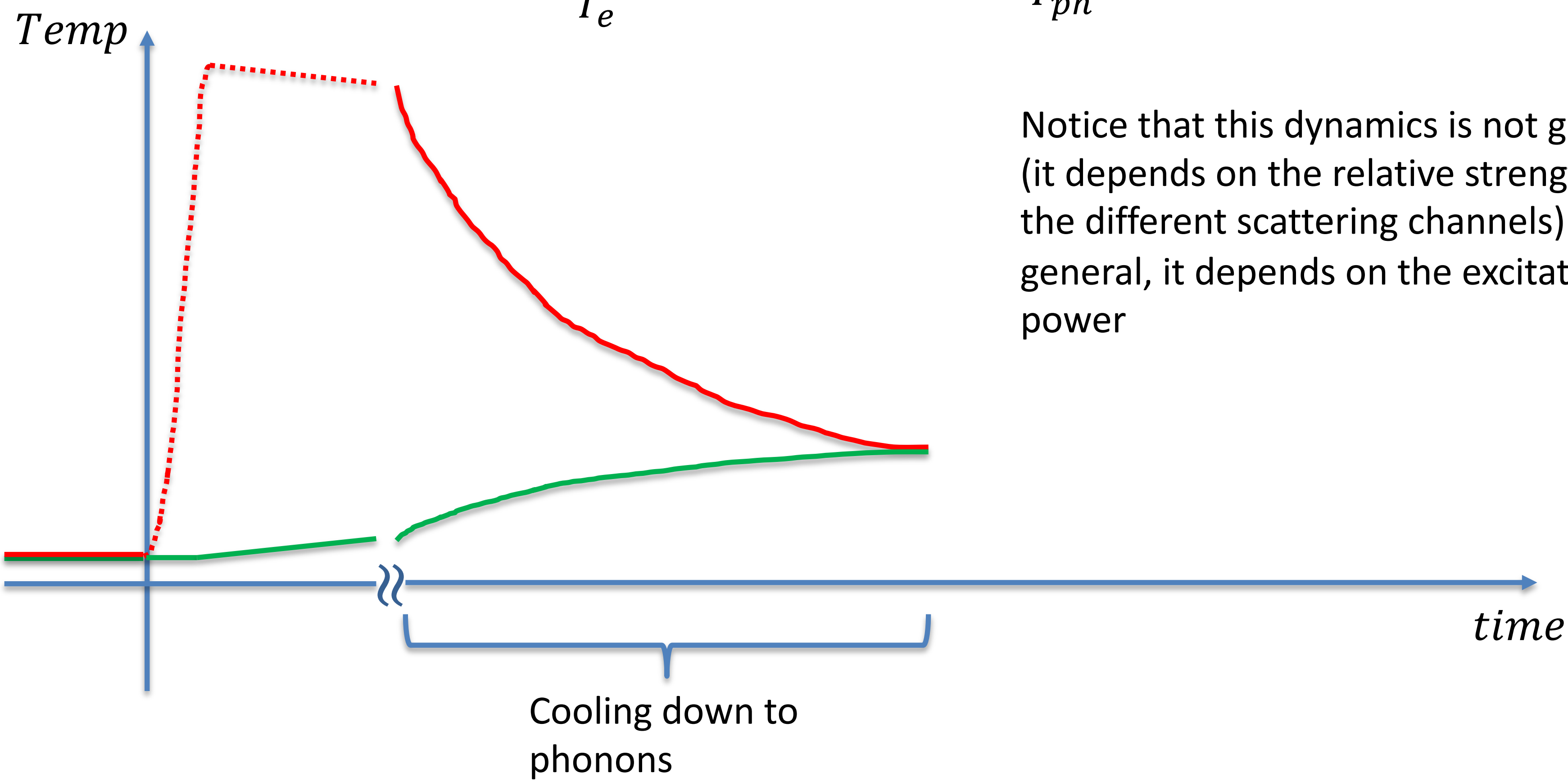
Electronic temperature is still undefined: the population slowly tends to resemble a Fermi Dirac more and more

Energy in the electronic system is slightly decreasing because of transfer to phonons



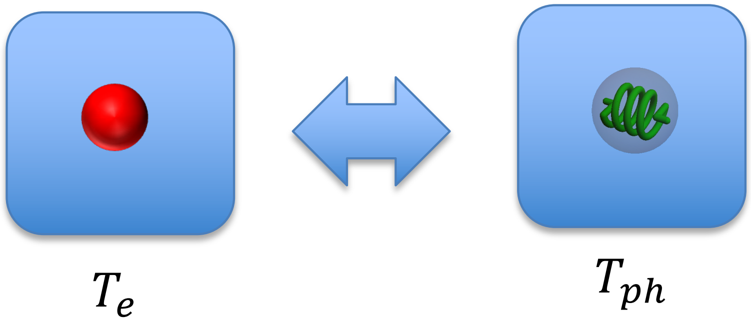
Summary so far

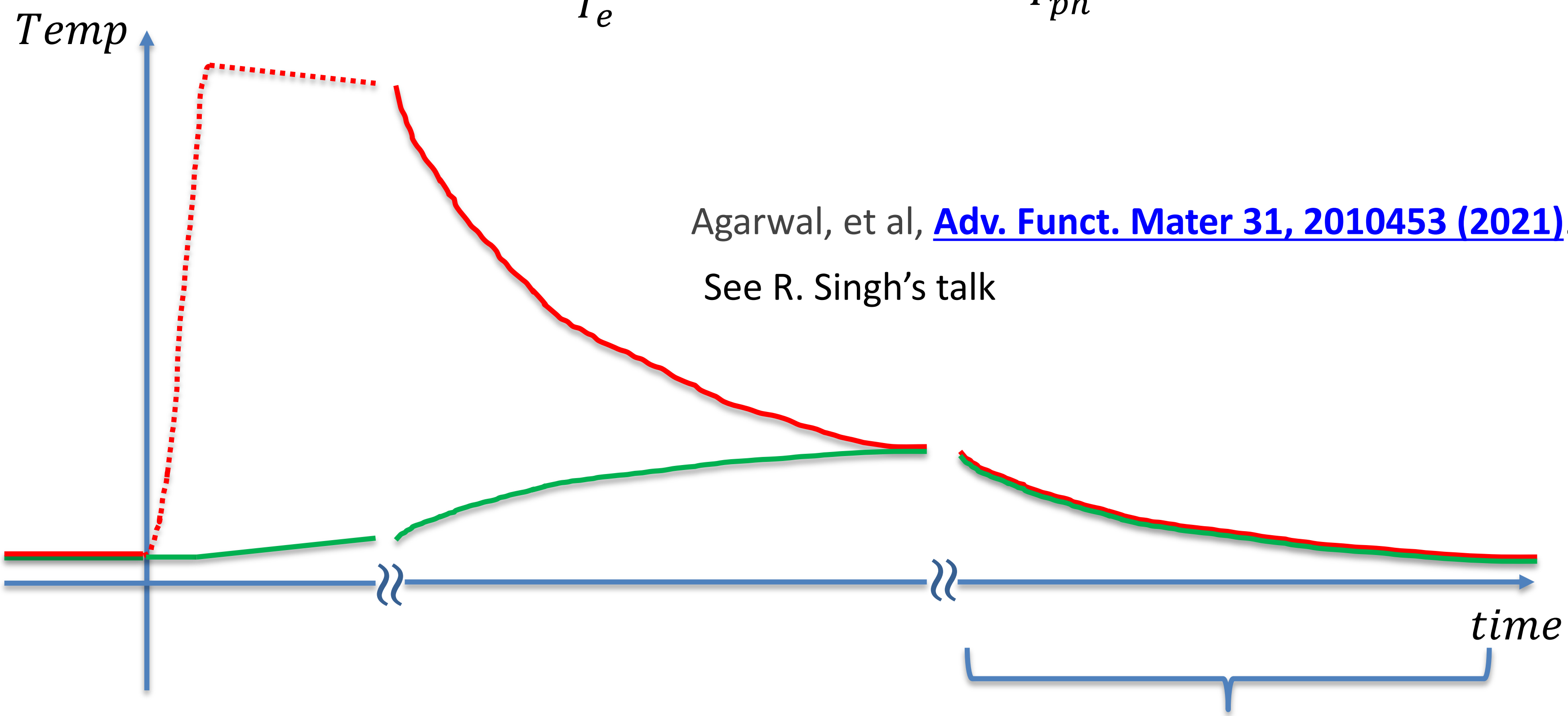




Notice that this dynamics is not general (it depends on the relative strength of the different scattering channels) and, in general, it depends on the excitation power

Summary so far





Agarwal, et al, [Adv. Funct. Mater 31, 2010453 (2021)].

See R. Singh's talk

Cooling down through heat diffusion to substrate

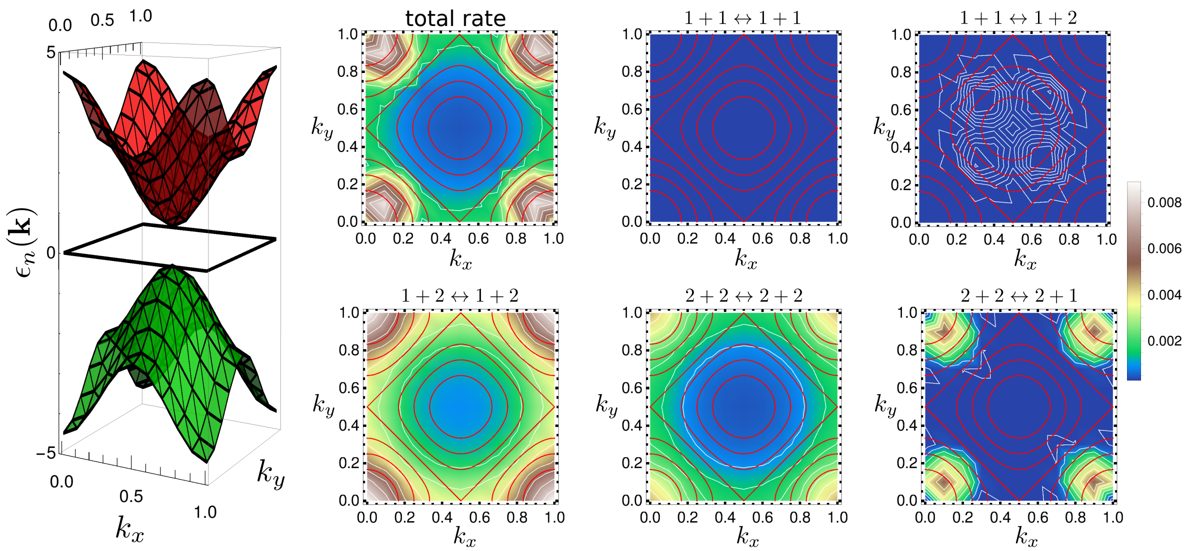
Timescales

Despite what seemed from the previous slides, pinning down timescales is far from trivial

The decay time of excided states is a complex interplay of the decay timescales of higher (and to a certain extent, also lower) energy excitations and scattering lifetimes of the states.

The decay time of excided states is a complex interplay of the decay timescales of higher (and to a certain extent, also lower) energy excitations and scattering lifetimes of the states.

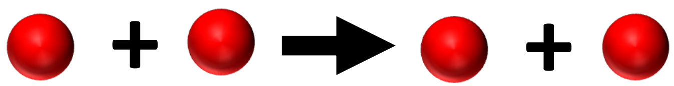
Scattering times also depend on the (excited) population.
However, if the excitation is not too strong, we can look at equilibrium lifetimes

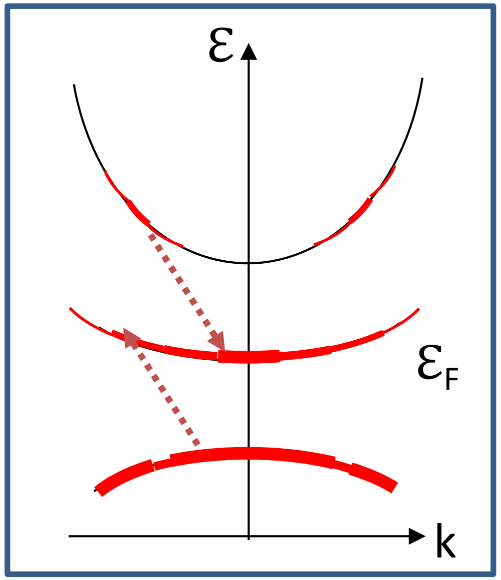


Wais, Held, Battiato, Comput. Phys. Commun. 264, 107877 (2021)
Wadgaonkar, Jain, Battiato, Comput. Phys. Commun 263, 107863 (2021)
Wadgaonkar, Wais, Battiato, Comput. Phys. Commun 271, 108207 (2021)

Timescales

The lifetime of a state





$$\frac{1}{\tau(k_1)} \propto \sum_{\substack{all\ allowed\\ transitions\\ for\ given\ h\nu}} W_{n_1,n_2}(k_1,k_2,k_3,k_4)\, f_{n_1}(k_1) f_{n_2}(k_2)\left(1-f_{n_3}(k_3)\right)\left(1-f_{n_4}(k_4)\right)$$

NOTE: Please notice that the one above is not the correct equation, but I did not want to spend time on technical details which are not really relevant for intuition. Check the refs below for the correct treatment

Wais, Held, Battiato, Comput. Phys. Commun. 264, 107877 (2021)
Wadgaonkar, Jain, Battiato, Comput. Phys. Commun 263, 107863 (2021)
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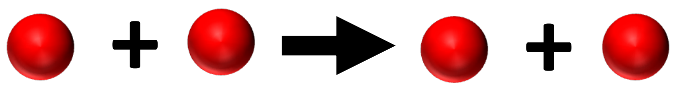
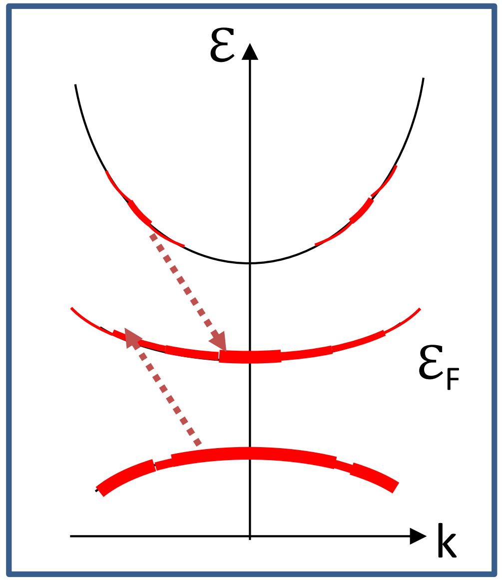
Timescales

The lifetime of a state





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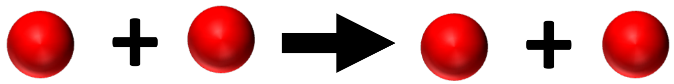
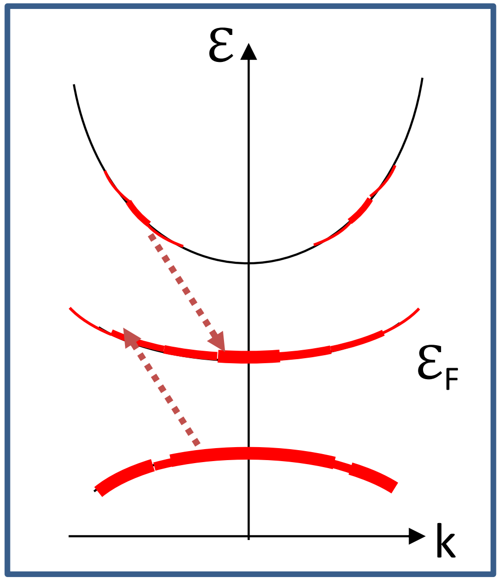
Timescales

The lifetime of a state





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Wadgaonkar, Jain, Battiato, Comput. Phys. Commun 263, 107863 (2021)
Wadgaonkar, Wais, Battiato, Comput. Phys. Commun 271, 108207 (2021)

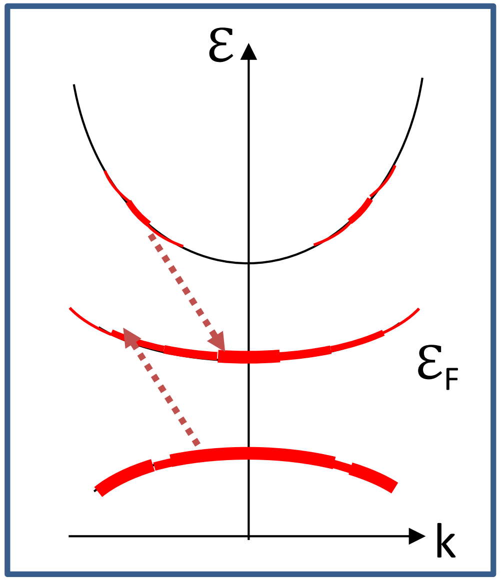
Timescales

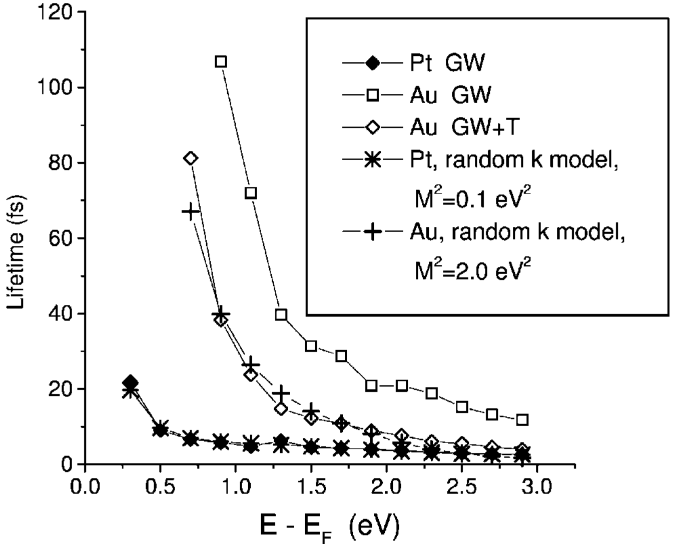
As a rule of thumb, in general (for generic metals)

Energy of the excitation

Number of allowed transitions

Lifetime





V. Zhukov et al., Phys. Rev. B 73, 125105 (2006)

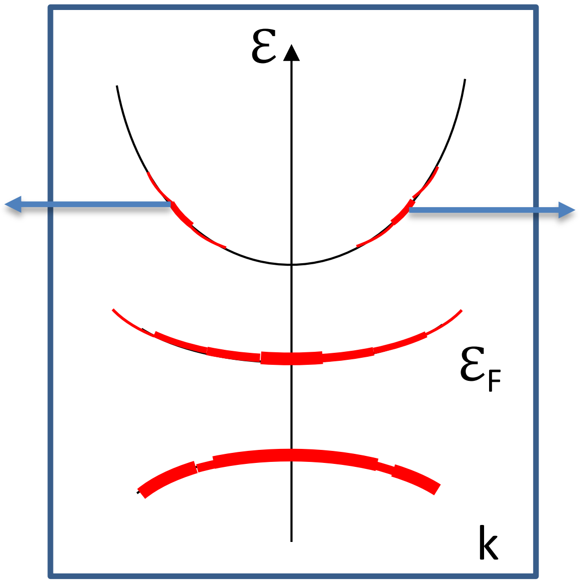
YOU: So? When can I consider the electronic system to be thermalized?

ME: Well, it depends on the energy you are looking at.

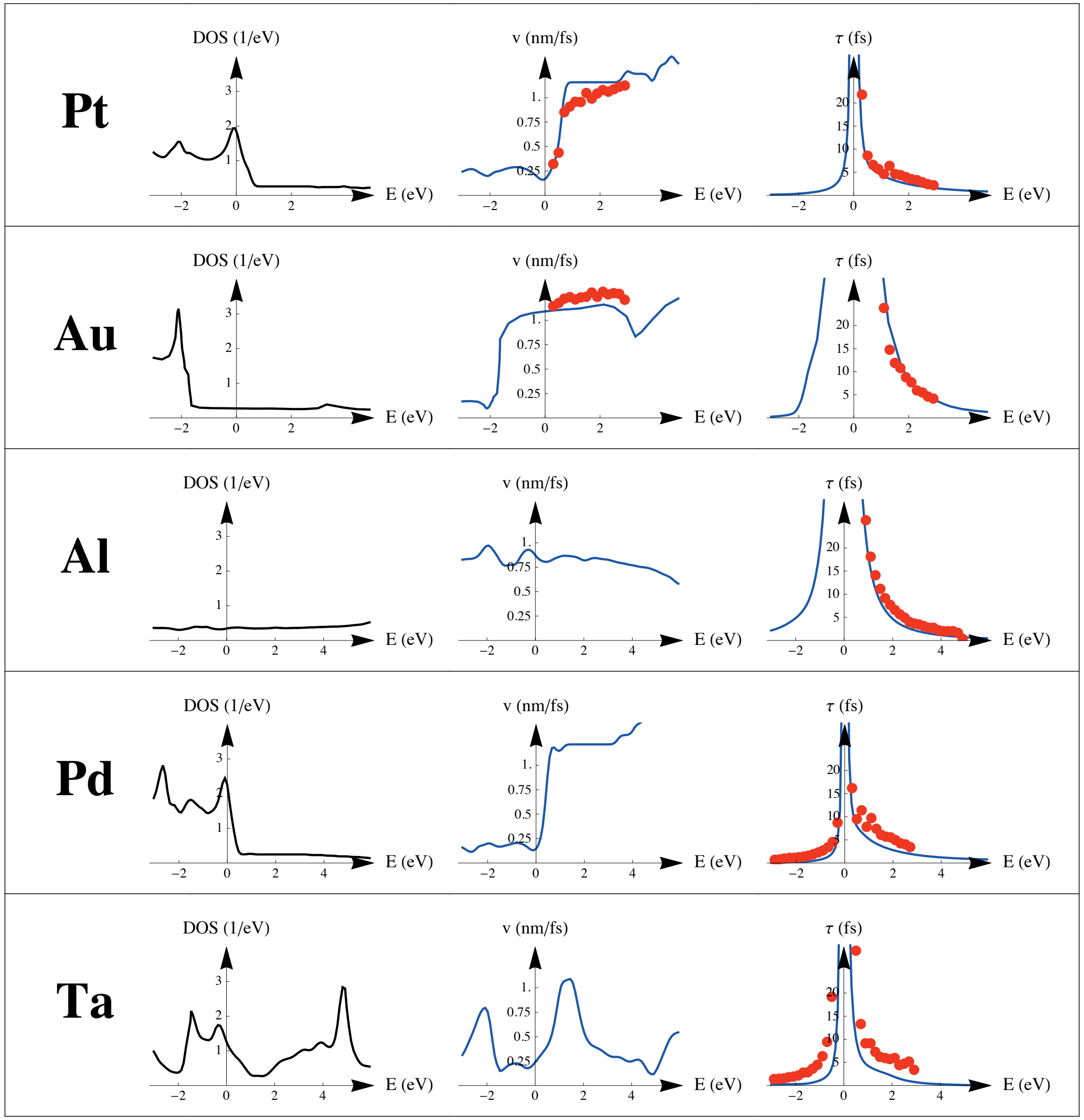
YOU: Fine, but which energy should I look at?

ME: Well, it depends… sorry

Transport out-of-equilibrium

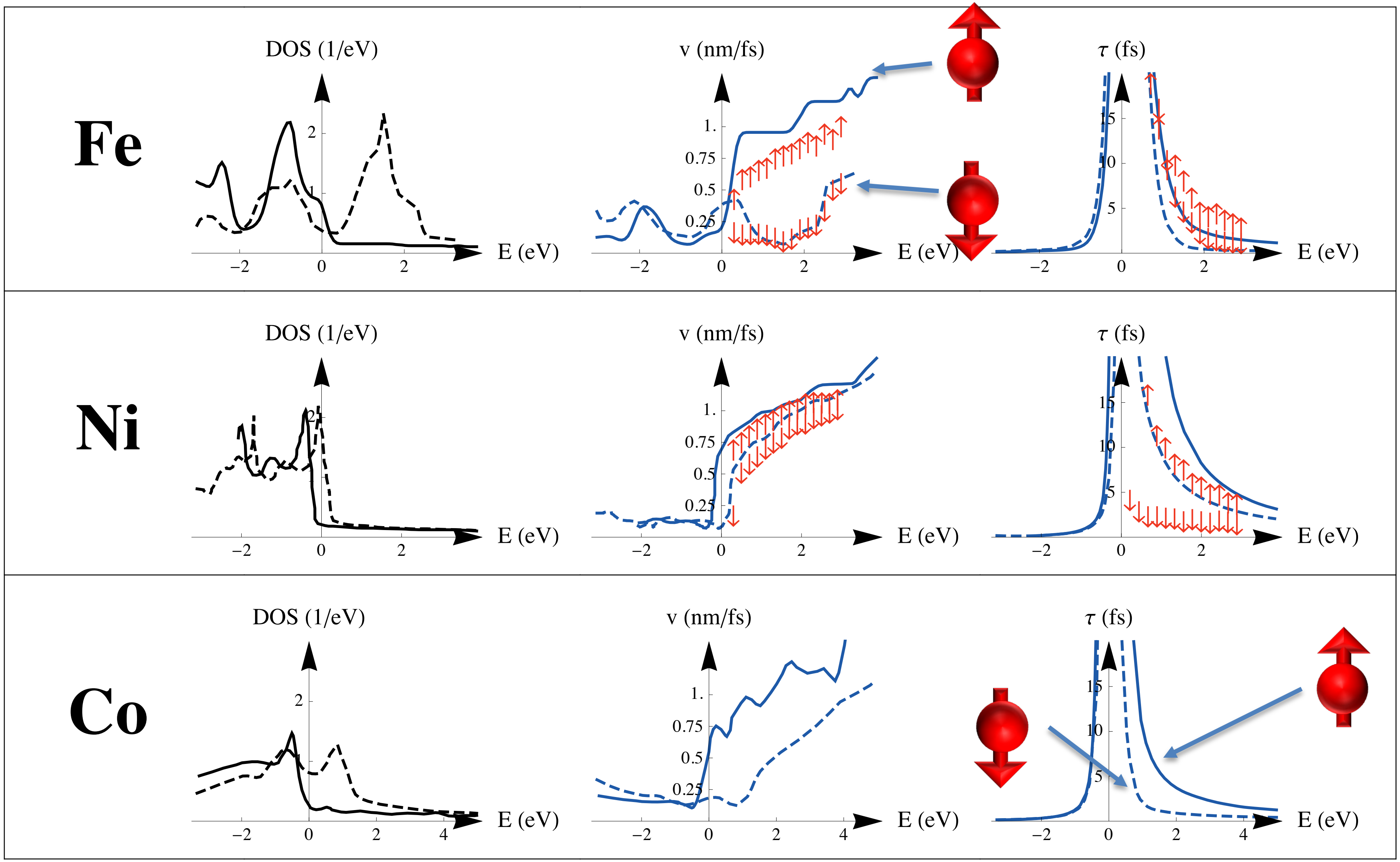


$$v(k) = \frac{1}{\hbar}\frac{\partial \mathcal{E}(k)}{\partial k}$$



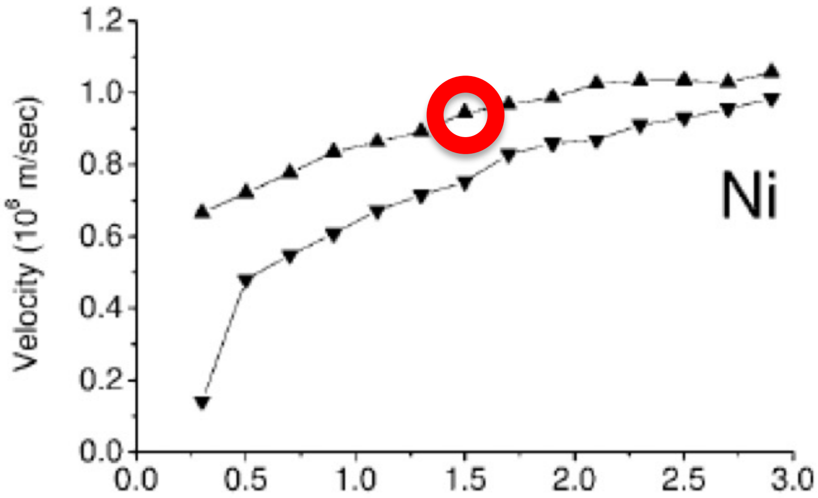
M. Battiato, PhD Thesis

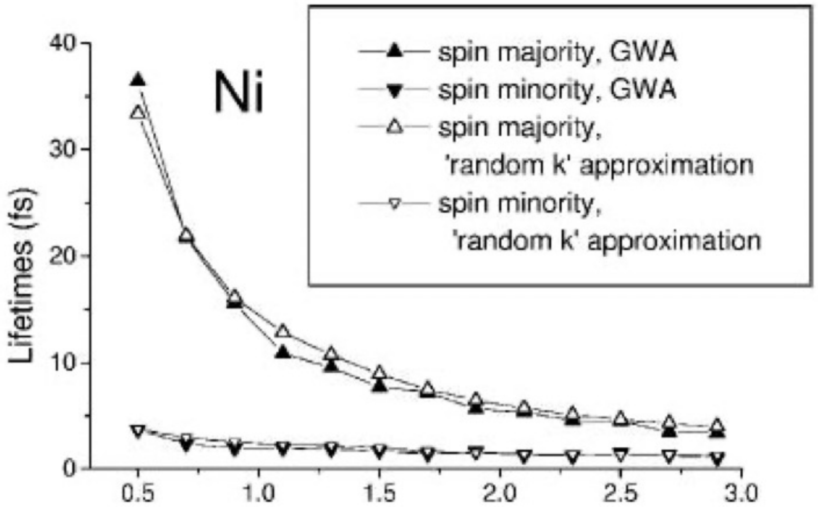
Transport out-of-equilibrium with spin

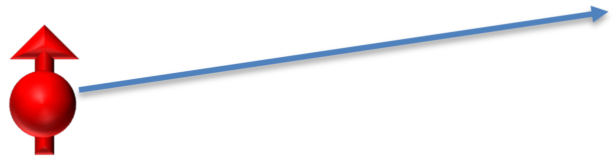


M. Battiato, PhD Thesis

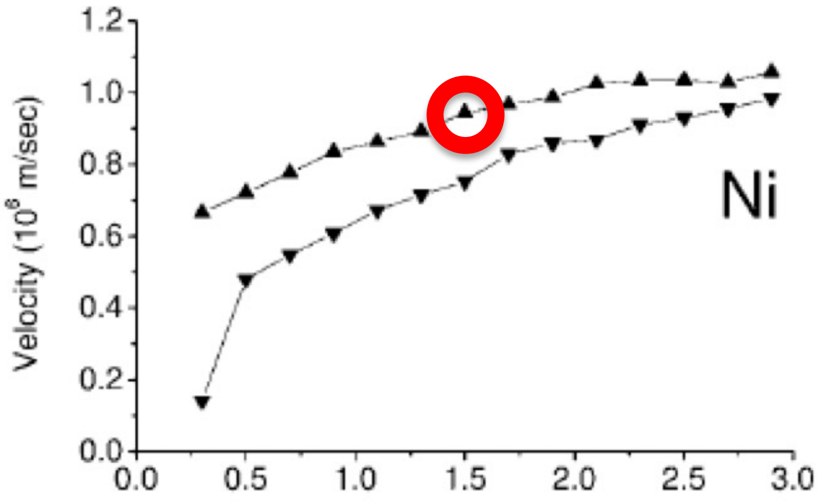
Transport out of equilibrium with spin

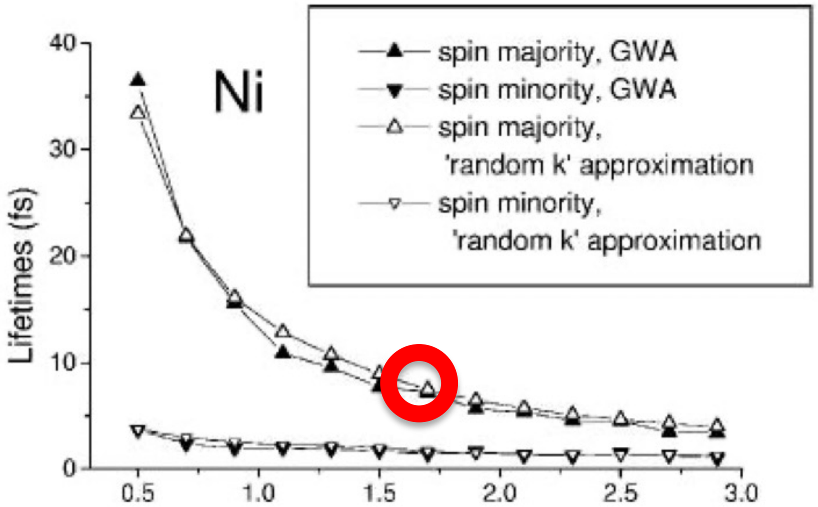


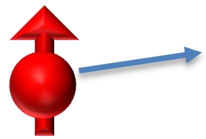




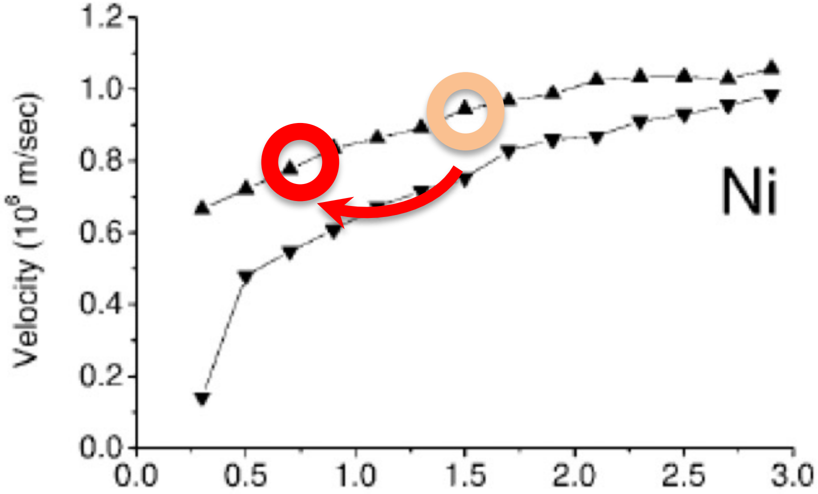
Transport out of equilibrium with spin

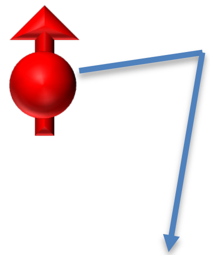


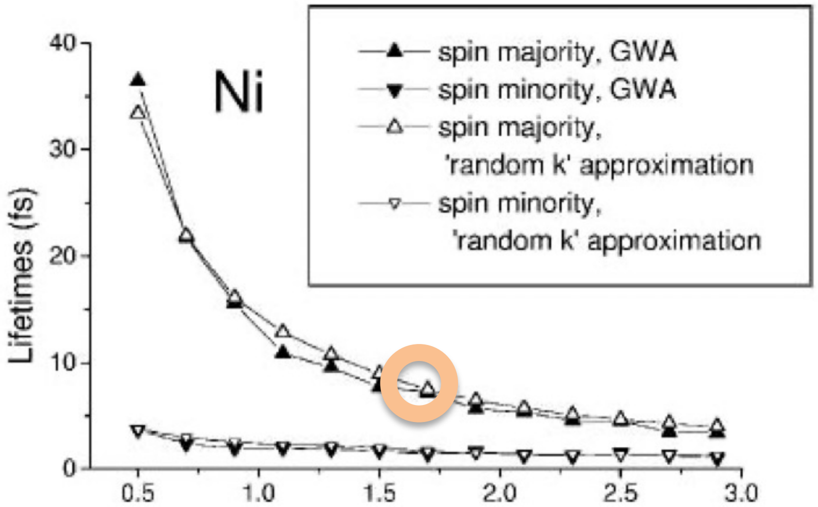




Transport out of equilibrium with spin







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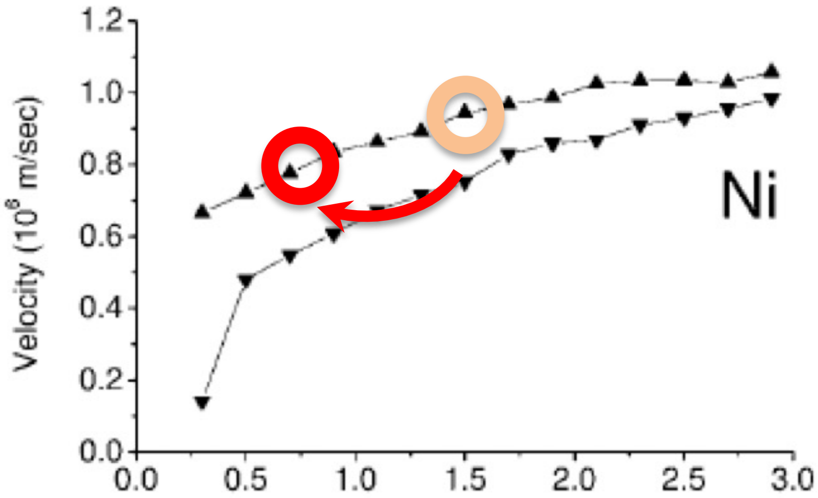
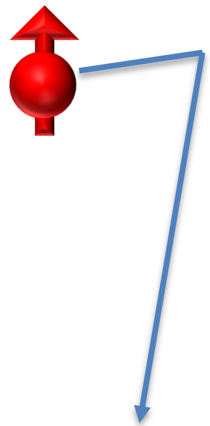
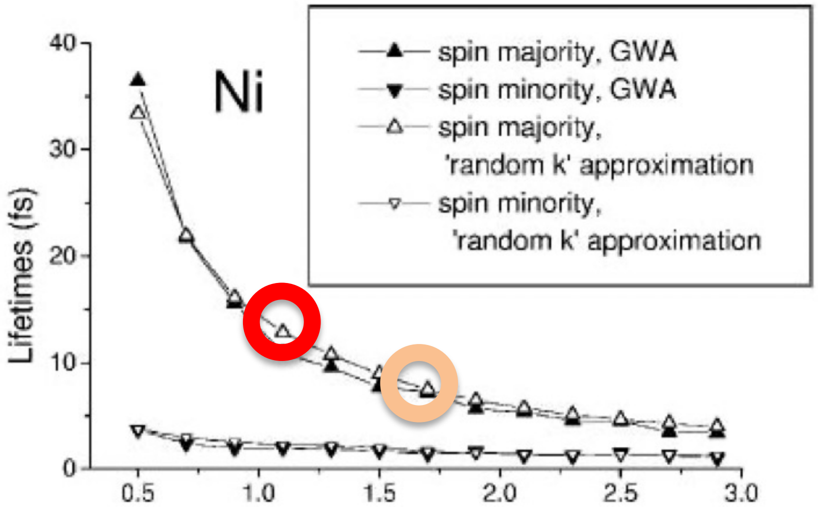
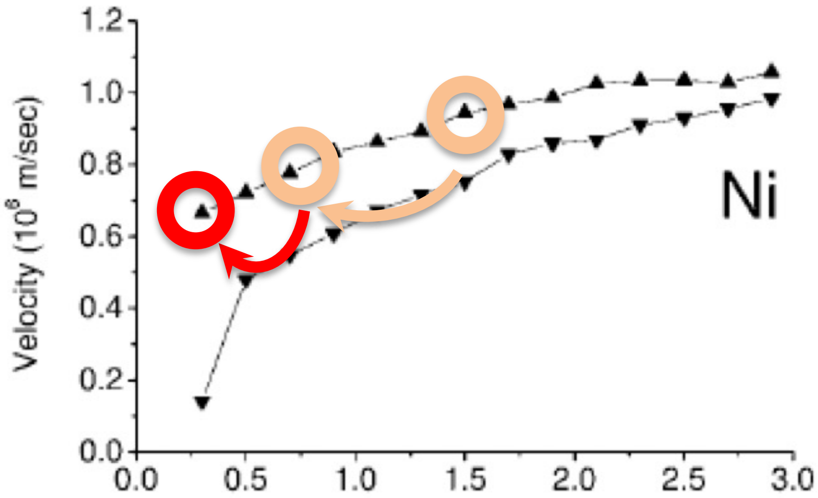
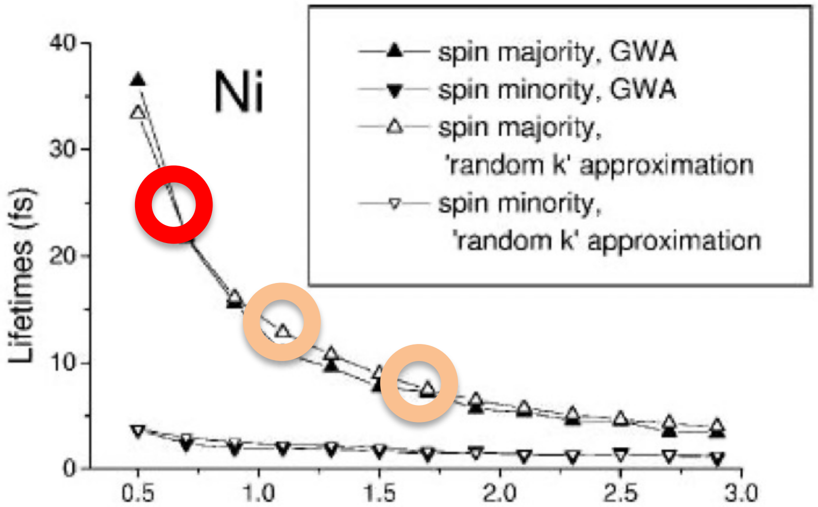


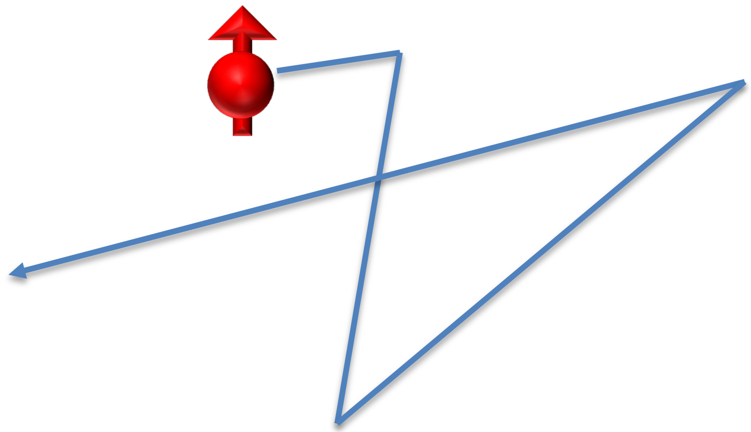




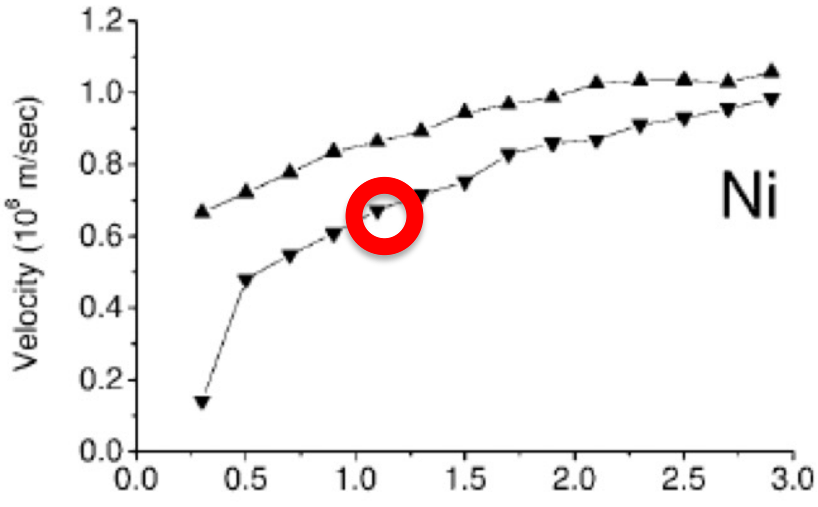
Transport out of equilibrium with spin

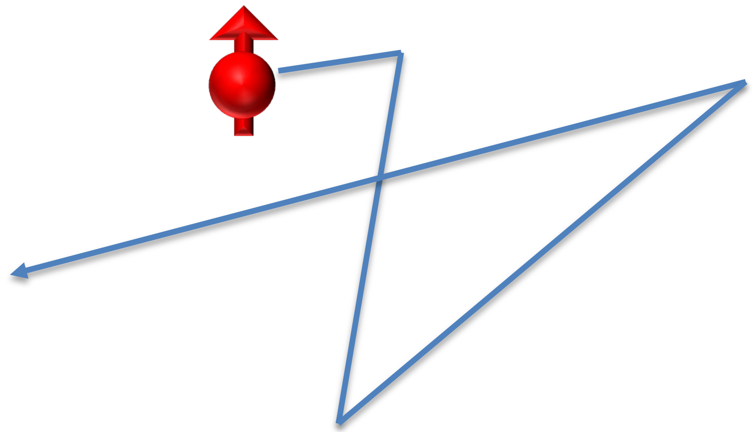




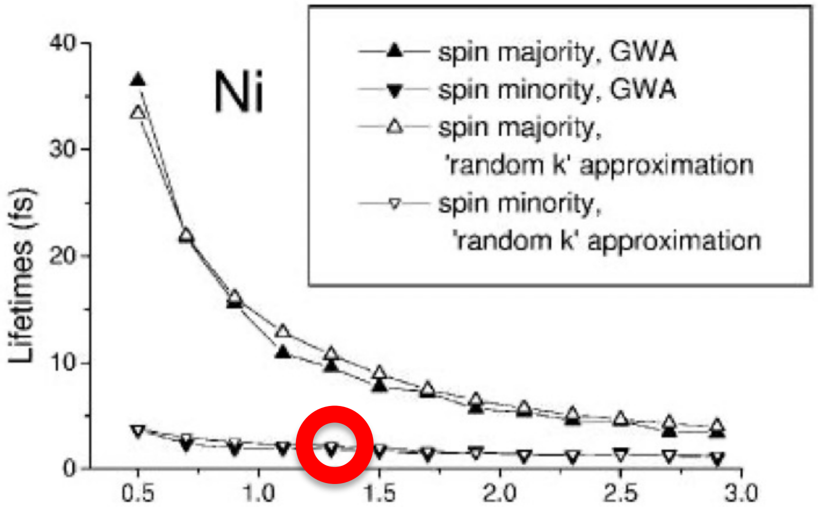


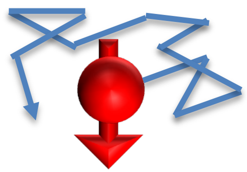
Transport out of equilibrium with spin





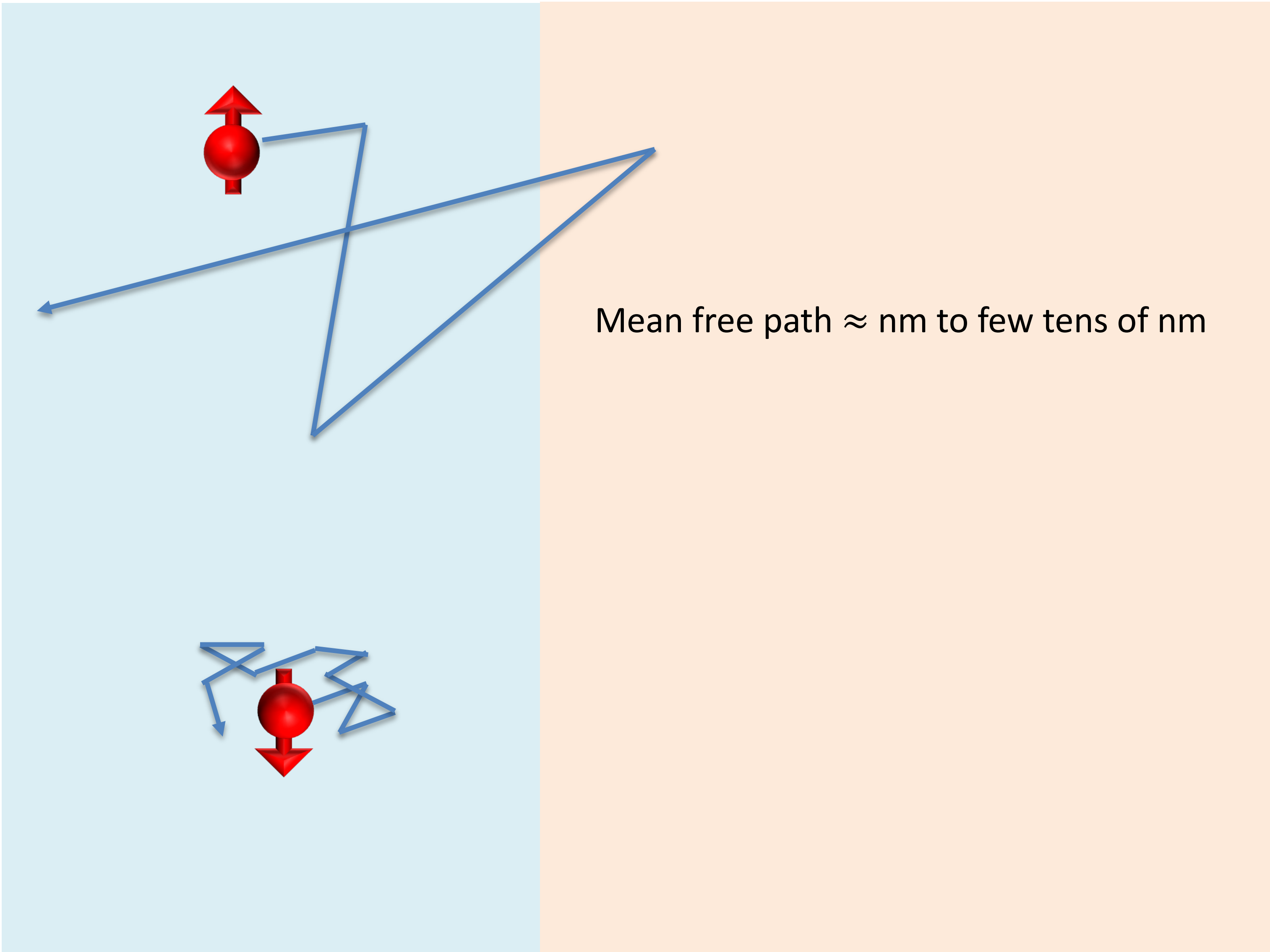
Superdiffusive regime -> efficient



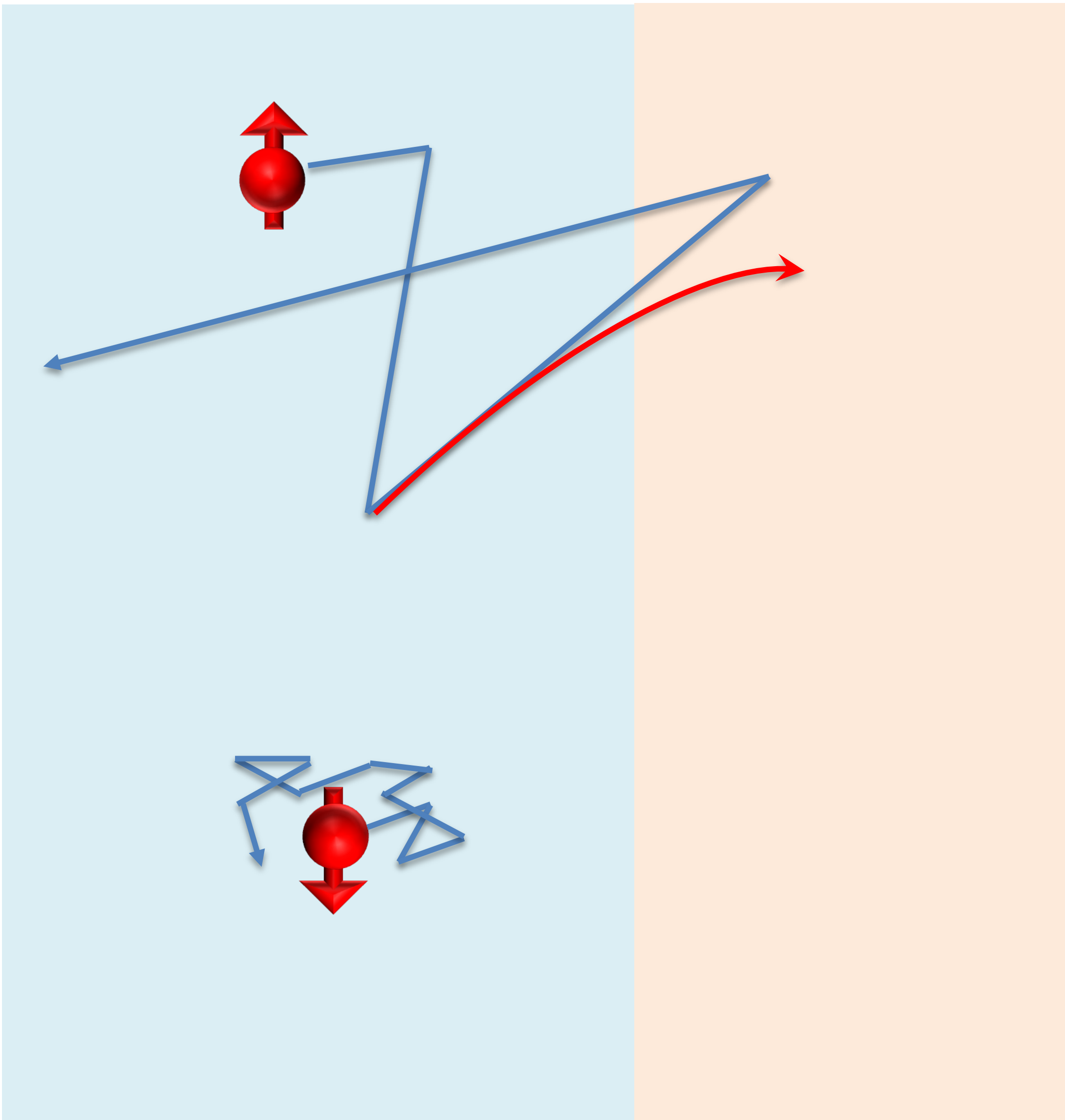


Close to the diffusive regime -> inefficient

Diffusion regimes



What about drift?



Group velocity
≈ 0.1-1 nm/fs
≈ 0.1-1 10^6 m/s

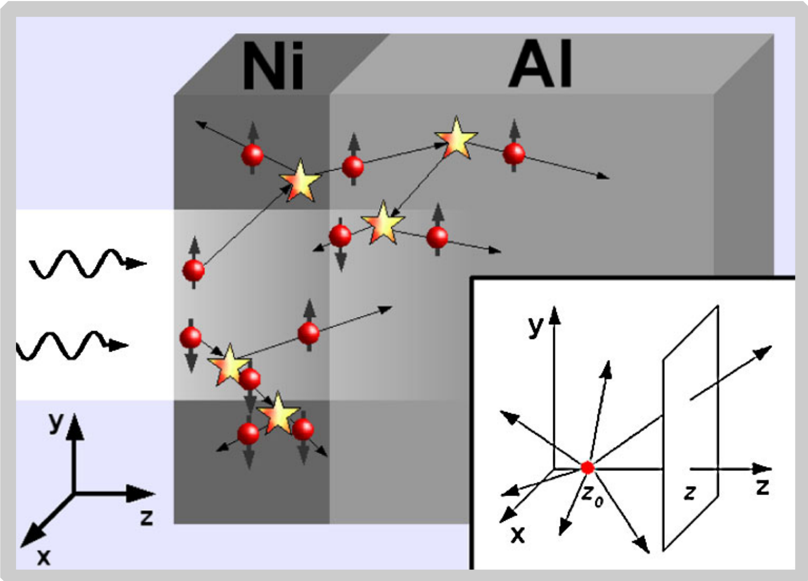
Typical mobility
≈ 10^{-3} $m^2/V\ s$

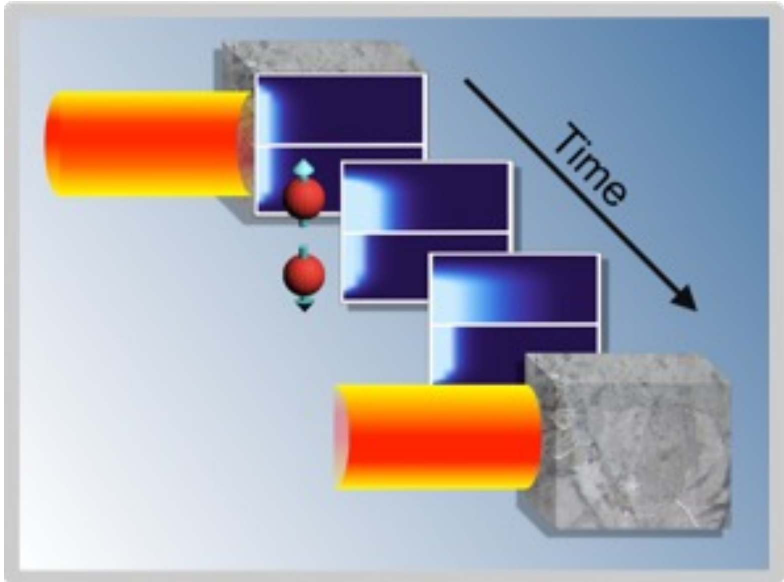
To have drift velocities comparable to group velocities we need electric fields of
≈ 0.1-1 V/nm

Marco BATTIATO

Superdiffusive spin transport

Simplistically, majority carriers diffuse more efficiently than minority carriers and therefore there is a nest spin diffusion away from the excited area.



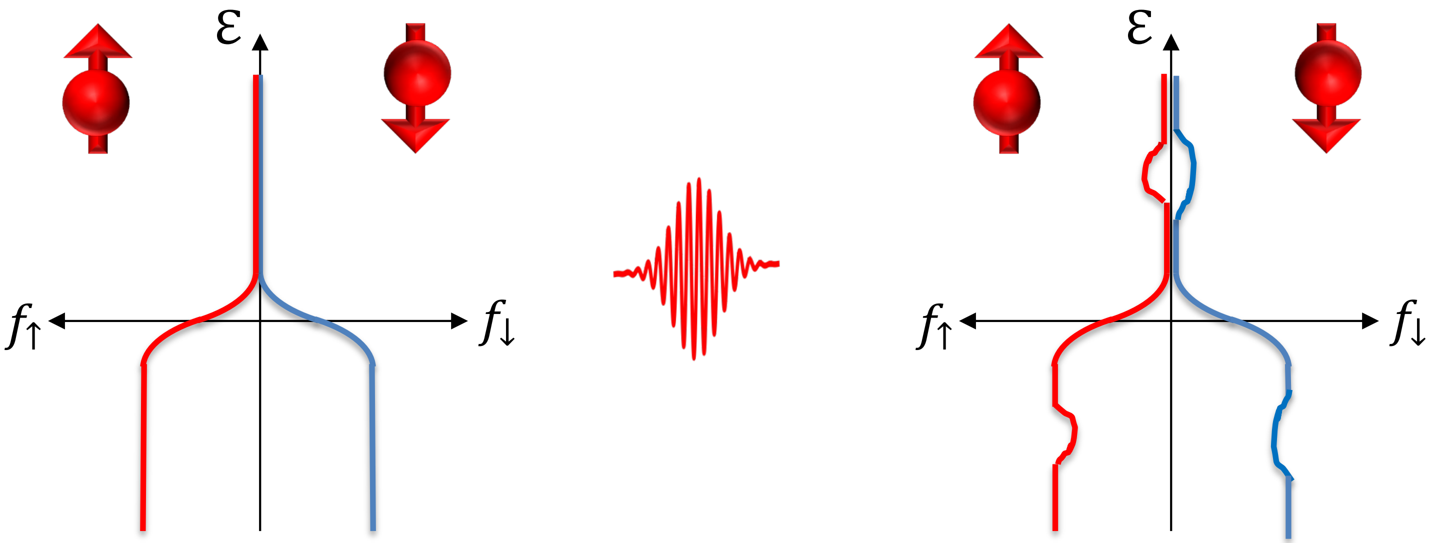


Battiato, Carva, Oppeneer, **Phys. Rev. Lett.** 105, 027203 (2010)
Battiato, Carva, Oppeneer, **Phys. Rev. B** 86, 024404 (2012)
Battiato, Maldonado, Oppeneer, **J. Appl. Phys.** 115, 172611 (2014).

Superdiffusive spin transport: energy

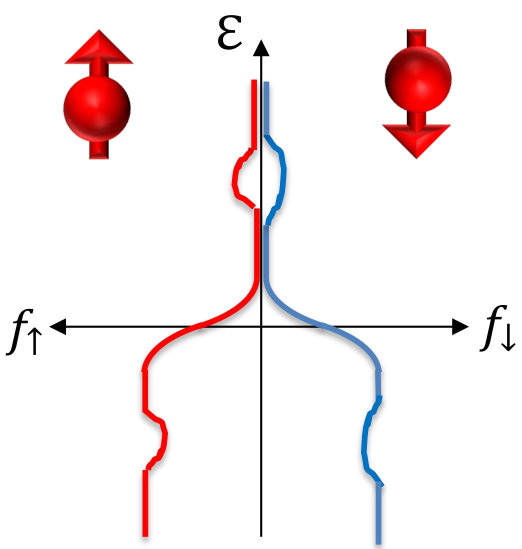
Carriers are excited at several energies (and their energy changes during thermalization).
The question is: what are the most effective energies contributing to the spin transport?

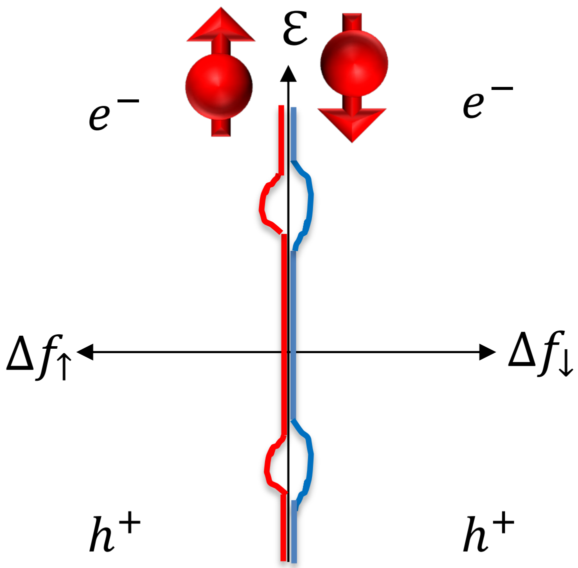
After the laser excitation, carriers in both spin channels are excited



Superdiffusive spin transport: energy

Let us display only the excitation's population (since we know that the transport of the equilibrium population integrates to zero)

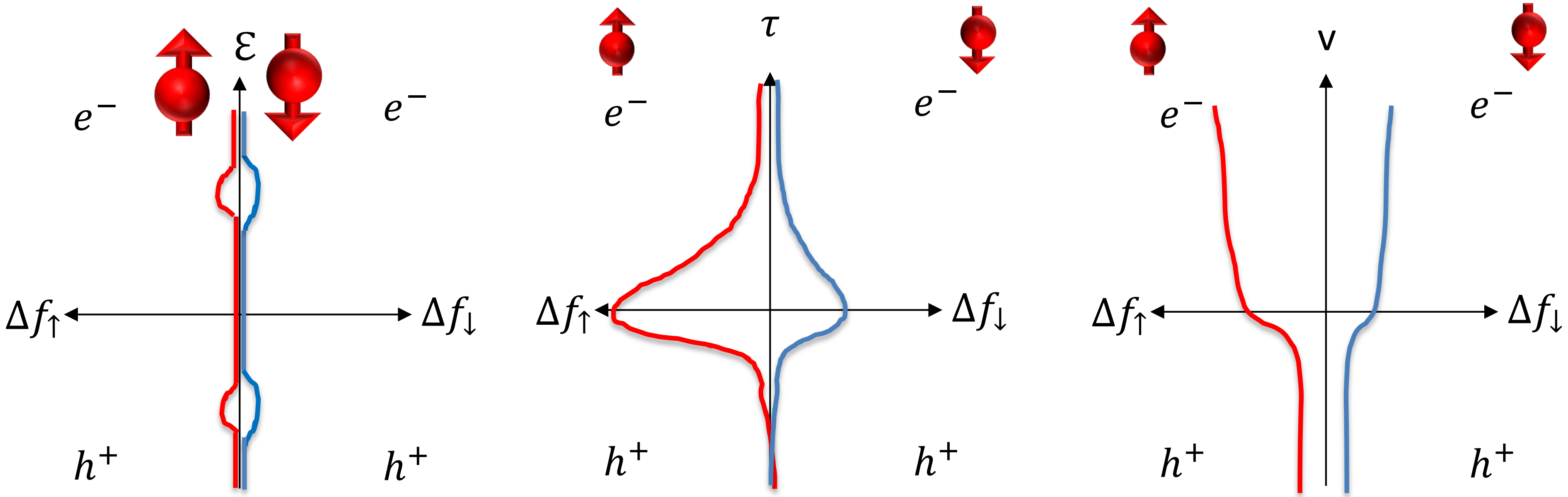




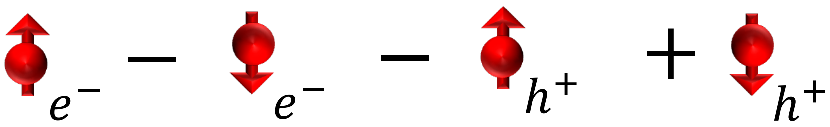
Both excited electrons and holes undergo diffusion
Careful since spin up holes carry spin down

Superdiffusive spin transport: energy

How do they behave?

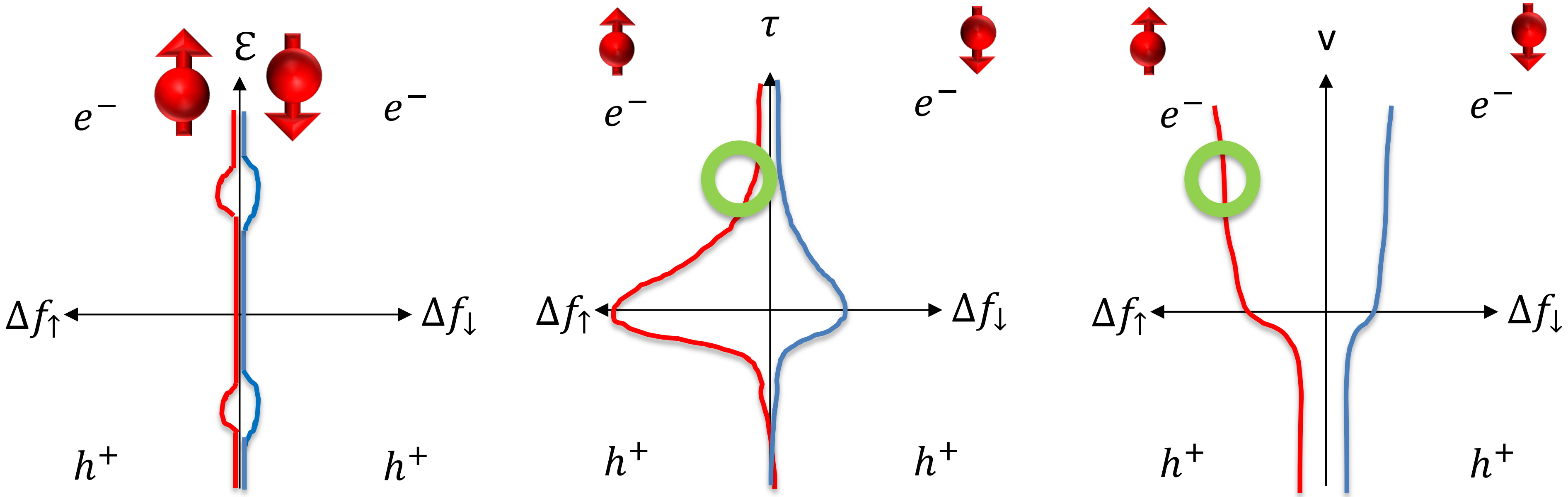


The net spin transport is



Superdiffusive spin transport: energy

How do they behave?



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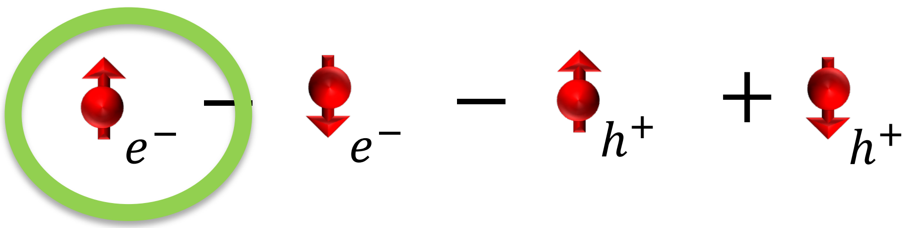
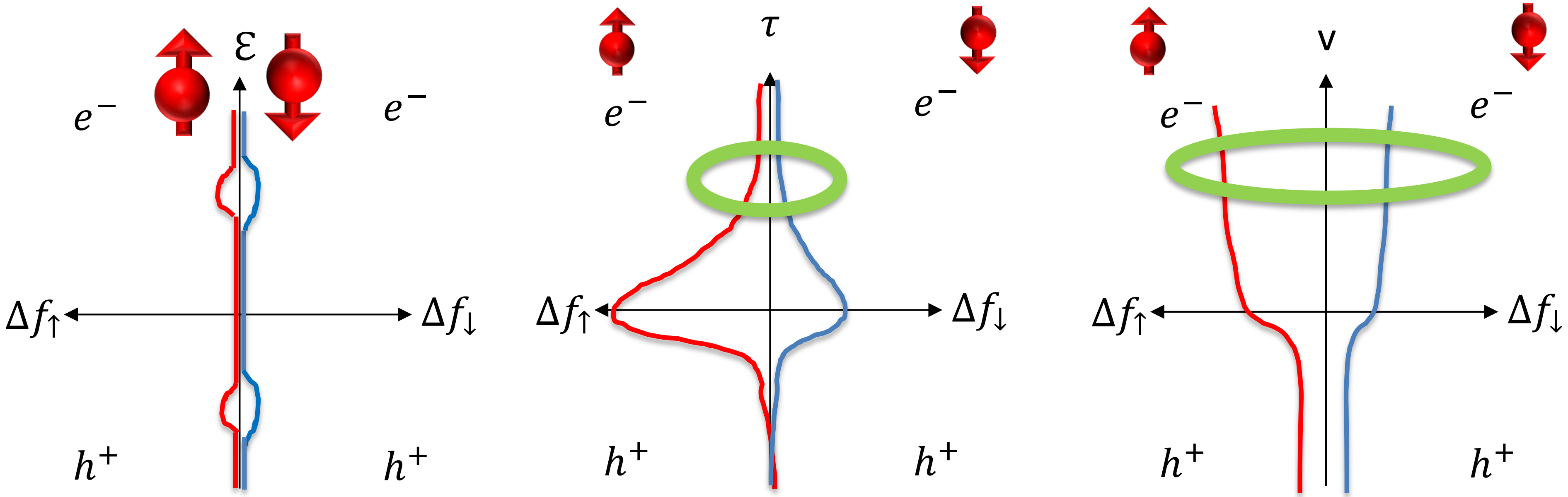


At high energy, the lifetimes are short,
- ➔ the mean free paths are short
- ➔ transport closer to standard diffusion
- ➔ inefficient transport

Superdiffusive spin transport: energy

How do they behave?

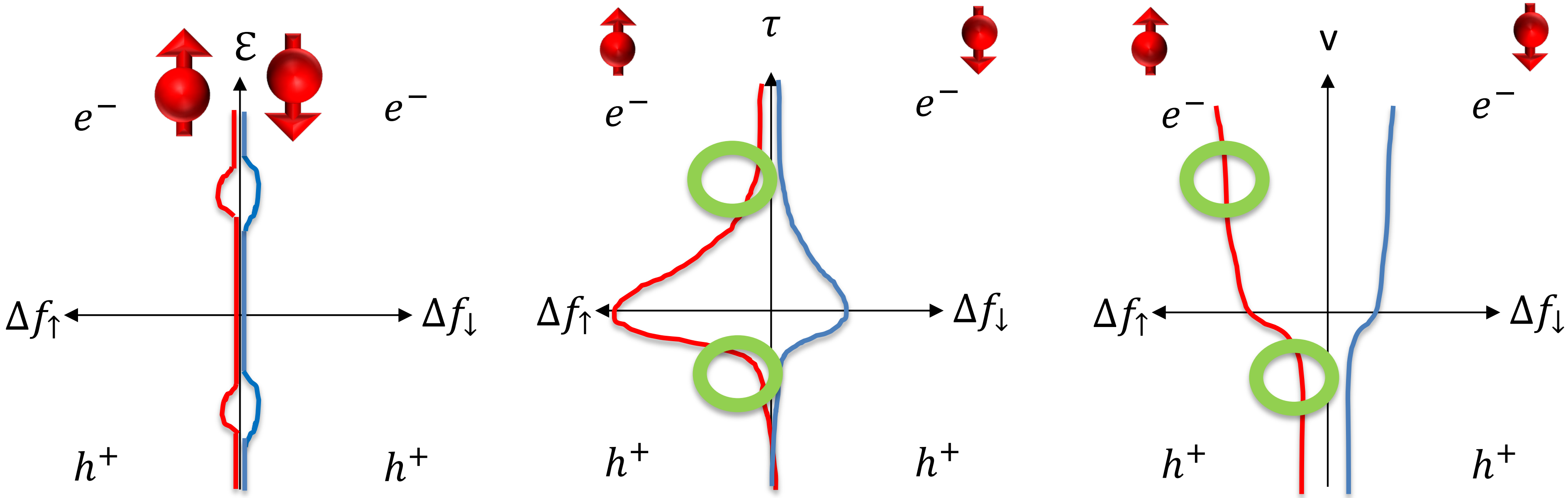


The net spin transport is

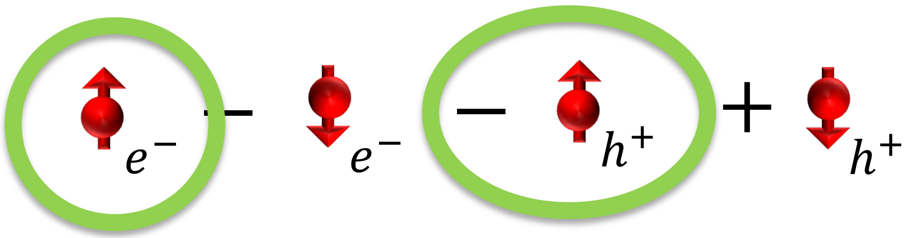
Where the maximal asymmetry is located usually depends on the ferromagnet

Superdiffusive spin transport: energy

How do they behave?



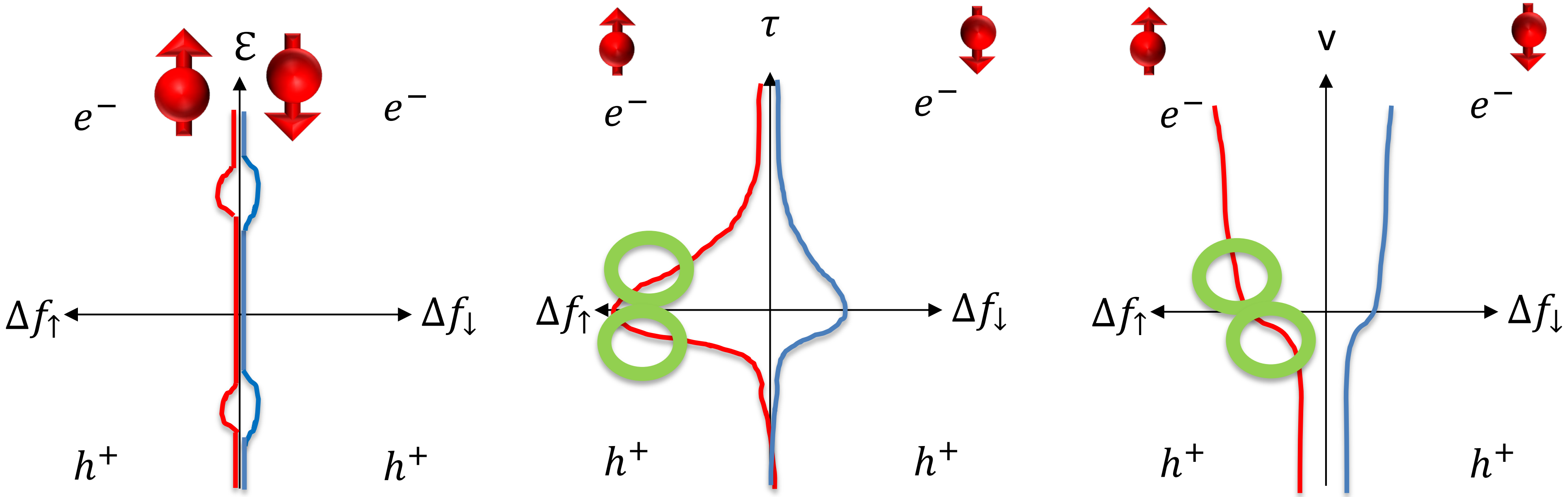
The net spin transport is



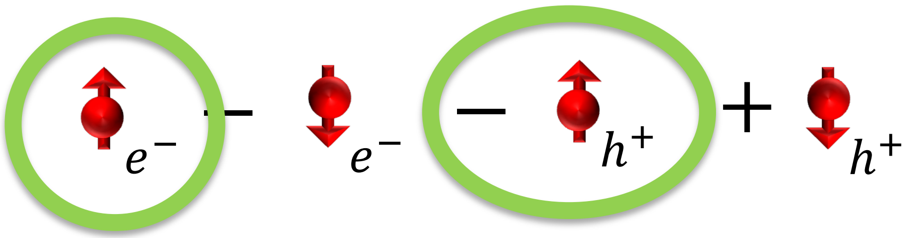
Usually holes considerably slower and/or much shorter lifetimes, except…

Superdiffusive spin transport: energy

How do they behave?

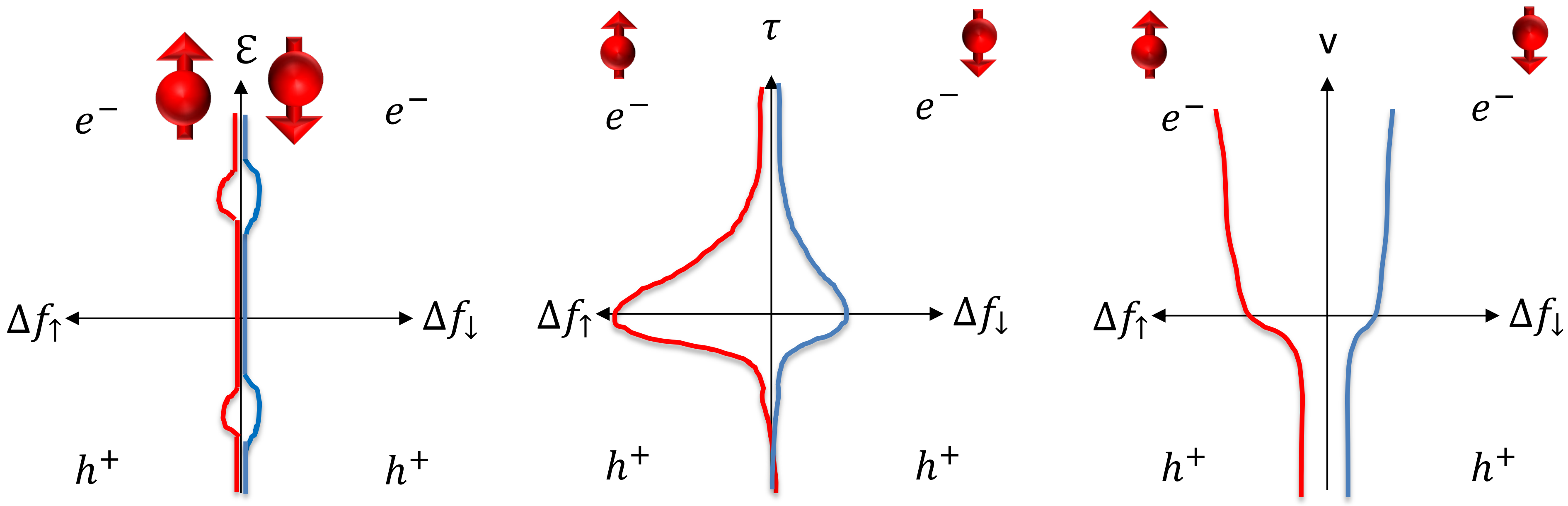


The net spin transport is



Usually holes considerably slower and/or much shorter lifetimes, except…
when both electrons and holes are close to the Fermi level, then their transport cancels

Superdiffusive spin transport: energy



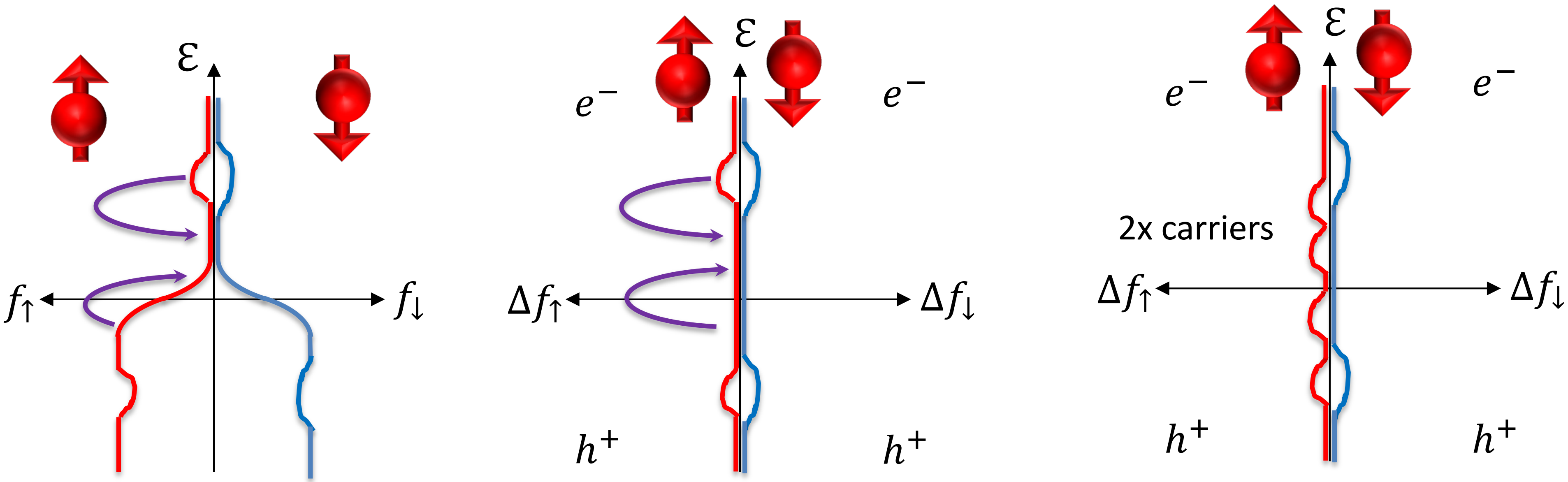
The states that contribute the most to the spin diffusion are at relatively low energies: high energies have too short lifetimes and their transport is inefficient
(Notice that only a theoretical treatment that can describe superdiffusion can account for this difference)

However, the energies should not be too low because in that case electron and hole transport cancel each other

But there is another even more important effect that gives low energies an advantage…

Superdiffusive spin transport: energy

When an excitation scatters with other electrons



Carrier multiplication

During thermalization to each photon corresponds a single high energy excitation and many low energy excitations

Meaning that relatively low energy excitations (but not too low), not only are more efficient in producing spin diffusion, but they are also much more numerous

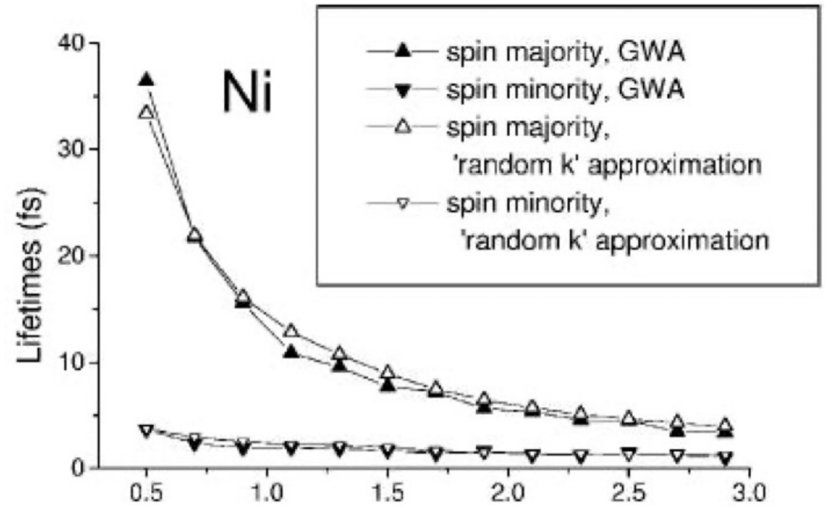
Superdiffusive spin transport: timescale

We are now in a slightly better position to estimate the timescales that are relevant to the superdiffusive spin transport.

For thermalization typically several scattering events are needed.

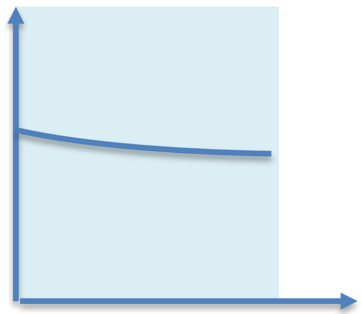
Therefore, different energies can be thought to thermalize with different speeds.

Since the most important energy scale is the low energy one, we expect the population within that energy to be different from a Fermi–Dirac for few hundreds of fs.

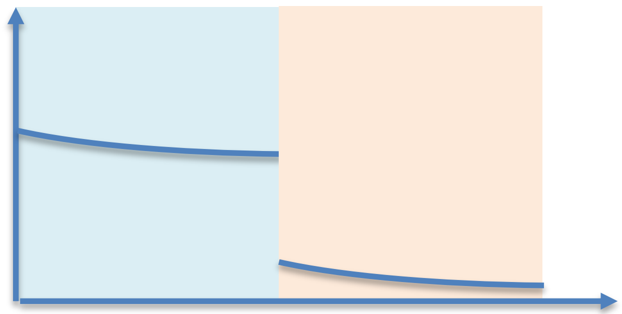


Superdiffusive spin transport: common misconceptions

What drives the directionality?



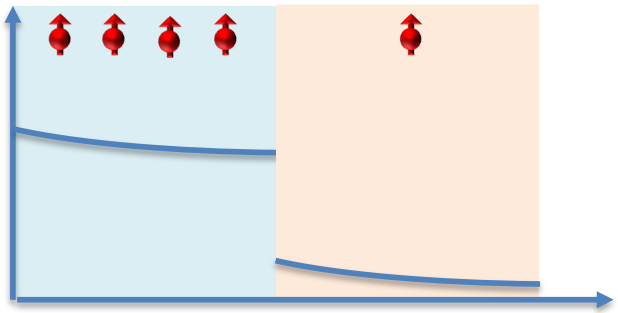
Except for very thick samples, the laser excitation profile is usually rather flat within a given layer (because of multiple reflections)



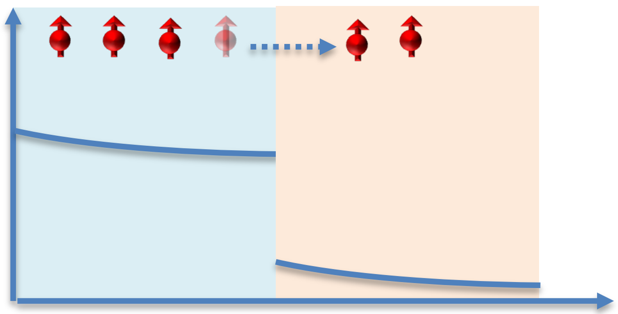
On the other hand, if there are different layers (with very different refractive indices) the absorption profile can be strongly non uniform…

However, that is way less important than what one might think at first.
Let's understand why

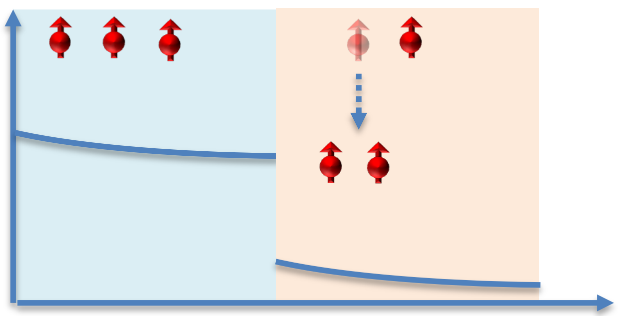
Superdiffusive spin transport: common misconceptions



The initial high energy excitation is surely very non uniform, however…



As the excitations diffuse and enter the other layer…



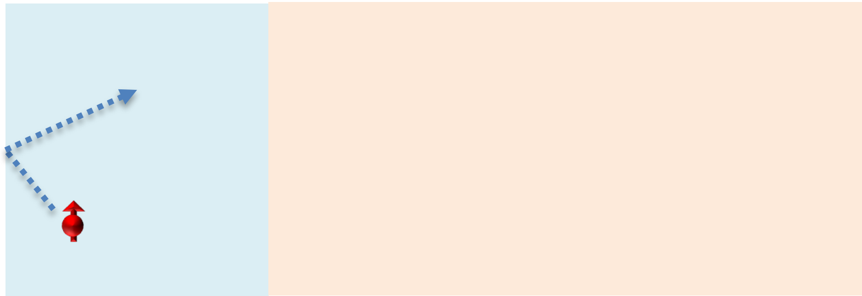
When they scatter, they act as source of lower energy carriers (which more importantly produce transport) and so on.

Secondary excitations make the excitation profile more uniform, compared to what one might think at first

Superdiffusive spin transport: directionality

Where does the directionality come from?

Interfaces with vacuum

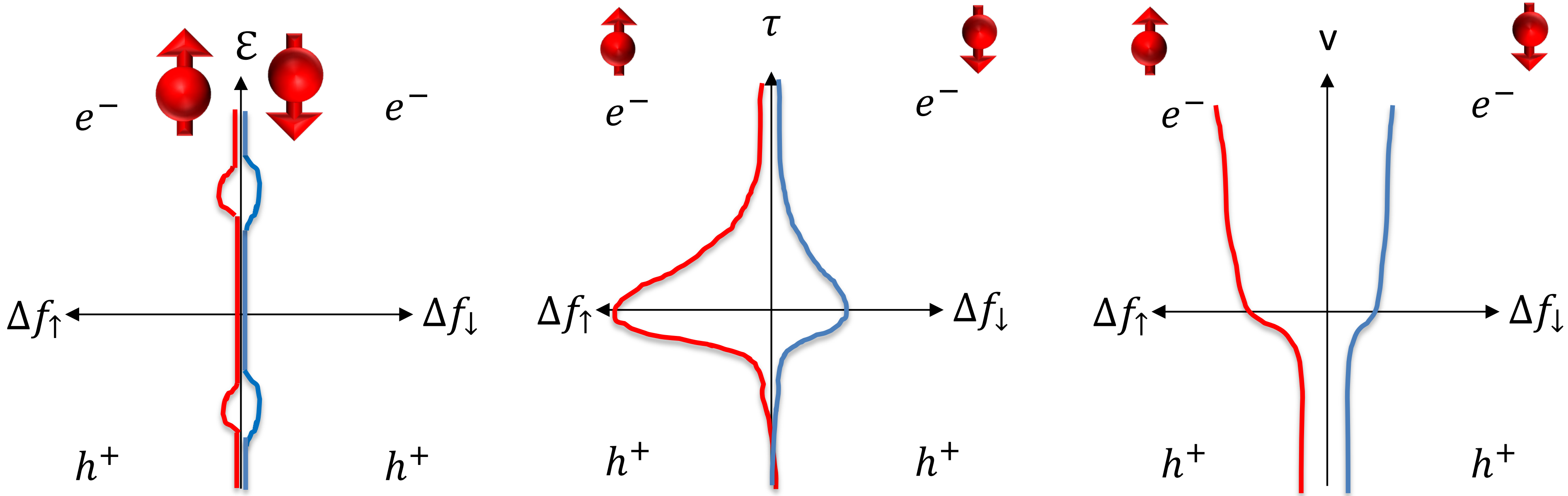


Different transport properties in different materials (differently for different spin channels)

Battiato, Carva, Oppeneer, **Phys. Rev. Lett.** 105, 027203 (2010)
Battiato, Carva, Oppeneer, **Phys. Rev. B** 86, 024404 (2012)
Battiato, Maldonado, Oppeneer, **J. Appl. Phys.** 115, 172611 (2014).

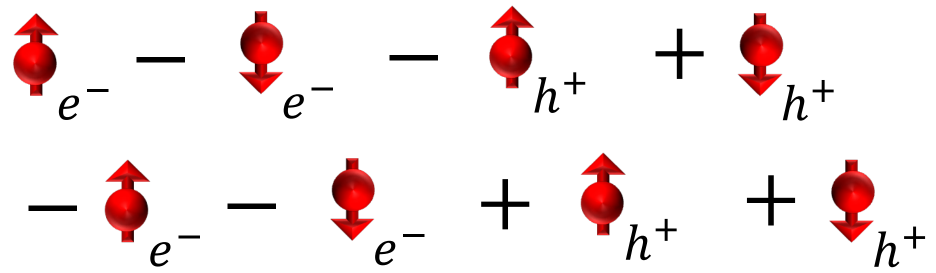
Superdiffusive spin transport: Charge current

One last important point: charge current



The net spin transport is

The net charge transport is



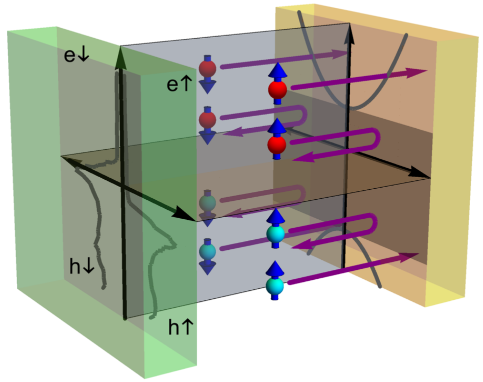
Superdiffusive spin transport: Charge current

This means that there is indeed an associated charge current

The net spin transport is $\uparrow_{e^-} - \downarrow_{e^-} - \uparrow_{h^+} + \downarrow_{h^+}$

The net charge transport is $-\uparrow_{e^-} - \downarrow_{e^-} + \uparrow_{h^+} + \downarrow_{h^+}$

It must be taken into account, since it generates electric fields that impact the transport. In metals, the carriers will try and screen the generated electric fields (and carry their spin while they move!!!)



See E. Chia's talk

To a first approximation, for low excitations, one can anyway expect that the majority of the screening is done by carriers around the Fermi energy. In most cases, this will lead to an enhancement of the spin current compared to what one might get neglecting the effect of the charge currents.

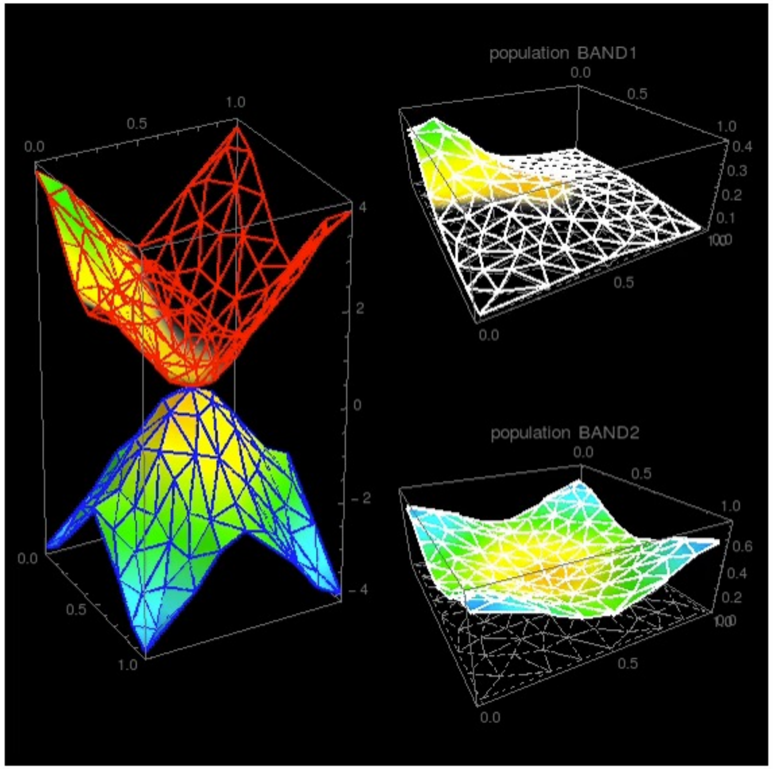
The effect becomes even more important when semiconductors are involved

Battiato, Held, **Phys. Rev. Lett.** 116, 196601 (2016).
M. Battiato, **J. Phys. Condens. Matter** 29, 174001 (2017).
Cheng, Wang, Yang, Chai, Yang, Chen, Wu, Chen, Chi, Goh, Zhu, Sun, Wang, Song, Battiato, Yang, Chia, **Nature Physics** (2019).

Boltzmann + Maxwell system

Electronic population $f_{n,\sigma}[t, \boldsymbol{x}, \boldsymbol{k}]$

Electromagnetic field $\mathbf{E}[t, \mathbf{x}]$ $\mathbf{B}[t, \mathbf{x}]$



$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}\cdot\nabla_{\mathbf{x}} f + \frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f - \left(\frac{\partial f}{\partial t}\right)_{\text{sc}} - \left(\frac{\partial f}{\partial t}\right)_{\text{ex}} = 0$$

$$\nabla\cdot\epsilon\mathbf{E} = \rho$$

$$\nabla\cdot\mathbf{B} = 0$$

$$\nabla\times\mathbf{E} = -\frac{\partial\mathbf{B}}{\partial t} \qquad \rho[t,\mathbf{x}] = -\frac{e}{(2\pi)^3}\int f[t,\mathbf{x},\mathbf{k}]d\mathbf{k}$$

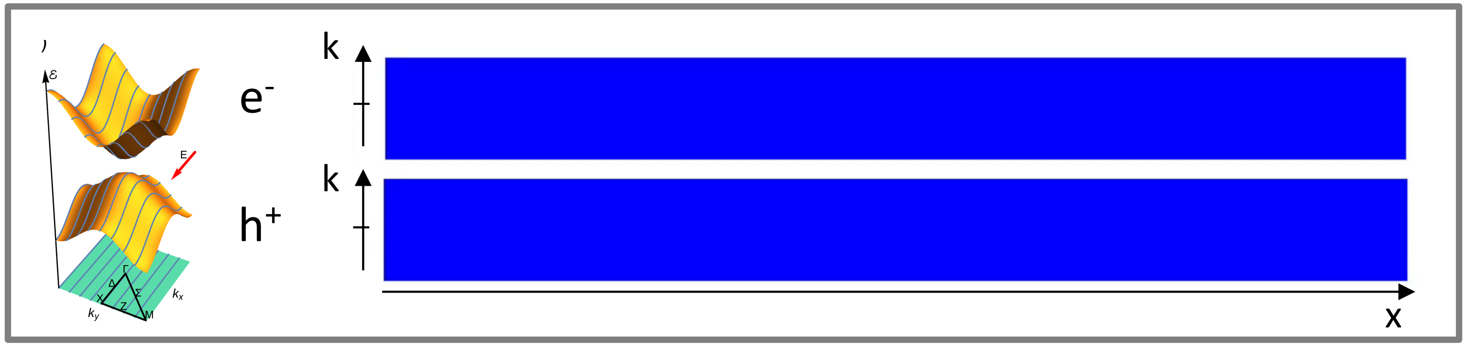
$$\nabla\times\frac{\mathbf{B}}{\mu} = \mathbf{j} + \frac{\partial\epsilon\mathbf{E}}{\partial t} \qquad \mathbf{j}[t,\mathbf{x}] = -\frac{e}{(2\pi)^3\hbar}\int\frac{\partial\mathcal{E}}{\partial\mathbf{k}} f[t,\mathbf{x},\mathbf{k}]d\mathbf{k}$$

Boltzmann equation

$$\frac{\partial f}{\partial t} + \boxed{\frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}\cdot\nabla_{\mathbf{x}}f + \frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}f} - \left(\frac{\partial f}{\partial t}\right)_{\mathrm{sc}} - \left(\frac{\partial f}{\partial t}\right)_{\mathrm{ex}} = 0$$

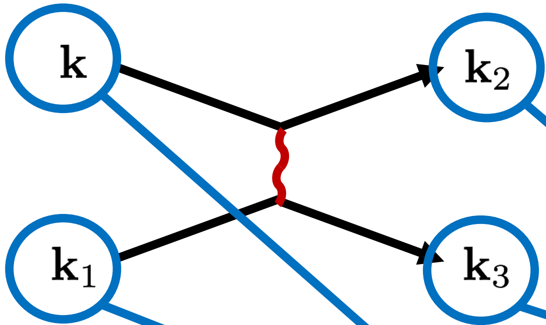
1+1+3 dimensional problem: not cheap, but can be handled

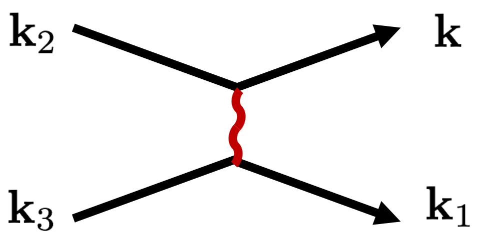
Runge Kutta Discontinuous Galerkin
- Unstructured meshes
- Arbitrarily high order of convergence (depending on max polynomial power)
- Mass, energy and momentum conserving
- High stability in presence of shocks



Boltzmann equation

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}\cdot\nabla_{\mathbf{x}} f + \frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f - \left(\frac{\partial f}{\partial t}\right)_{\mathrm{sc}} - \left(\frac{\partial f}{\partial t}\right)_{\mathrm{ex}} = 0$$





$$\left(\frac{\partial f}{\partial t}\right)_{col}(t,\mathbf{x},\mathbf{k}) =$$

$$\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3\, W(\mathbf{x},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\left[(1-f(t,\mathbf{x},\mathbf{k}))(1-f(t,\mathbf{x},\mathbf{k}_1))f(t,\mathbf{x},\mathbf{k}_2)f(t,\mathbf{x},\mathbf{k}_3)+\right.$$

$$\left.-f(t,\mathbf{x},\mathbf{k})f(t,\mathbf{x},\mathbf{k}_1)(1-f(t,\mathbf{x},\mathbf{k}_2))(1-f(t,\mathbf{x},\mathbf{k}_3))\right]$$

$$W(\mathbf{x},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3) =$$

$$= \sum_{\mathbf{G}} w(\mathbf{x},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\,\delta(\mathbf{k}+\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3+\mathbf{G})\,\delta(\mathcal{E}(\mathbf{k})+\mathcal{E}(\mathbf{k}_1)-\mathcal{E}(\mathbf{k}_2)-\mathcal{E}(\mathbf{k}_3))$$

k-conservation (umklapp)

energy-conservation

Scattering term

$$S_{ijklm} = \sum_{\mathbf{G}} \int d\mathbf{k} d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$

$$\Big(w(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \cdot$$

$$\delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 + \mathbf{G})\ \delta(\mathcal{E}(\mathbf{k}) + \mathcal{E}(\mathbf{k}_1) - \mathcal{E}(\mathbf{k}_2) - \mathcal{E}(\mathbf{k}_3)) \cdot$$

$$b_i(\mathbf{k}) b_j(\mathbf{k}) b_k(\mathbf{k}_1) b_l(\mathbf{k}_2) b_m(\mathbf{k}_3) \Big)$$

Scattering term

$$S_{ijklm} = \sum_{\mathbf{G}} \int d\mathbf{k} d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$
$$\Big(w(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \cdot$$
$$\delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 + \mathbf{G})\ \delta(\mathcal{E}(\mathbf{k}) + \mathcal{E}(\mathbf{k}_1) - \mathcal{E}(\mathbf{k}_2) - \mathcal{E}(\mathbf{k}_3)) \cdot$$
$$b_i(\mathbf{k}) b_j(\mathbf{k}) b_k(\mathbf{k}_1) b_l(\mathbf{k}_2) b_m(\mathbf{k}_3) \Big)$$

- 5 dimensional tensor: number of entries is N^5
  (400 basis functions -> 10^{13} integrals to calculate and 10TB to load in memory)

Scattering term

$$S_{ijklm} = \sum_{\mathbf{G}} \int \boxed{d\mathbf{k} d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3} \Big(w(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \cdot \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 + \mathbf{G}) \, \delta(\mathcal{E}(\mathbf{k}) + \mathcal{E}(\mathbf{k}_1) - \mathcal{E}(\mathbf{k}_2) - \mathcal{E}(\mathbf{k}_3)) \cdot b_i(\mathbf{k}) b_j(\mathbf{k}) b_k(\mathbf{k}_1) b_l(\mathbf{k}_2) b_m(\mathbf{k}_3) \Big)$$

- 5 dimensional tensor: number of entries is N^5
  (400 basis functions -> 10^{13} integrals to calculate and 10TB to load in memory)
- 12 dimensional integral

Scattering term

$$S_{ijklm} = \sum_{\mathbf{G}} \int d\mathbf{k} d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$

$$\Big(w(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \cdot$$

$$\delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 + \mathbf{G}) \, \delta(\mathcal{E}(\mathbf{k}) + \mathcal{E}(\mathbf{k}_1) - \mathcal{E}(\mathbf{k}_2) - \mathcal{E}(\mathbf{k}_3)) \cdot$$

$$b_i(\mathbf{k}) b_j(\mathbf{k}) b_k(\mathbf{k}_1) b_l(\mathbf{k}_2) b_m(\mathbf{k}_3) \Big)$$

- 5 dimensional tensor: number of entries is N^5
  (400 basis functions -> 10^{13} integrals to calculate and 10TB to load in memory)
- 12 dimensional integral
- Dirac deltas inside the integral

Scattering term

$$S_{ijklm} = \sum_{\mathbf{G}} \int d\mathbf{k} d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3$$
$$\Big(w(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \cdot$$
$$\delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3 + \mathbf{G}) \; \delta(\mathcal{E}(\mathbf{k}) + \mathcal{E}(\mathbf{k}_1) - \mathcal{E}(\mathbf{k}_2) - \mathcal{E}(\mathbf{k}_3)) \cdot$$
$$b_i(\mathbf{k}) b_j(\mathbf{k}) b_k(\mathbf{k}_1) b_l(\mathbf{k}_2) b_m(\mathbf{k}_3) \Big)$$

- 5 dimensional tensor: number of entries is N^5
  (400 basis functions -> 10^{13} integrals to calculate and 10TB to load in memory)
- 12 dimensional integral
- Dirac deltas inside the integral
- Failure to integrate to extreme precision leads to breaking of particle, energy and momentum conservation

Scattering term

Usually used approaches to bypass the problem

$$\left(\frac{\partial f}{\partial t}\right)_{col}(t,\mathbf{x},\mathbf{k}) =$$

$$\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3\, W(\mathbf{x},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\big[\,(1-f(t,\mathbf{x},\mathbf{k}))\,\cancel{(1-f(t,\mathbf{x},\mathbf{k}_1))}\,f(t,\mathbf{x},\mathbf{k}_2)\cancel{f(t,\mathbf{x},\mathbf{k}_3)}+$$

$$-\,f(t,\mathbf{x},\mathbf{k})\cancel{f(t,\mathbf{x},\mathbf{k}_1)}\,(1-f(t,\mathbf{x},\mathbf{k}_2))\,\cancel{(1-f(t,\mathbf{x},\mathbf{k}_3))}\,\big]$$

- Only electron-phonon scatterings included (phonons treated as bath)

Scattering term

Usually used approaches to bypass the problem

$$\left(\frac{\partial f}{\partial t}\right)_{col}(t,\mathbf{x},\mathbf{k}) =$$

$$\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3\, W(\mathbf{x},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\big[\,(1-f(t,\mathbf{x},\mathbf{k}))\,(1-f(t,\mathbf{x},\mathbf{k}_1))\,f(t,\mathbf{x},\mathbf{k}_2)f(t,\mathbf{x},\mathbf{k}_3)+$$

$$-\,f(t,\mathbf{x},\mathbf{k})\,f(t,\mathbf{x},\mathbf{k}_1)\,(1-f(t,\mathbf{x},\mathbf{k}_2))\,(1-f(t,\mathbf{x},\mathbf{k}_3))\big]$$

- Only electron-phonon scatterings included (phonons treated as bath)
- Close to equilibrium approximation

Scattering term

Usually used approaches to bypass the problem

$$\left(\frac{\partial f}{\partial t}\right)_{col}(t,\mathbf{x},\mathbf{k}) =$$

$$\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3\, W(\mathbf{x},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\Big[\,(1-f(t,\mathbf{x},\mathbf{k}))\,(1-f(t,\mathbf{x},\mathbf{k}_1))\,f(t,\mathbf{x},\mathbf{k}_2)f(t,\mathbf{x},\mathbf{k}_3)+$$
$$-\,f(t,\mathbf{x},\mathbf{k})f(t,\mathbf{x},\mathbf{k}_1)\,(1-f(t,\mathbf{x},\mathbf{k}_2))\,(1-f(t,\mathbf{x},\mathbf{k}_3))\,\Big]$$

- Only electron-phonon scatterings included (phonons treated as bath)
- Close to equilibrium approximation
- Low (electron or hole) population

Scattering term

Usually used approaches to bypass the problem

$$\left(\frac{\partial f}{\partial t}\right)_{col}(t,\mathbf{x},\mathbf{k}) =$$

$$\int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3\, W(\mathbf{x},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)\Big[\,(1-f(t,\mathbf{x},\mathbf{k}))\,(1-f(t,\mathbf{x},\mathbf{k}_1))\,f(t,\mathbf{x},\mathbf{k}_2)f(t,\mathbf{x},\mathbf{k}_3)+$$
$$-\,f(t,\mathbf{x},\mathbf{k})f(t,\mathbf{x},\mathbf{k}_1)\,(1-f(t,\mathbf{x},\mathbf{k}_2))\,(1-f(t,\mathbf{x},\mathbf{k}_3))\,\Big]$$

- Only electron-phonon scatterings included (phonons treated as bath)
- Close to equilibrium approximation
- Low (electron or hole) population
- Relaxation time approximation

Strongly out-of-equilibrium thermalisation and transport

Wais, Held, Battiato, Comput. Phys. Commun. 264, 107877 (2021)
Wadgaonkar, Jain, Battiato, Comput. Phys. Commun 263, 107863 (2021)
Wadgaonkar, Wais, Battiato, Comput. Phys. Commun 271, 108207 (2021)

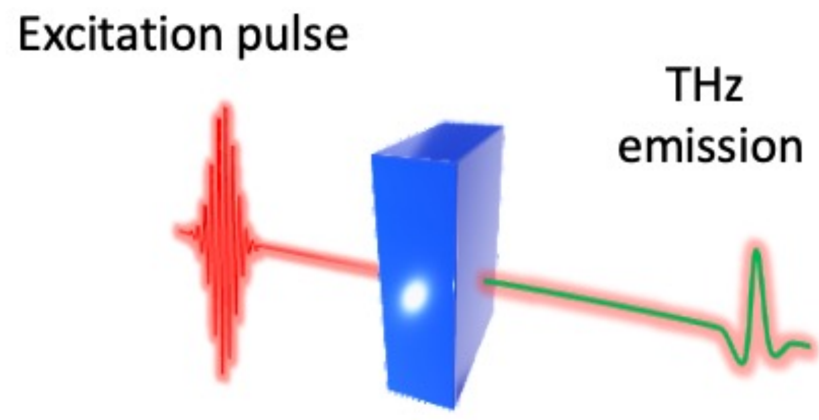
Boltzmann equation

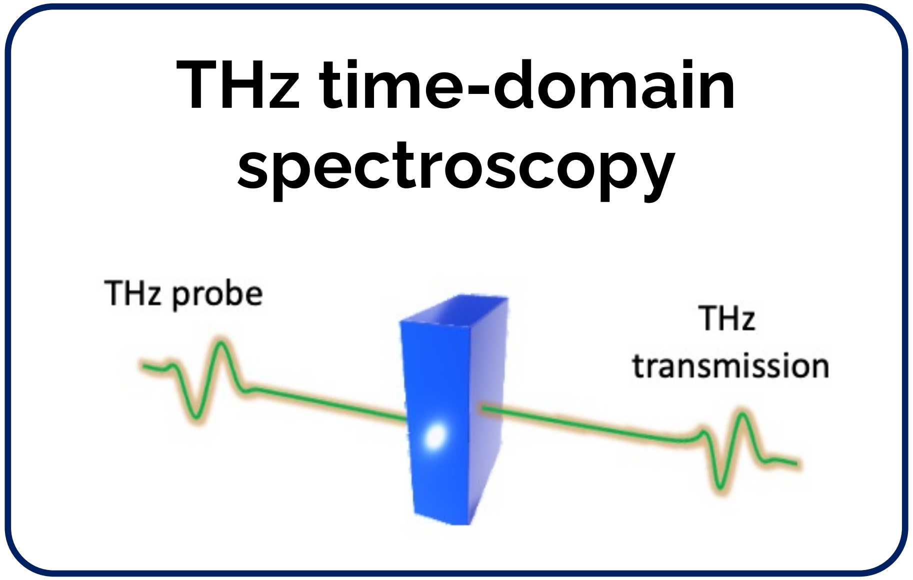
$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar}\nabla_k \mathcal{E} \cdot \nabla_x f - \frac{e}{\hbar} E \cdot \nabla_k f + \left(\frac{df}{dt}\right)_{scatt}$$

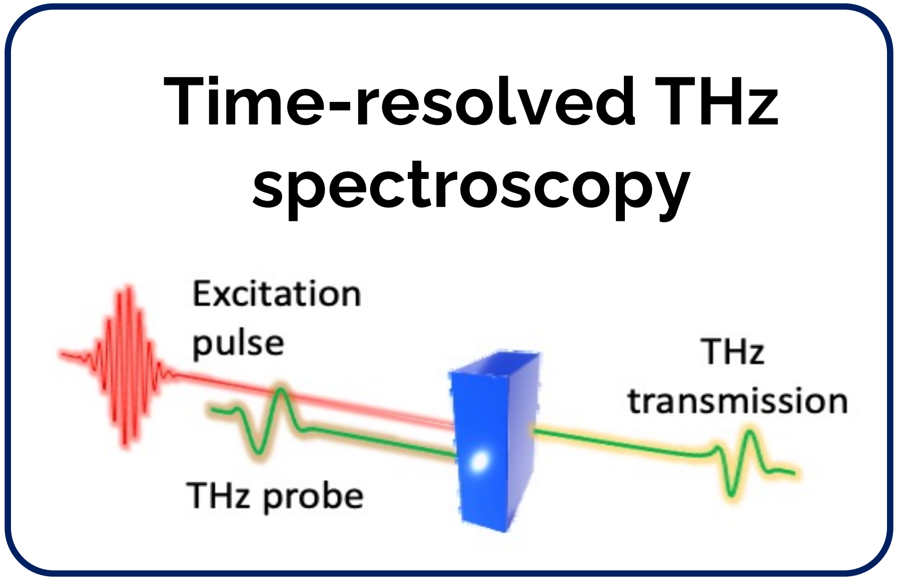
- No close to equilibrium assumptions
- No fixed population assumptions
- Any number of quasiparticles and bands
- Arbitrary dispersion (dispersion as input)
- Any number of scattering channels
- Scattering channels with 2, 3, and 4 legs (soon >4)
- Arbitrary scattering amplitude (required as input)
- Excellent scaling with precision
- Exact conservation of particle, energy and momentum

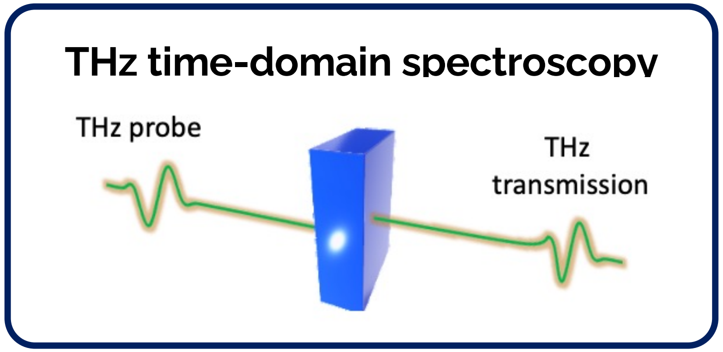
C++ library

THz from and through excited materials



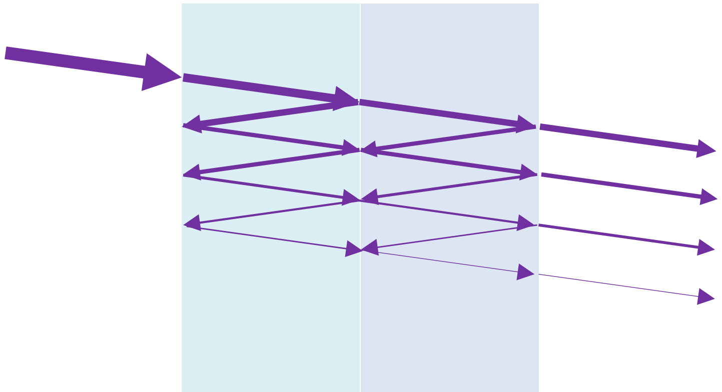






THz through non exited multilayers

Transfer Matrix Method (TMM)



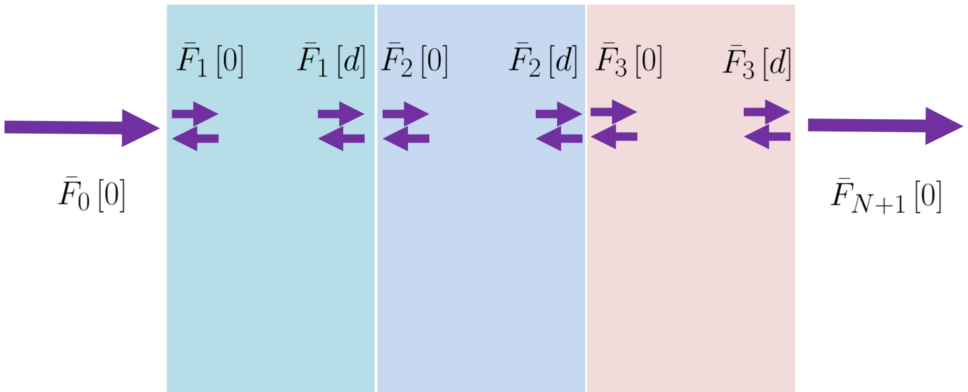
$$\partial_z E\,[z,t] = \mu\,\partial_t H\,[z,t]$$

$$\partial_z H\,[z,t] = \epsilon\,\partial_t E\,[z,t]$$

Maxwell's equations

$$E[z,t] = f^{>}[t]e^{ikz} + f^{<}[t]e^{-ikz}$$

$$H[z,t] = \sqrt{\frac{\epsilon}{\mu}} f^{>}[t]e^{ikz} - \sqrt{\frac{\epsilon}{\mu}} f^{<}[t]e^{-ikz}$$



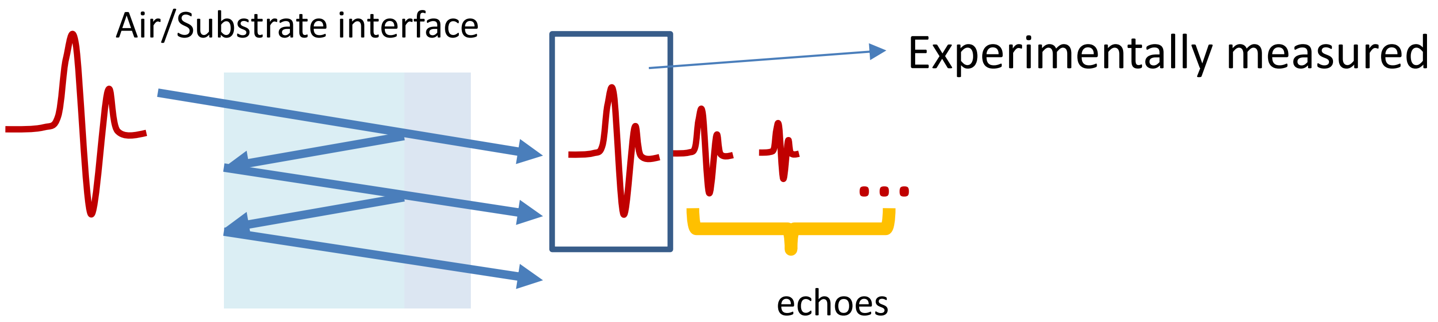
$$\bar{F}\,[\omega,z] = a[\omega,z]\bar{f}\,[\omega]$$

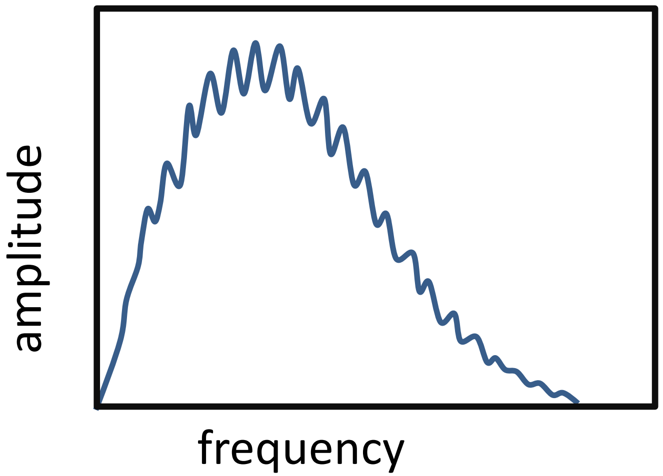
$$\bar{f}_{N+1} = (a_{N+1}[0])^{-1}\left(\prod_{j=N}^{1} M_j[d_j]\right) a_0[0]\bar{f}_0 = T_{[0,N+1]}\bar{f}_0$$

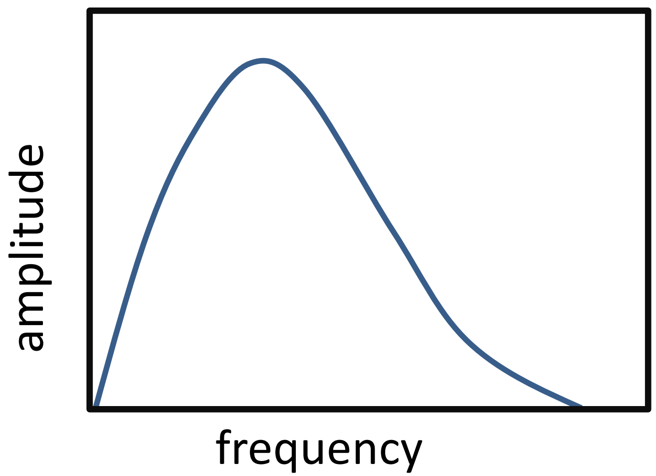
$$\begin{bmatrix} f^{>}_{N+1} \\ 0 \end{bmatrix} = T_{[0,N+1]} \begin{bmatrix} f^{>}_0 \\ f^{<}_0 \end{bmatrix}$$

An annoying issue: echo

Y Yang, S Dal Forno, M Battiato, J Infr Millim, 42 1142 (2021)

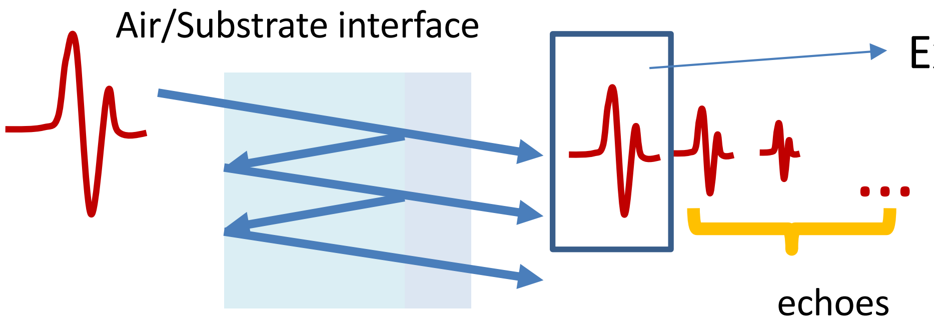






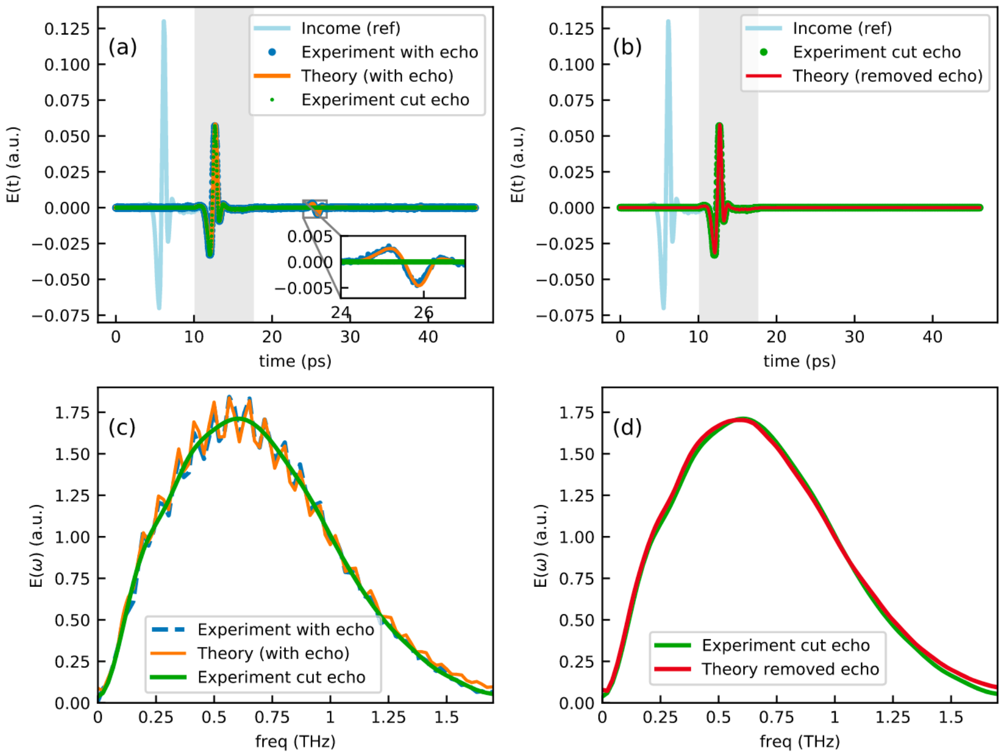
An annoying issue: echo

Y Yang, S Dal Forno, M Battiato, J Infr Millim, 42 1142 (2021)

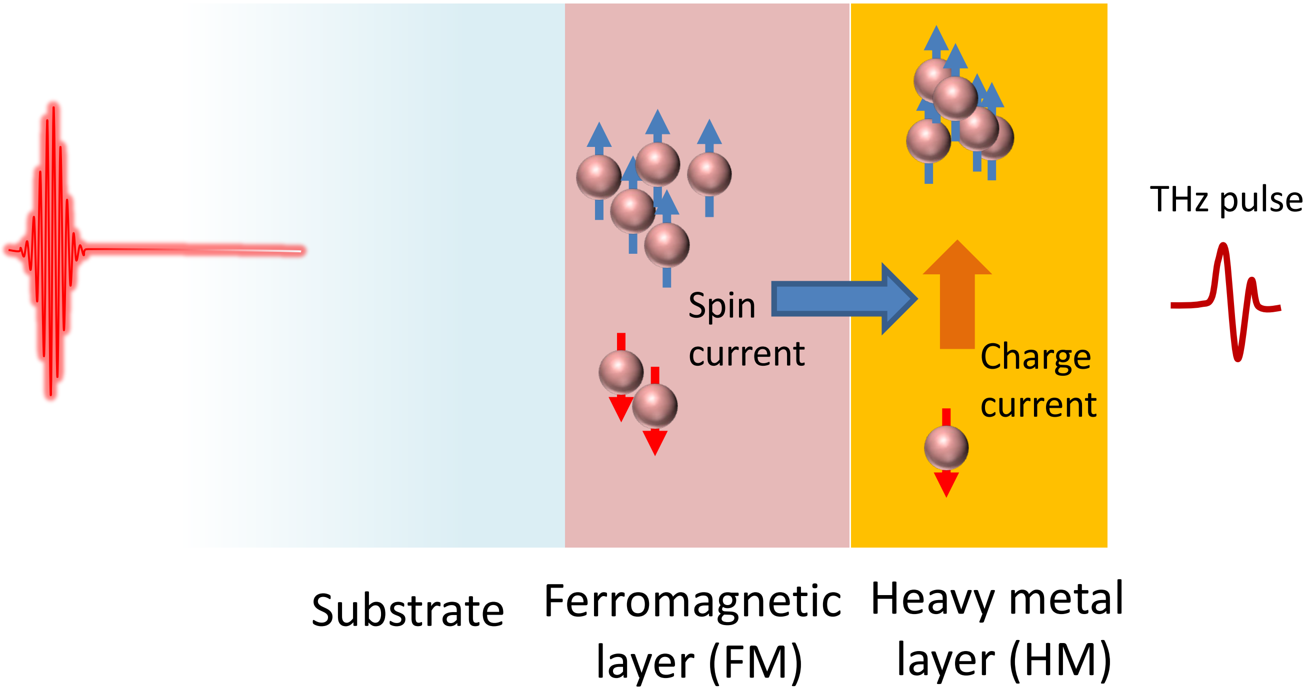


$$\begin{bmatrix} f_{N+1}^{>\text{no echo}} \\ 0 \end{bmatrix} = T_{[S,N+1]} \begin{bmatrix} f_S^{>*} \\ f_S^{<*} \end{bmatrix} = T_{[S,N+1]} \begin{bmatrix} t_{[0,S]} f_0^{>} \\ f_S^{<*} \end{bmatrix}$$

$$f_S^{>*} = t_{[0,S]} f_0^{>} \qquad f_{N+1}^{>\text{no echo}} = t_{[0,S]} t_{[S,N+1]} f_0^{>} .$$



Modelling of spintronics THz emitters



Stage1: Sample excitation

Stage2: Spin current generation

Stage3: Spin current injection to HM

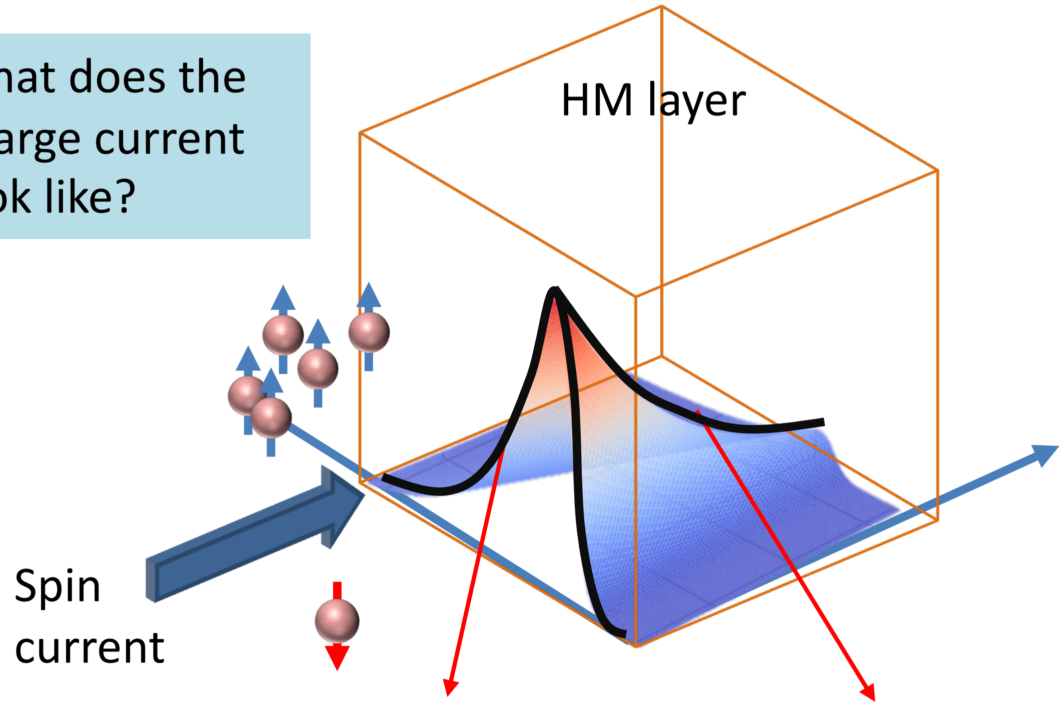
Stage4: Spin to charge conversion

Stage5: THz emission from charge current

Stage6: THz propagation through the multilayer

Modelling of spintronics THz emitters

What does the charge current look like?

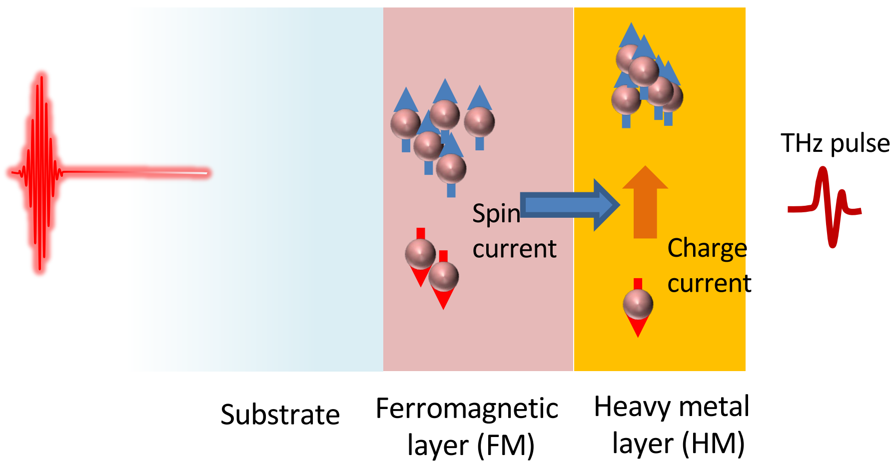


Temporal profile: Charge current generation in time

Spatial profile: Charge current distribution along the HM layer

Modelling of spintronics THz emitters

Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437



Stage1: Sample excitation

Stage2: Spin current generation

Stage3: Spin current injection to HM

Stage4: Spin to charge conversion

Stage5: THz emission from charge current

Stage6: THz propagation through the multilayer

A. Pump laser absorption profile

$$Q_{\text{loss}} = -\int_{-\infty}^{+\infty} \mathrm{d}t \oint_S (\mathbf{E} \times \mathbf{H}) \cdot \mathrm{d}\boldsymbol{S}.$$

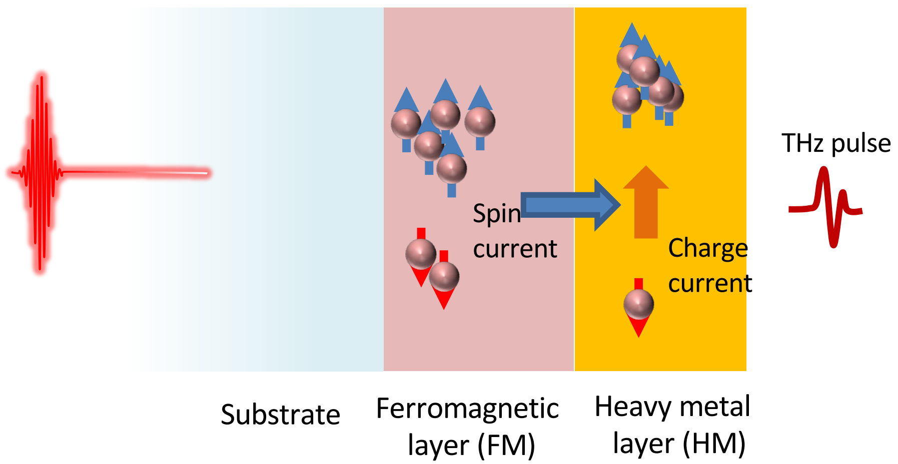
$$\Phi(z) = -\int_{-\infty}^{+\infty} E[t, z]H[t, z]\mathrm{d}t,$$

$$A_{\text{layer}} = \frac{Q_{\text{loss}}}{Q_{in}} = \frac{\Phi(z_0) - \Phi(z_0 + d)}{Q_{in}},$$

$$D(z) = -\frac{d(\Phi(z)/Q_{in})}{dz}.$$

Modelling of spintronics THz emitters

Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437



Stage1: Sample excitation

Stage2: Spin current generation

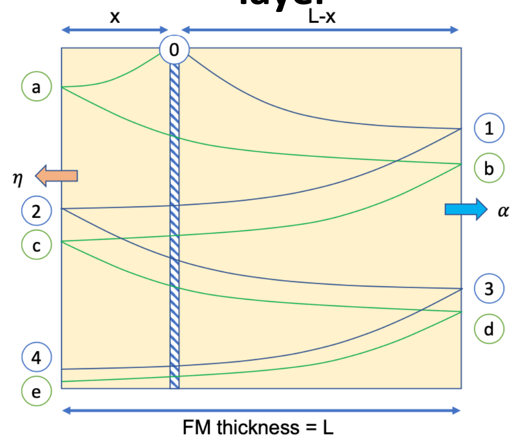
Stage3: Spin current injection to HM

Stage4: Spin to charge conversion

Stage5: THz emission from charge current

Stage6: THz propagation through the multilayer

B. Spin generation profile in the FM layer



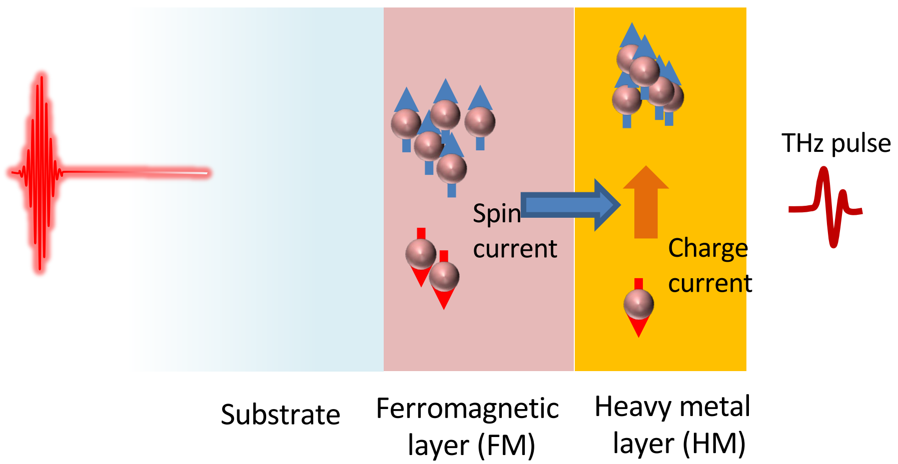
$$\zeta_R(z) = \frac{\alpha}{N}\left[e^{-\frac{d-z}{\lambda}} + \bar{\beta} e^{-\frac{d+z}{\lambda}}\right],$$

$$\zeta_L(z) = \frac{\beta}{N}\left[e^{-\frac{z}{\lambda}} + \bar{\alpha} e^{-\frac{2d-z}{\lambda}}\right],$$

$$N = 1 - \bar{\alpha}\bar{\beta} e^{-\frac{2d}{\lambda}}, \bar{\alpha} = 1 - \alpha, \bar{\beta} = 1 - \beta.$$

Modelling of spintronics THz emitters

Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437



Stage1: Sample excitation

Stage2: Spin current generation

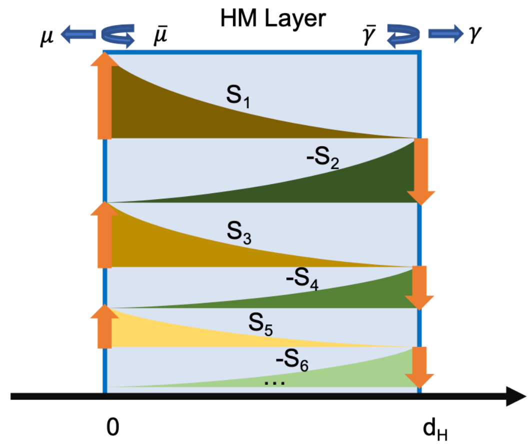
Stage3: Spin current injection to HM

Stage4: Spin to charge conversion

Stage5: THz emission from charge current

Stage6: THz propagation through the multilayer

C. Charge current profile in the HM layer



$$\sigma(z,d) = \frac{1}{N}\left[e^{-\frac{z}{\lambda}} + \bar{\gamma} e^{-\frac{2d-z}{\lambda}}\right],$$

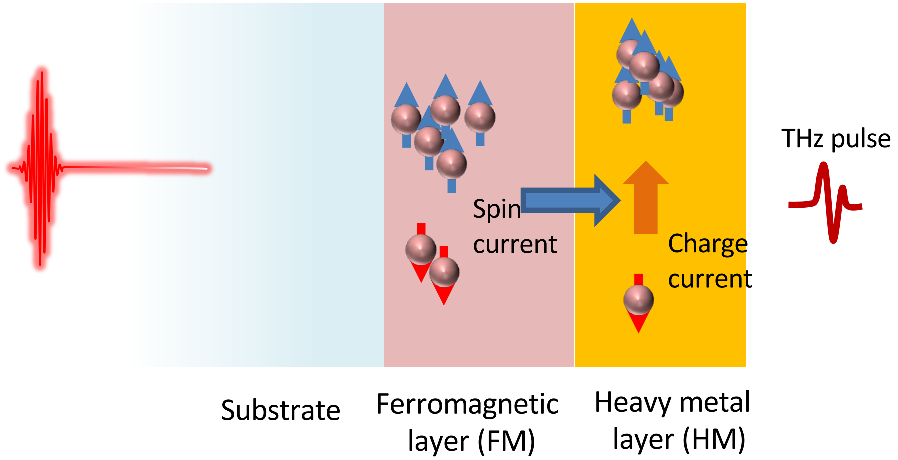
$$N = 1 - \bar{\gamma}\bar{\mu}e^{-\frac{2d}{\lambda}}$$

$$\bar{\gamma} = 1-\gamma, \bar{\mu} = 1-\mu$$

λ Spin diffusion length

Modelling of spintronics THz emitters

Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437



Stage1: Sample excitation

Stage2: Spin current generation

Stage3: Spin current injection to HM

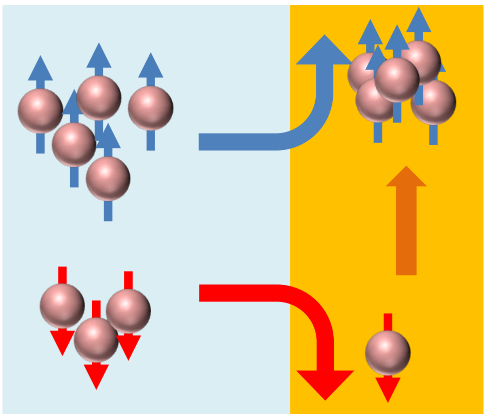
Stage4: Spin to charge conversion

Stage5: THz emission from charge current

Stage6: THz propagation through the multilayer

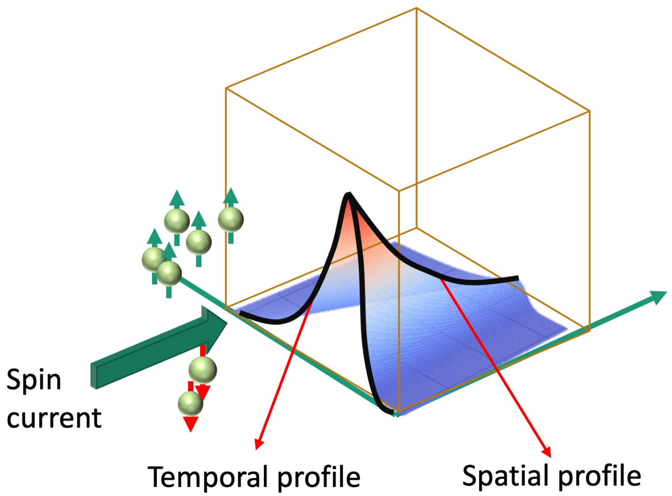
Modelling of spintronics THz emitters

Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437



$$\partial_z E\left[t,z\right] = \mu\, \partial_t H\left[t,z\right]$$
$$\partial_z H\left[t,z\right] = \epsilon\, \partial_t E\left[t,z\right] + J e^{i(kz-\omega t)}$$

$$\bar{F}\left[\omega,z\right] = \begin{bmatrix} E\left[\omega,z\right] \\ H\left[\omega,z\right] \end{bmatrix} = \bar{\bar{a}}\left[\omega,z\right] \begin{bmatrix} f^{>} \\ f^{<} \end{bmatrix} + J \begin{bmatrix} \frac{-i\omega\mu e^{ikz}}{\epsilon\mu\omega^2-k^2} \\ \frac{ike^{ikz}}{\epsilon\mu\omega^2-k^2} \end{bmatrix},$$



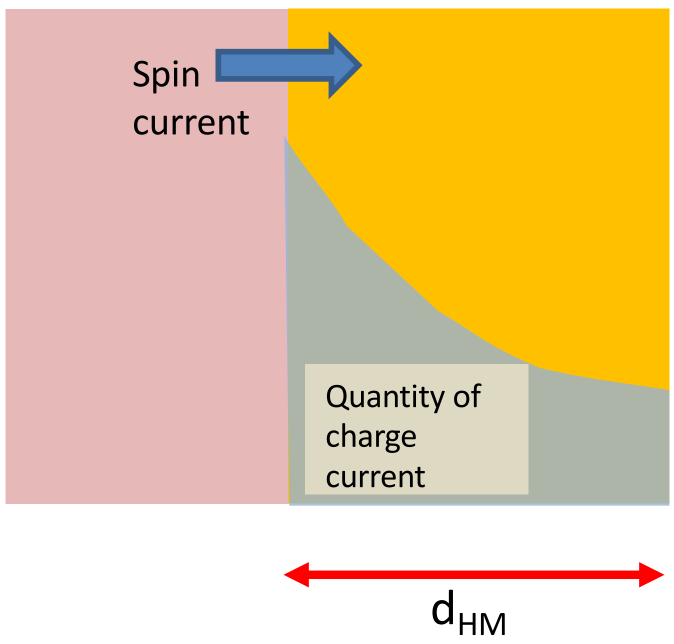
$$\begin{bmatrix} f^{>}_{N+1} \\ 0 \end{bmatrix} = \bar{\bar{T}}_{[0,N+1]} \begin{bmatrix} 0 \\ f^{<}_{0} \end{bmatrix} + \begin{bmatrix} J^{>} \\ J^{<} \end{bmatrix},$$

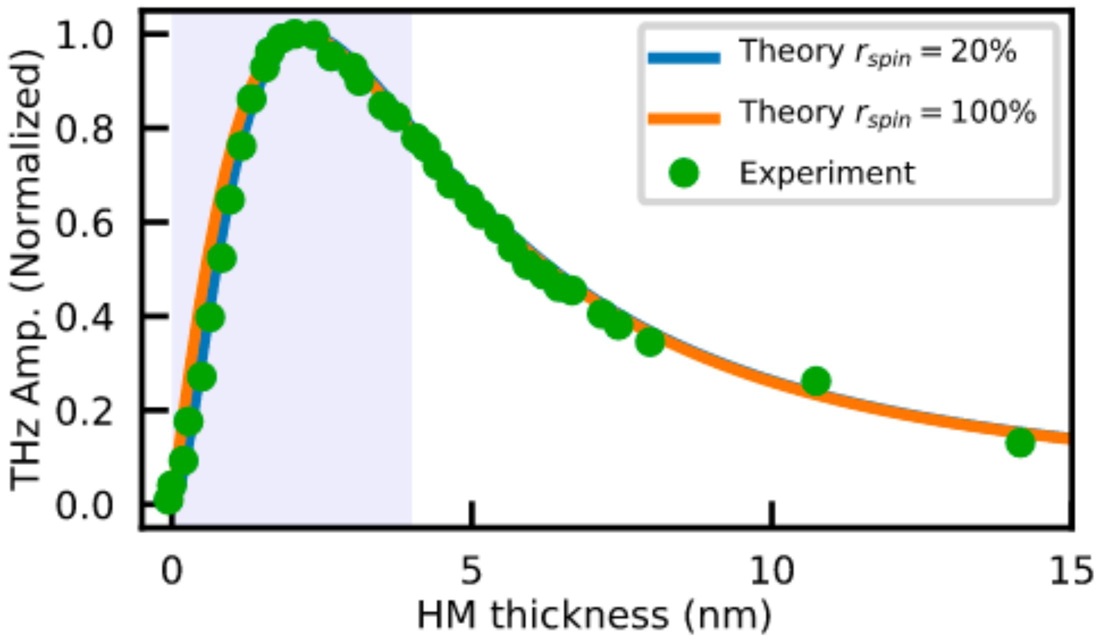
$$f^{>}_{N+1} = J^{>} - \frac{T_{[0,N+1],12}}{T_{[0,N+1],22}} J^{<}$$

Transfer Matrix Method with Source (TMMS)

Modelling of spintronics THz emitters

Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437

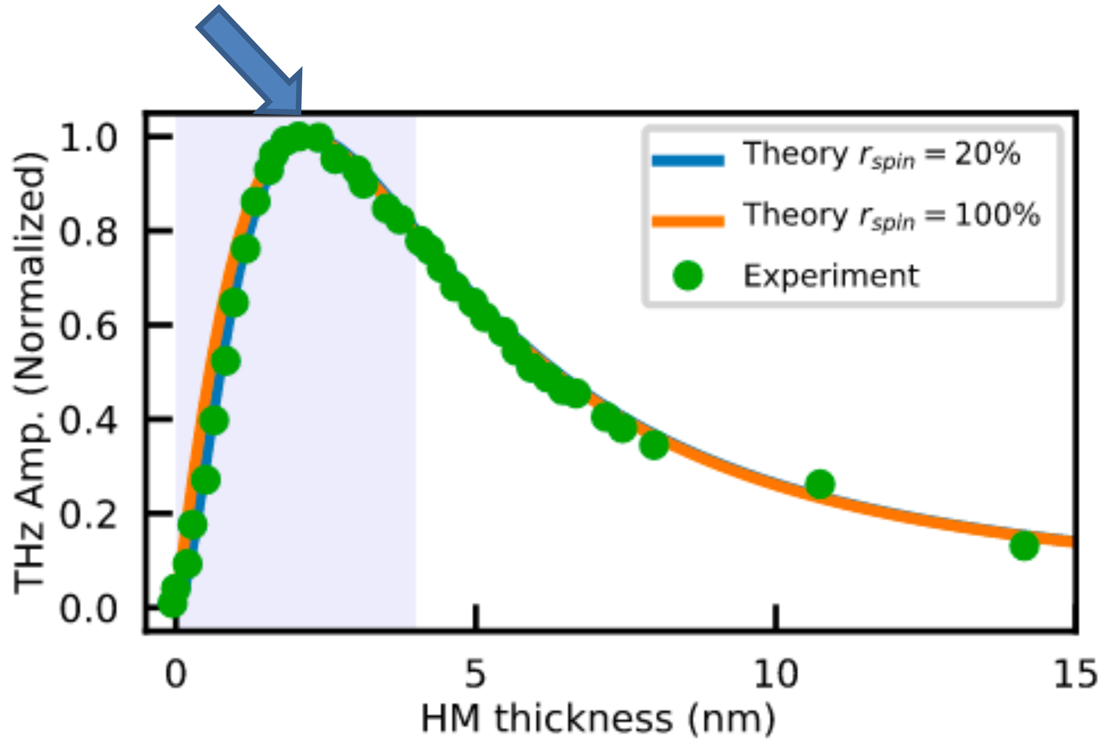




The large-thickness decay is controlled by the absorption of the THz emission within the metallic multilayer itself

Modelling of spintronics THz emitters

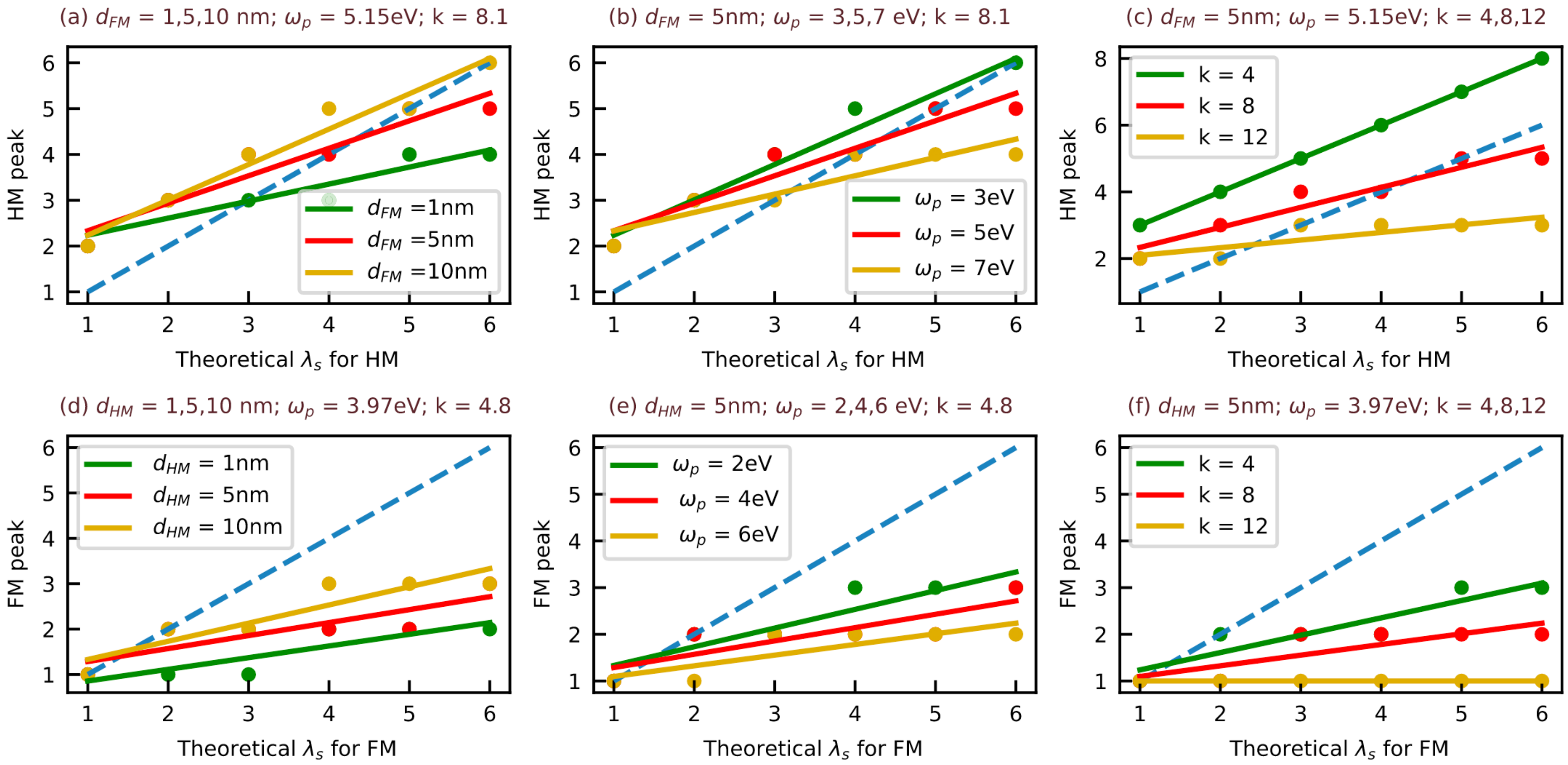
Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437



Is the thickness corresponding to the maximal emission really indicative of the spin diffusion length?

Modelling of spintronics THz emitters

Y Yang, S Dal Forno, M Battiato, Phys Rev B 104 (15), 155437

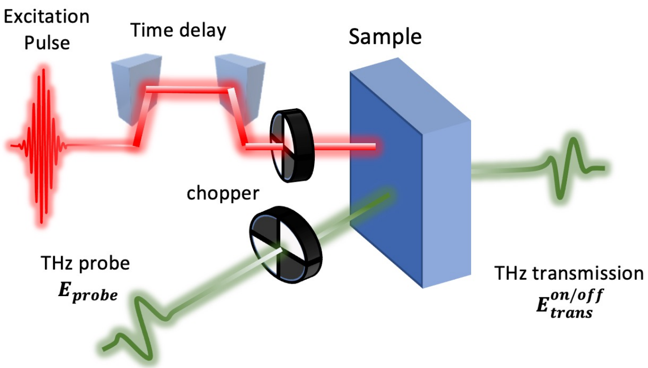


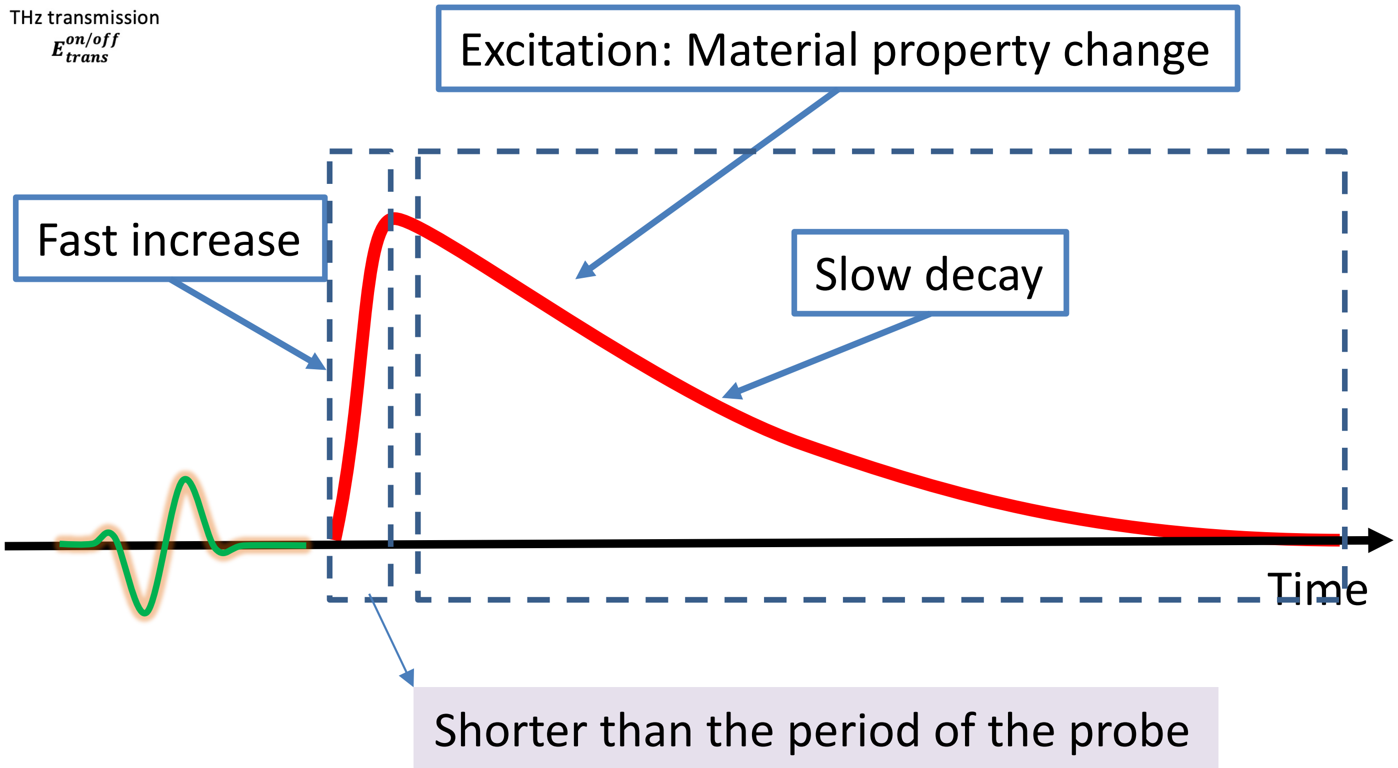
Blue dashed line represents when Spin diffusion length = peak position

The thickness corresponding to the maximal emission is **not indicative at all** of the spin diffusion length

Time resolved THz spectroscopy below ps

Y Yang, SD Forno, M Battiato, arXiv preprint arXiv:2206.00895





Time resolved THz spectroscopy below ps

Y Yang, SD Forno, M Battiato, arXiv preprint arXiv:2206.00895

$$\partial_z E\,[z,\omega] = -i\,\omega\,\mu[\omega]\,H\,[z,\omega]\,,$$
$$\partial_z H\,[z,\omega] = -i\,\omega\,\epsilon_B[\omega]\,E\,[z,\omega] + J[z,\omega]$$
$$\partial_t J[z,t] = -\gamma J[z,t] + \frac{ne^2}{m}E[z,t],$$

$$\gamma[z,t] = \gamma^{[0]} + \gamma^{[1]}[z,t]$$
$$n[z,t] = n^{[0]} + n^{[1]}[z,t]$$
$$E[z,t] \approx E^{[0]}[z,t] + E^{[1]}[z,t]$$
$$H[z,t] \approx H^{[0]}[z,t] + H^{[1]}[z,t]$$
$$J[z,t] \approx J^{[0]}[z,t] + J^{[1]}[z,t]$$

0th order

$$\partial_z E^{[0]}[z,\omega] = -i\omega\mu[\omega]H^{[0]}[z,\omega],$$
$$\partial_z H^{[0]}[z,\omega] = -i\omega\epsilon_T[\omega]E^{[0]}[z,\omega].$$

Solved using TMM

1st order

$$\partial_z E^{[1]}[z,\omega] = -\,i\omega\mu[\omega]H^{[1]}[z,\omega],$$
$$\partial_z H^{[1]}[z,\omega] = -\,i\omega\epsilon_B[\omega]E^{[1]}[z,\omega] + J^{[1]}[z,\omega],$$
$$\partial_t J^{[1]}[z,t] = -\,\gamma^{[0]}J^{[1]}[z,t] + \frac{n^{[0]}e^2}{m}E^{[1]}[z,t] - \gamma^{[1]}J^{[0]}[z,t] + \frac{n^{[1]}e^2}{m}E^{[0]}[z,t].$$

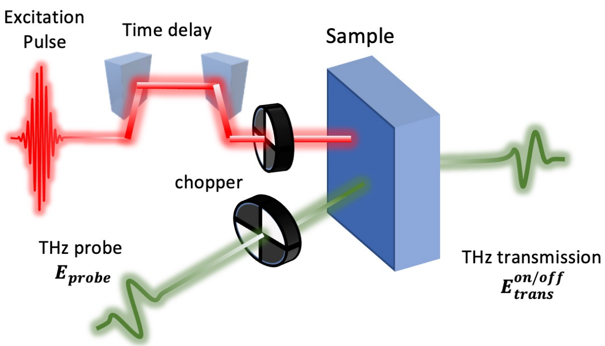
Similar to what we solved for TMMS

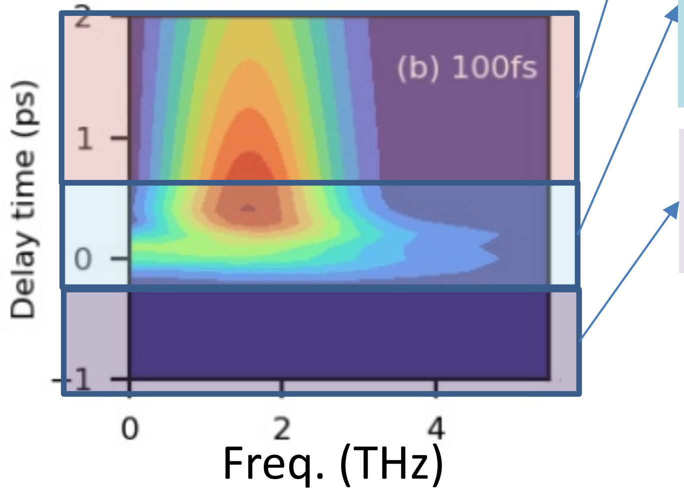
$$\partial_z E^{[1]}\,[z,\omega] = -i\,\omega\,\mu[\omega]\,H^{[1]}\,[z,\omega]\,,$$
$$\partial_z H^{[1]}\,[z,\omega] = -i\,\omega\,\epsilon_T[\omega]\,E^{[1]}\,[z,\omega] + \mathcal{J}[z,\omega],$$

$$\mathcal{J}[z,\omega] = \sigma_D^{[0]}[\omega] \times \mathcal{F}\left[\frac{n^{[1]}[t]}{n^{[0]}}E^{[0]}[z,t] - \frac{m\,\gamma^{[1]}[t]}{n^{[0]}\,e^2}J^{[0]}[z,t],\omega\right]$$

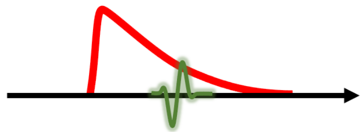
Time resolved THz spectroscopy below ps

Y Yang, SD Forno, M Battiato, arXiv preprint arXiv:2206.00895

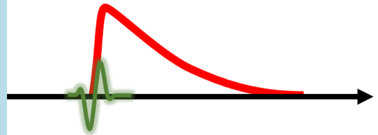




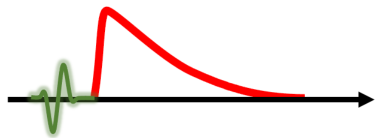
ΔE when probe arrives after system excited for a long time



ΔE when fast increase of material change overlaps with probe

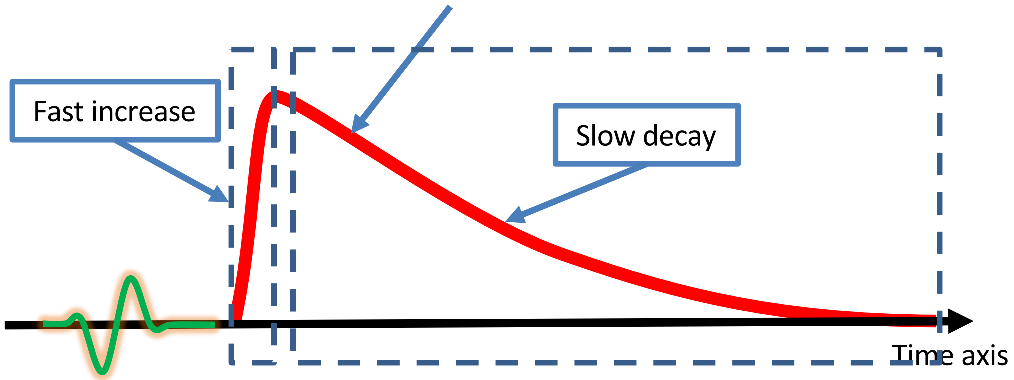


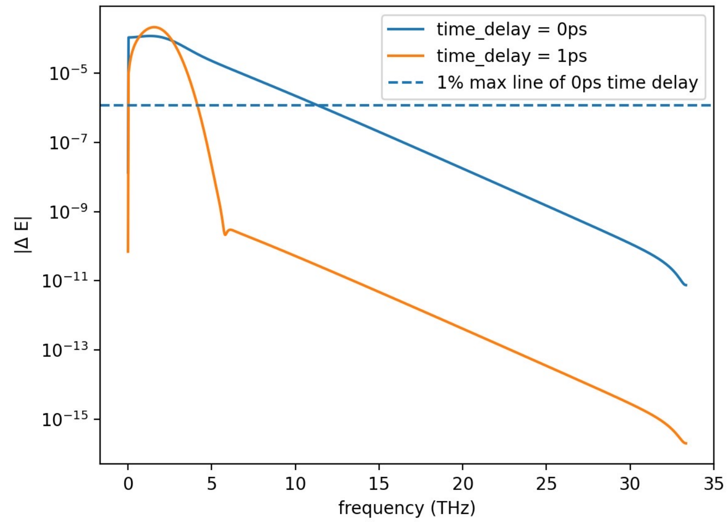
ΔE when probe arrives before excitation

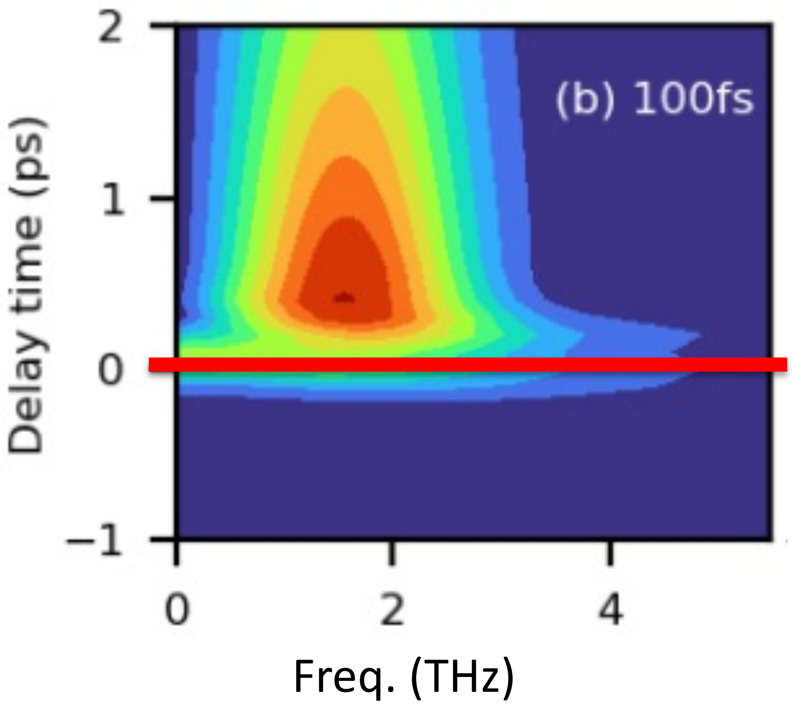


Time resolved THz spectroscopy below ps

Y Yang, SD Forno, M Battiato, arXiv preprint arXiv:2206.00895







$$increase\ time = \frac{1}{f_{1\%} - 2 * f_c}$$

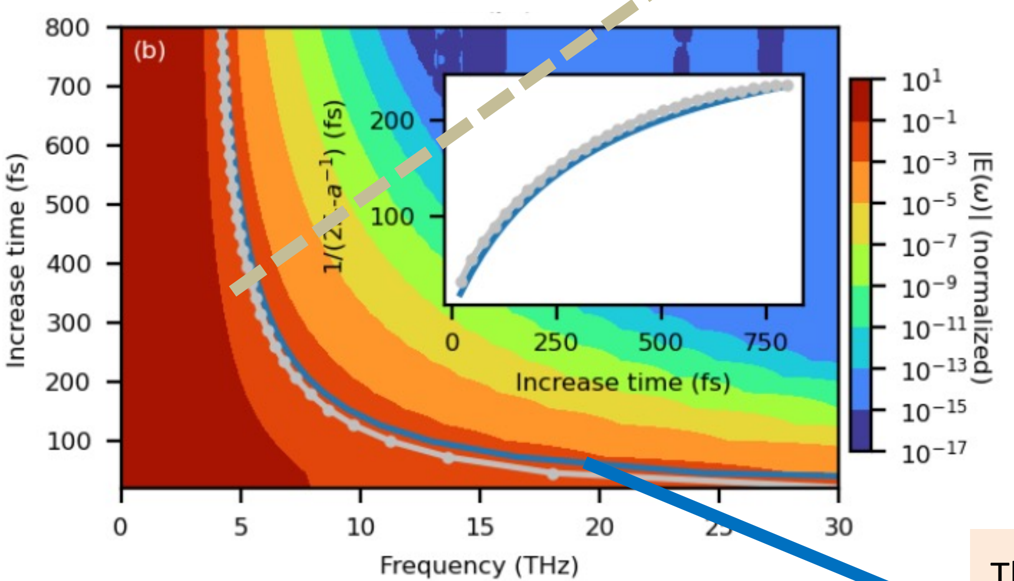
Frequency of 1% of spectrum maximum.

Central frequency of probe pulse

Time resolved THz spectroscopy below ps

Y Yang, SD Forno, M Battiato, arXiv preprint arXiv:2206.00895

The gray dotted line shows the region where the spectrum amplitude is 1% of its maximum ($f_{1\%}$).

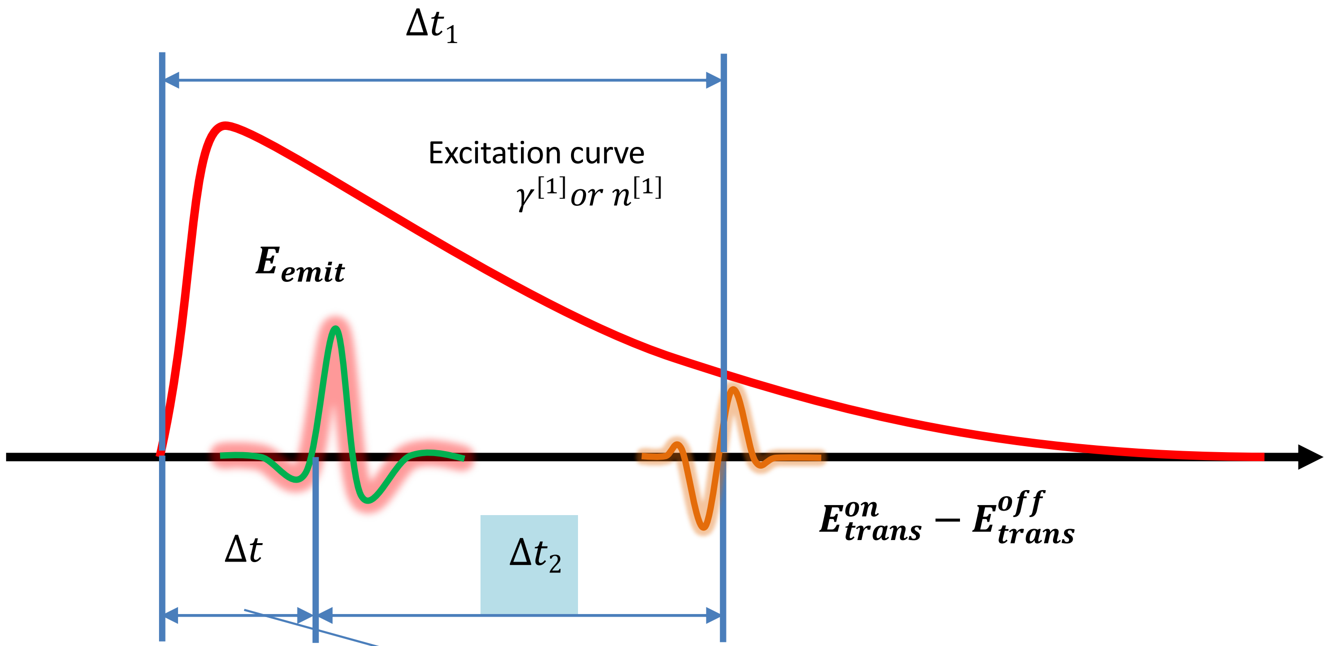


$$increase\ time = \frac{1}{f_{1\%} - 2 * f_c}$$

The blue line is $f_c * 2 + \frac{1}{\text{increase time}}$, where f_c is the center frequency of the probe.

How about spintronics THz emitters?

Y Yang, SD Forno, M Battiato, arXiv preprint arXiv:2206.00895

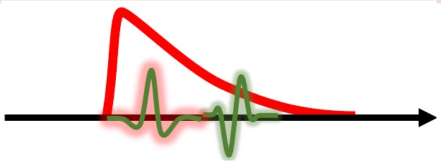


Aim:
How long does it take after the excitation for the THz to emit?

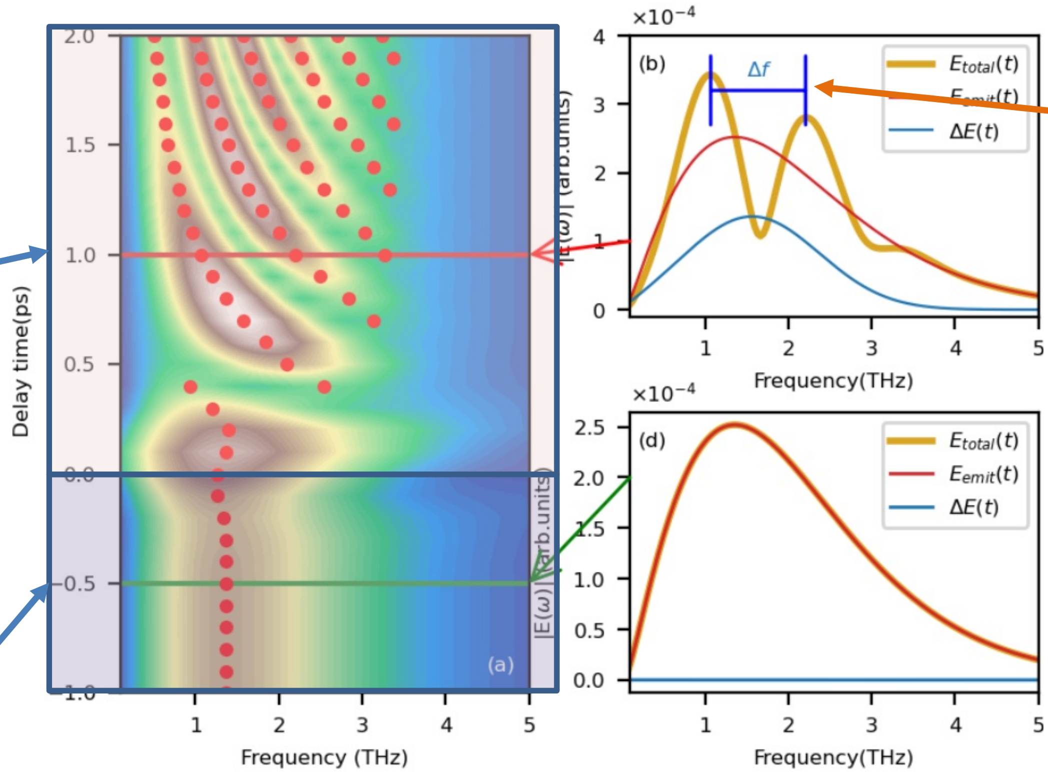
How about spintronics THz emitters?

Y Yang, SD Forno, M Battiato, arXiv preprint arXiv:2206.00895

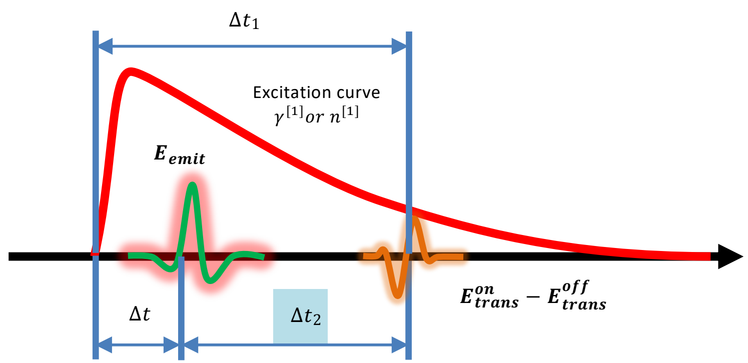
ΔE when probe arrives after the excitation.



ΔE when probe arrives before the excitation.

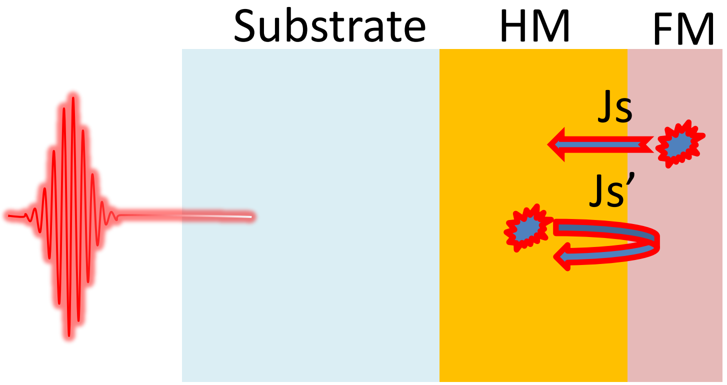


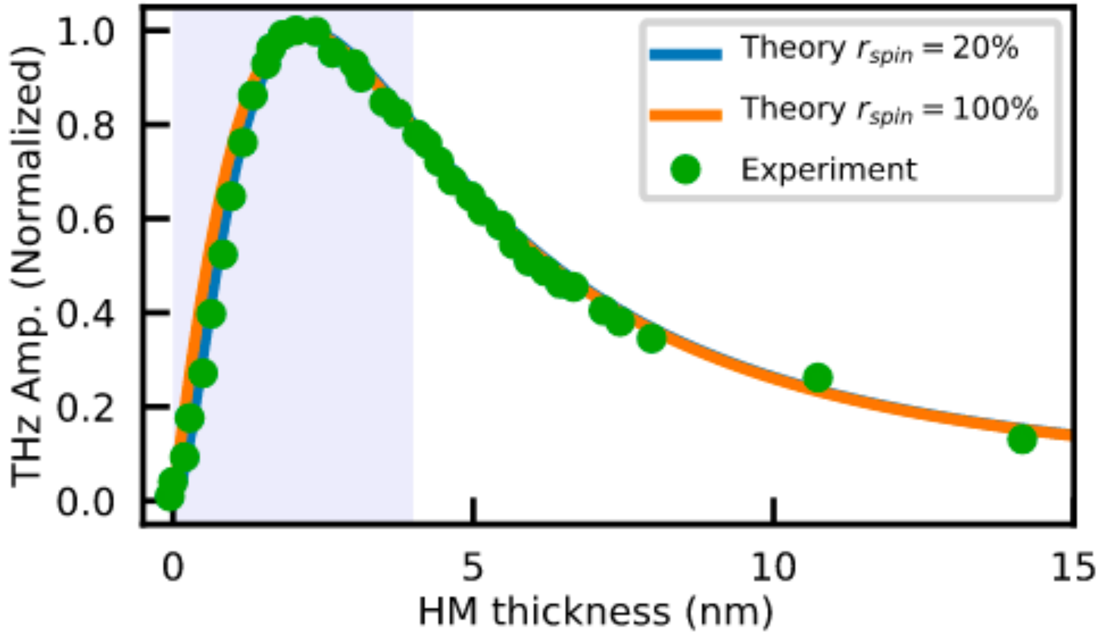
$$\Delta t_2 = \frac{1}{\Delta f}$$



What is contributing more to the THz?

P Agarwal*, Y Yang*, R Medwal, H Asada, Y Fukuma, M Battiato, R Singh arXiv:2211.15135



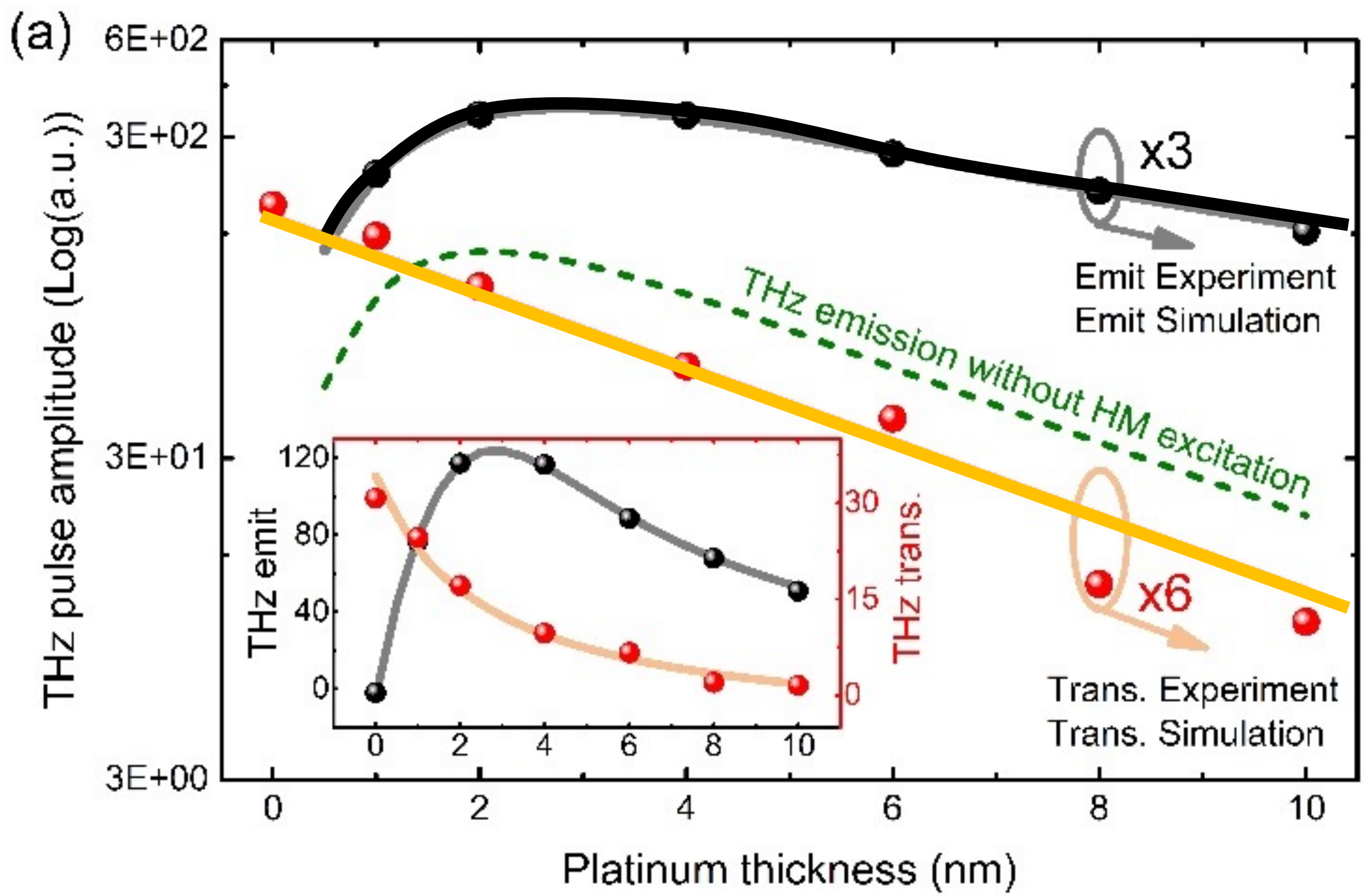


~~The large-thickness decay is controlled by the absorption of the THz emission within the metallic multilayer itself~~

I lied, sorry

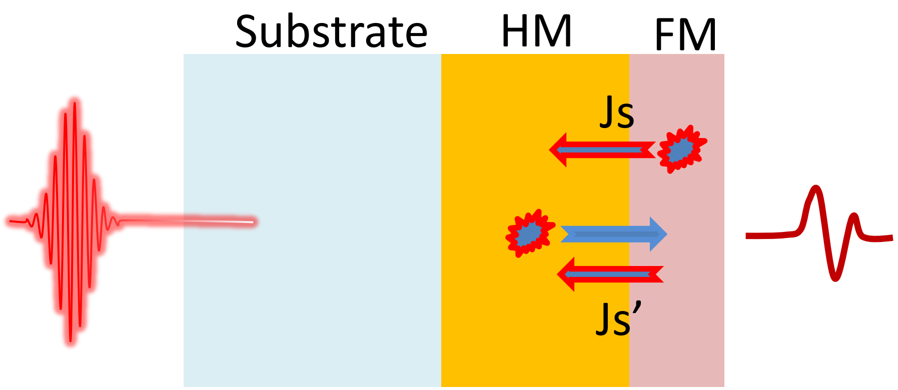
What is contributing more to the THz?

P Agarwal*, Y Yang*, R Medwal, H Asada, Y Fukuma, M Battiato, R Singh arXiv:2211.15135



What is contributing more to the THz?

P Agarwal*, Y Yang*, R Medwal, H Asada, Y Fukuma, M Battiato, R Singh arXiv:2211.15135



$$E_{THz}(d) = \alpha E_{THz}^{Pt}[\lambda_{sd}, \mathrm{d}]\mathrm{A}_{\mathrm{excite}}^{\mathrm{NiFe}}[\mathrm{d}] + \xi E_{THz}^{NiFe}[\lambda_{NiFe}, d]\mathrm{A}_{\mathrm{excite}}^{\mathrm{NiFe}}[\mathrm{d}] + \beta E_{THz}^{Pt}[\lambda_{sd}, d]\ \mathrm{A}_{\mathrm{excite}}^{\mathrm{Pt}}[\mathrm{d}] \int_0^d e^{-z/\lambda_E}\, dz$$

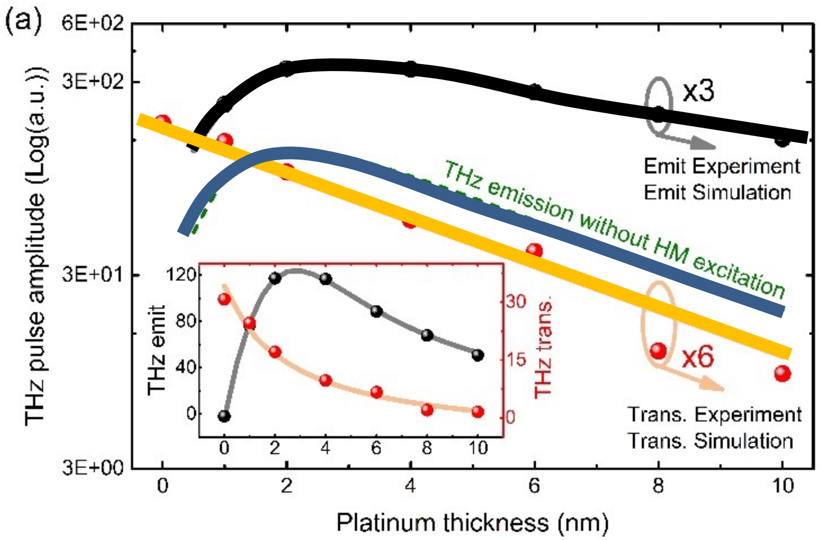
THz emission from Pt (HM) (FM excitation)

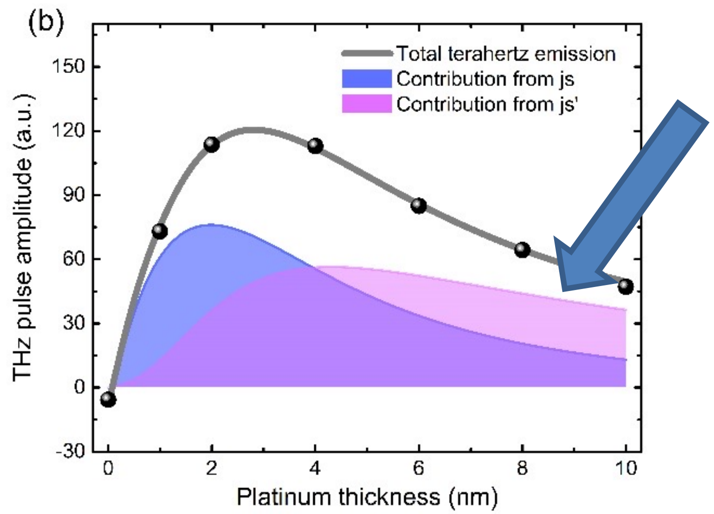
THz emission from NiFe(FM) (FM excitation)

THz emission from Pt (HM excitation)

What is contributing more to the THz?

P Agarwal*, Y Yang*, R Medwal, H Asada, Y Fukuma, M Battiato, R Singh arXiv:2211.15135





$$E_{THz}(d) = \alpha E_{THz}^{Pt}[\lambda_{sd}, \mathrm{d}]\mathrm{A}_{\mathrm{excite}}^{\mathrm{NiFe}}[\mathrm{d}] + \xi E_{THz}^{NiFe}[\lambda_{NiFe}, d]\mathrm{A}_{\mathrm{excite}}^{\mathrm{NiFe}}[\mathrm{d}] + \beta E_{THz}^{Pt}[\lambda_{sd}, d] \ldots [\mathrm{d}] \int_0^d e^{-z/\lambda_E}\, dz$$

THz emission from Pt (HM) (FM excitation)

THz emission from NiFe(FM) (FM excitation)

THz emission from Pt (HM excitation)

TORTOISE

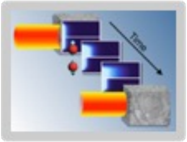
- No close to equilibrium assumptions
- No fixed population assumptions
- Any number of quasiparticles and bands
- Arbitrary dispersion (dispersion as input)
- Any number of scattering channels
- Scattering channels with 2, 3, and 4 legs (soon >4)
- Arbitrary scattering amplitude (required as input)
- Excellent scaling with precision
- Exact conservation of particle, energy and momentum

C++ library

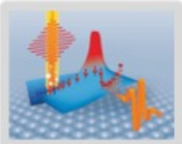
Wais, Held, Battiato, Comput. Phys. Commun. 264, 107877 (2021)
Wadgaonkar, Jain, Battiato, Comput. Phys. Commun 263, 107863 (2021)
Wadgaonkar, Wais, Battiato, Comput. Phys. Commun 271, 108207 (2021)
https://sites.google.com/view/battiatomarco/tortoise

https://github.com/MarcoBattiato/TORTOISE

Thanks to



P. Maldonado, K. Carva, P. M. Oppeneer

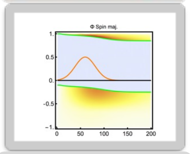


T. Kampfrath
G. Eilers
J. Nötzold

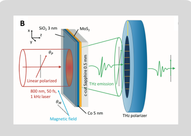
S. Mährlein
V. Zbarsky
F. Freimuth

Y. Mokrousov
S. Blügel
M. Wolf

I. Radu
M. Münzenberg



K. Held



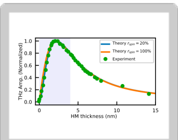
Liang Cheng
Xinbo Wang
Jianwei Chai
Weifeng Yang

Ming Yang
Mengji Chen
Yang Wu
Xiaoxuan Chen

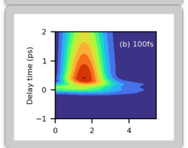
Dongzhi Chi
Kuan Eng Johnson Goh
Jian-Xin Zhu
Handong Sun

Shijie Wang
Justin C. W. Song
Hyunsoo Yang
Elbert E. M. Chia

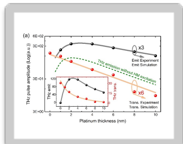
M. Wais, I. Wadgaonkar, Jain, K. Held



Y Yang, S Dal Forno

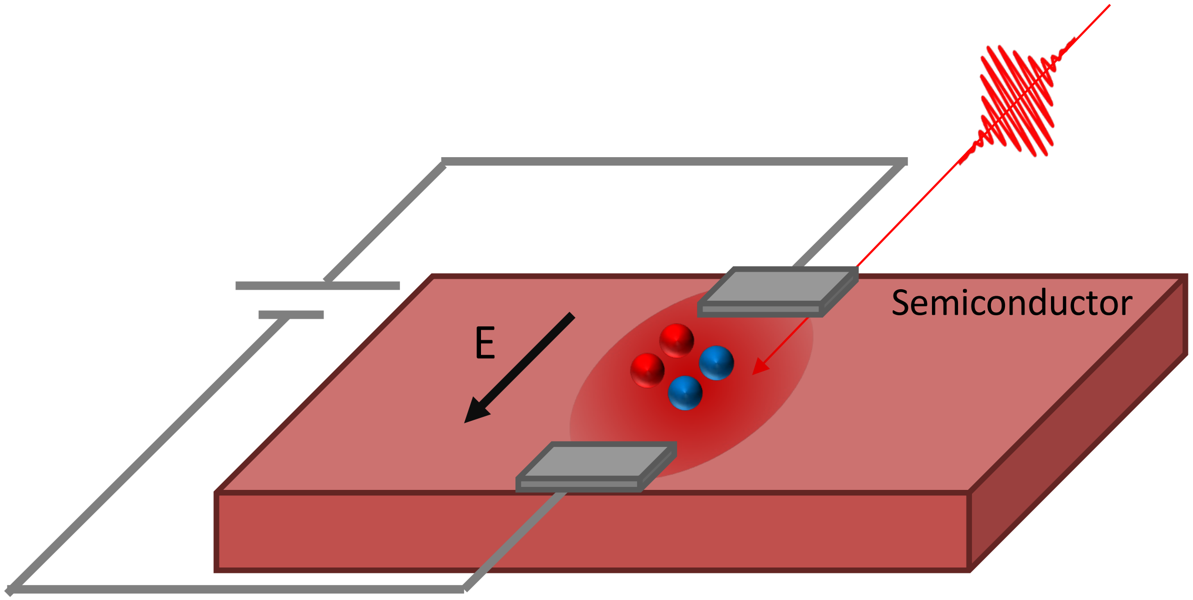


Y Yang, S Dal Forno

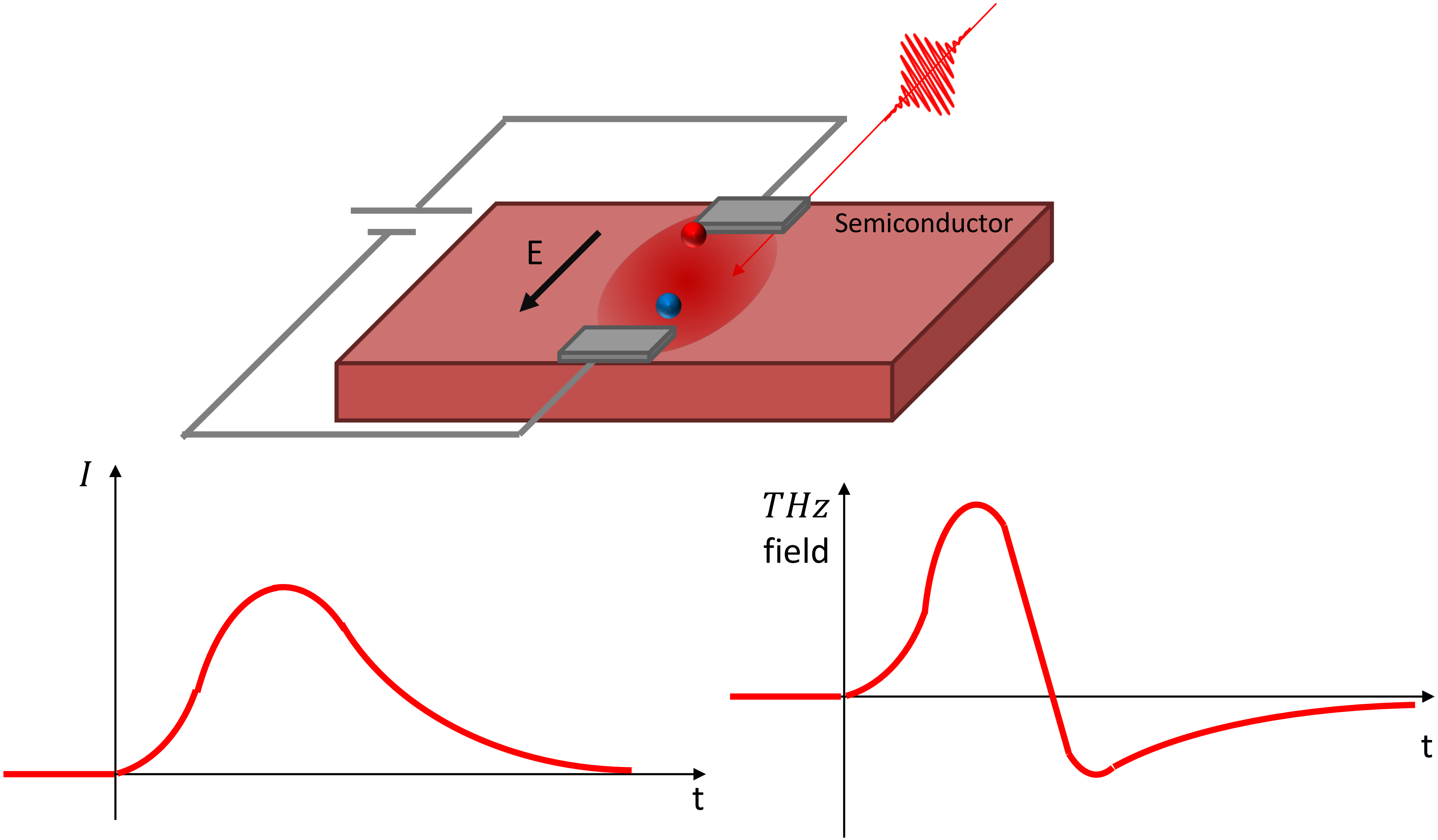


P Agarwal, Y Yang, R Medwal, H Asada, Y Fukuma, R. Singh

Photoconductive antennas

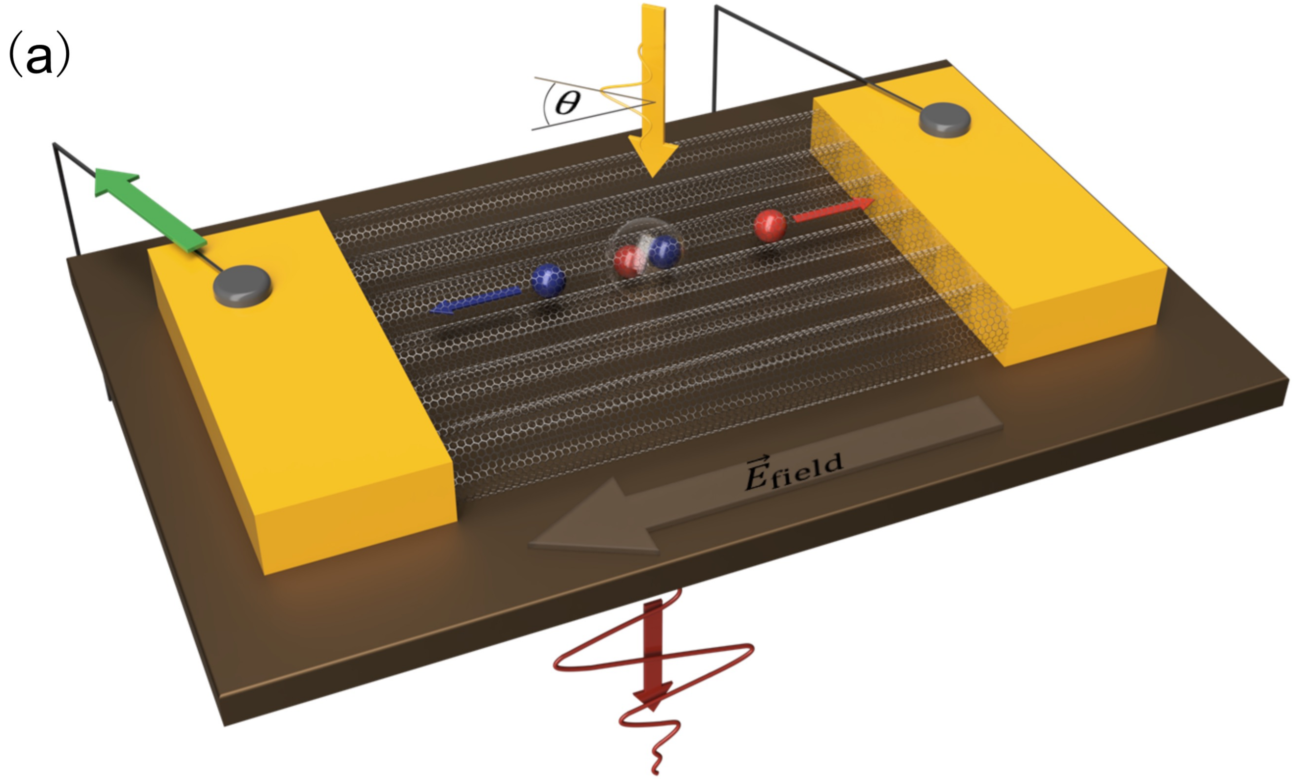


Photoconductive antennas



THz excitonics in carbon nanotubes

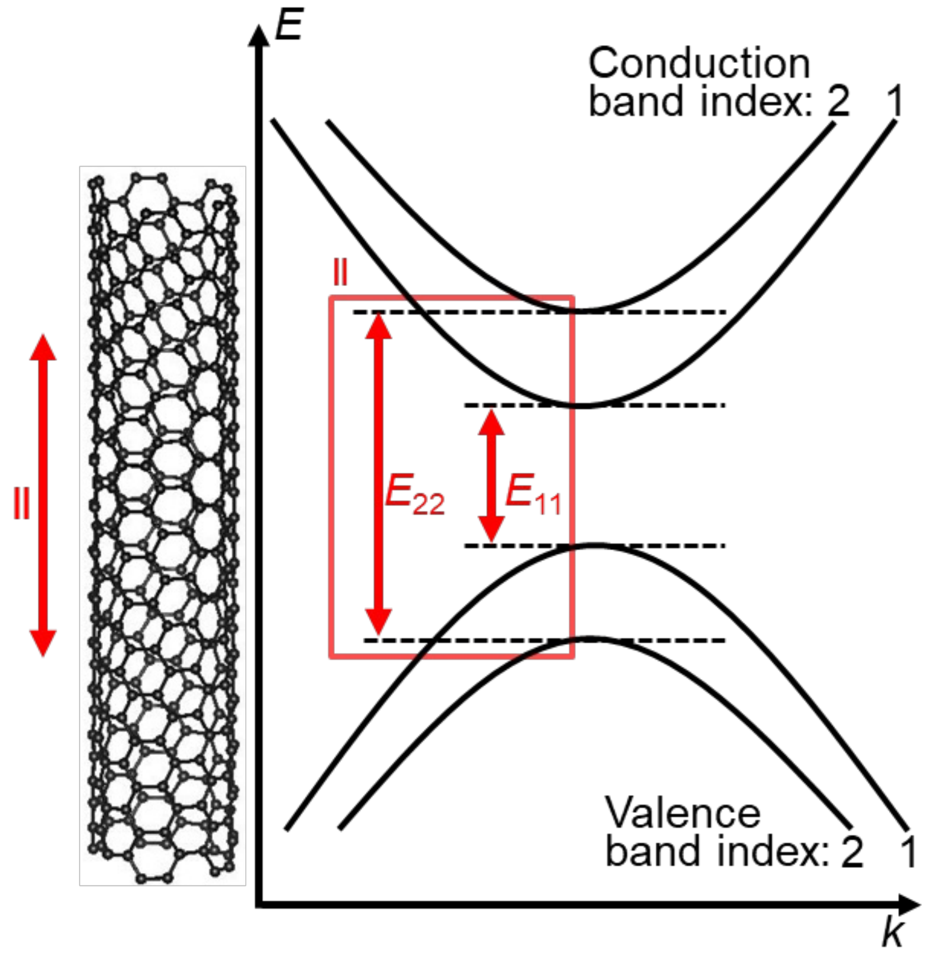
Bagsican, Wais, Komatsu, Gao, Weber, Serita, Murakami, Held, Hegmann, Tonouchi, Kono, Kawayama, Battiato, **Nano Letters** 20, 3098 (2020).

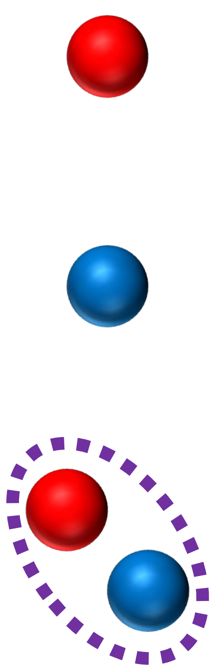


- Aligned
- Single walled
- Chirality enriched

THz excitonics in carbon nanotubes

Bagsican, Wais, Komatsu, Gao, Weber, Serita, Murakami, Held, Hegmann, Tonouchi, Kono, Kawayama, Battiato, **Nano Letters** 20, 3098 (2020).





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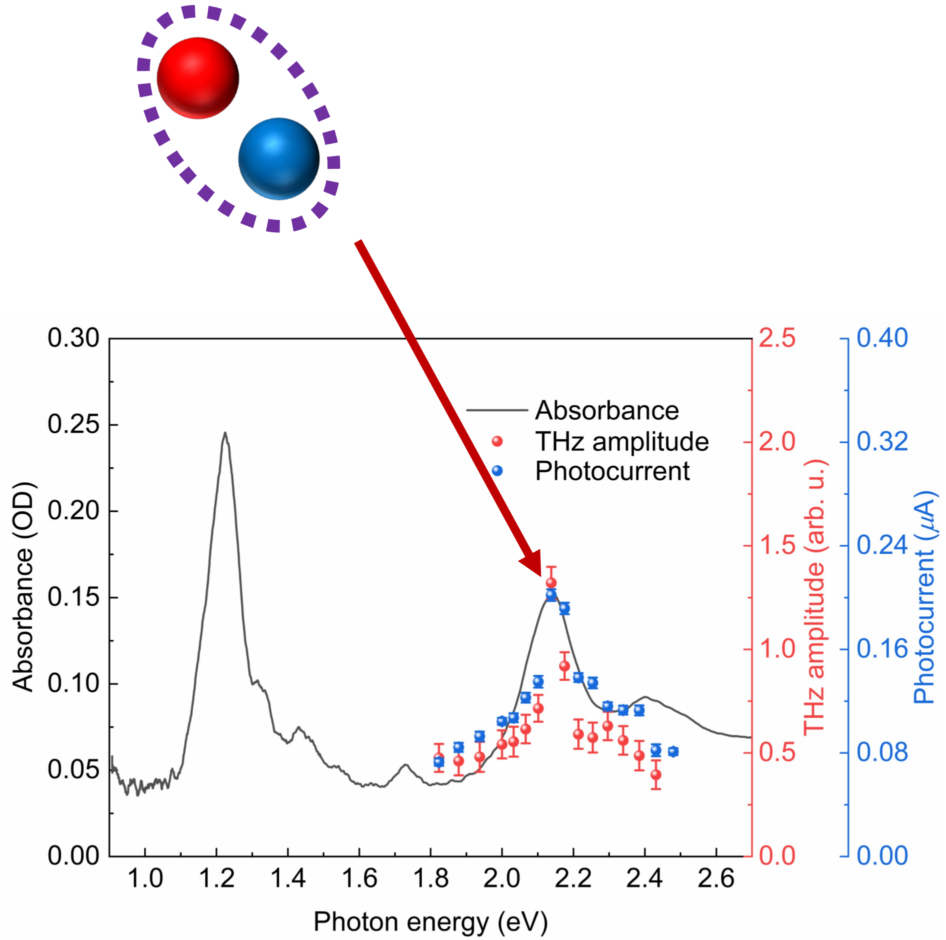

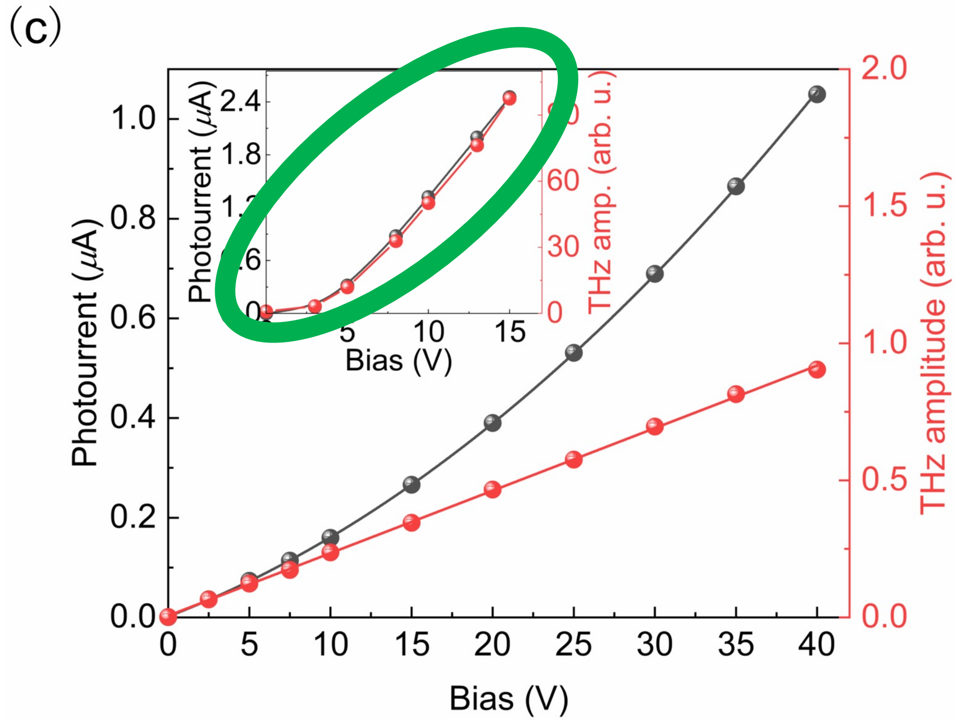

THz excitonics in carbon nanotubes

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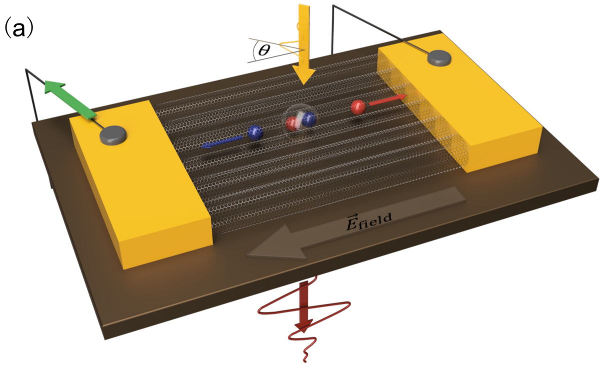

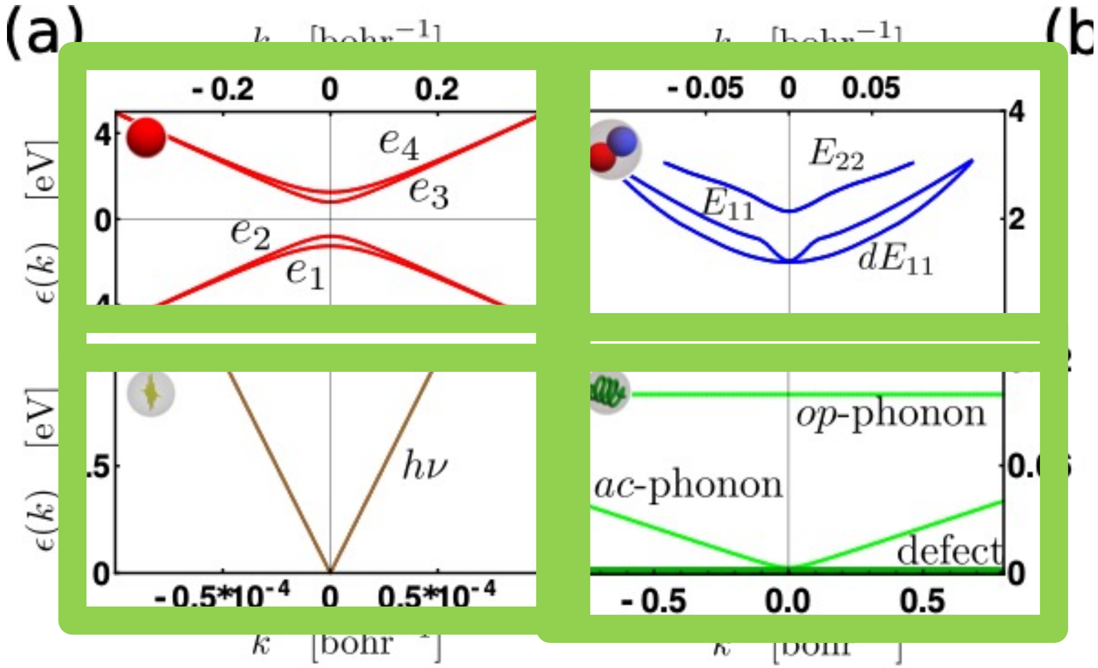

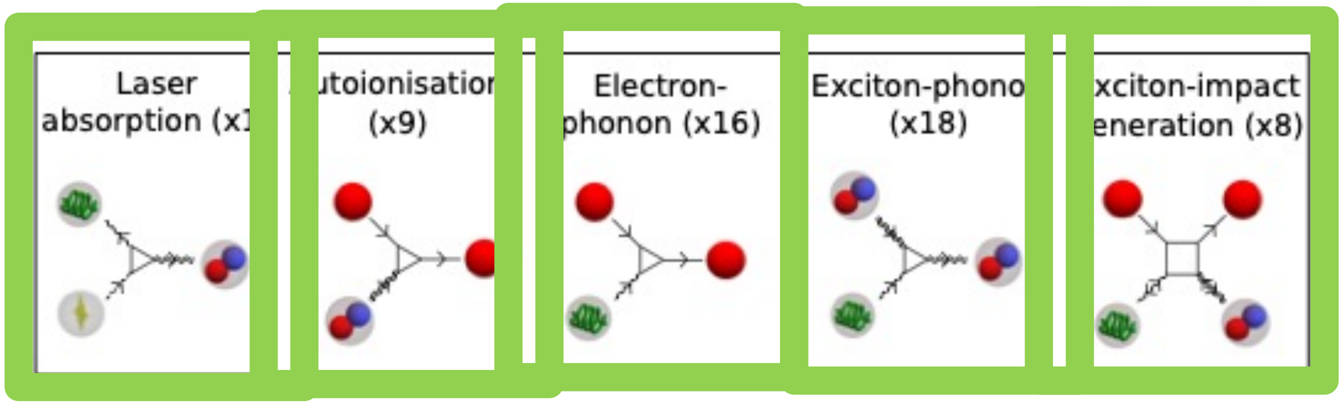

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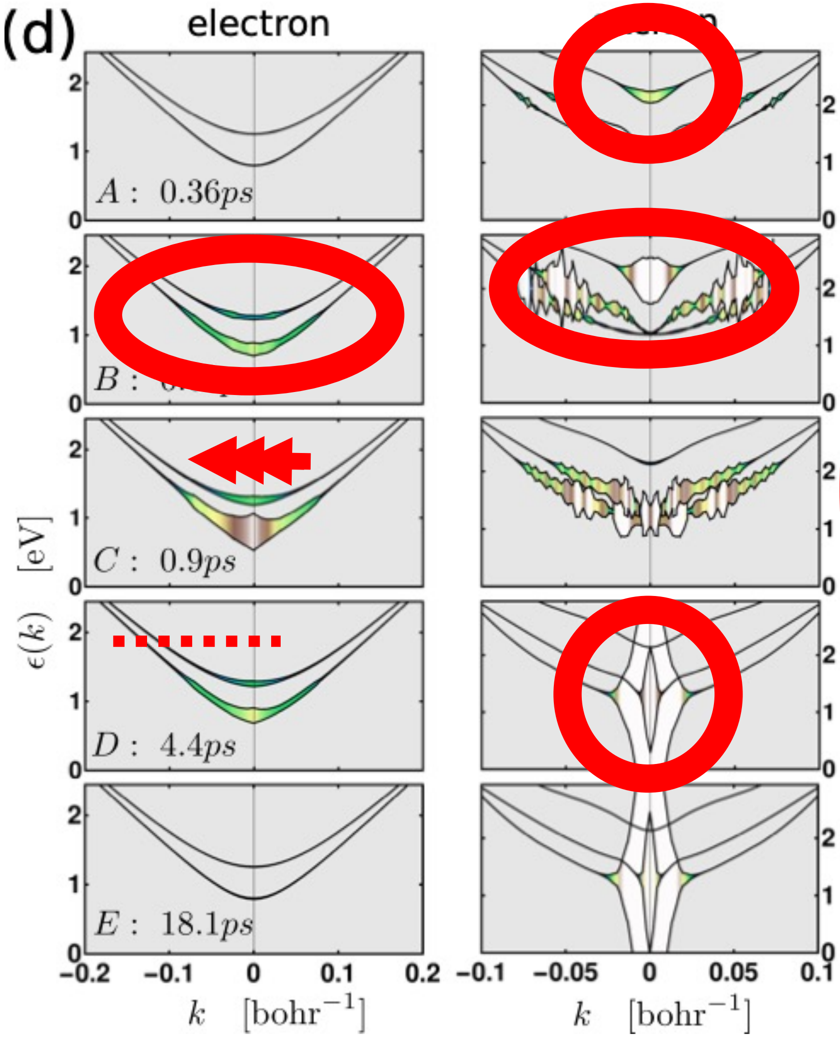

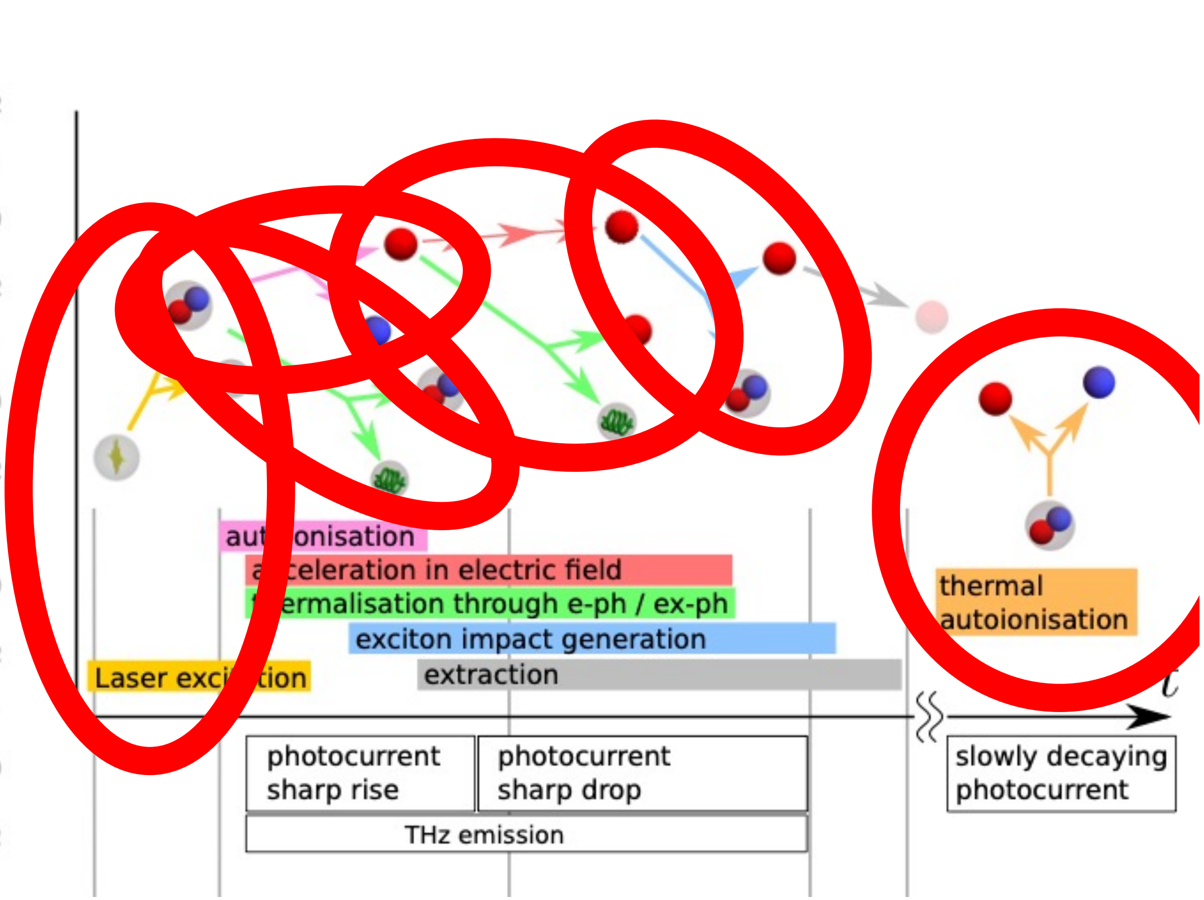

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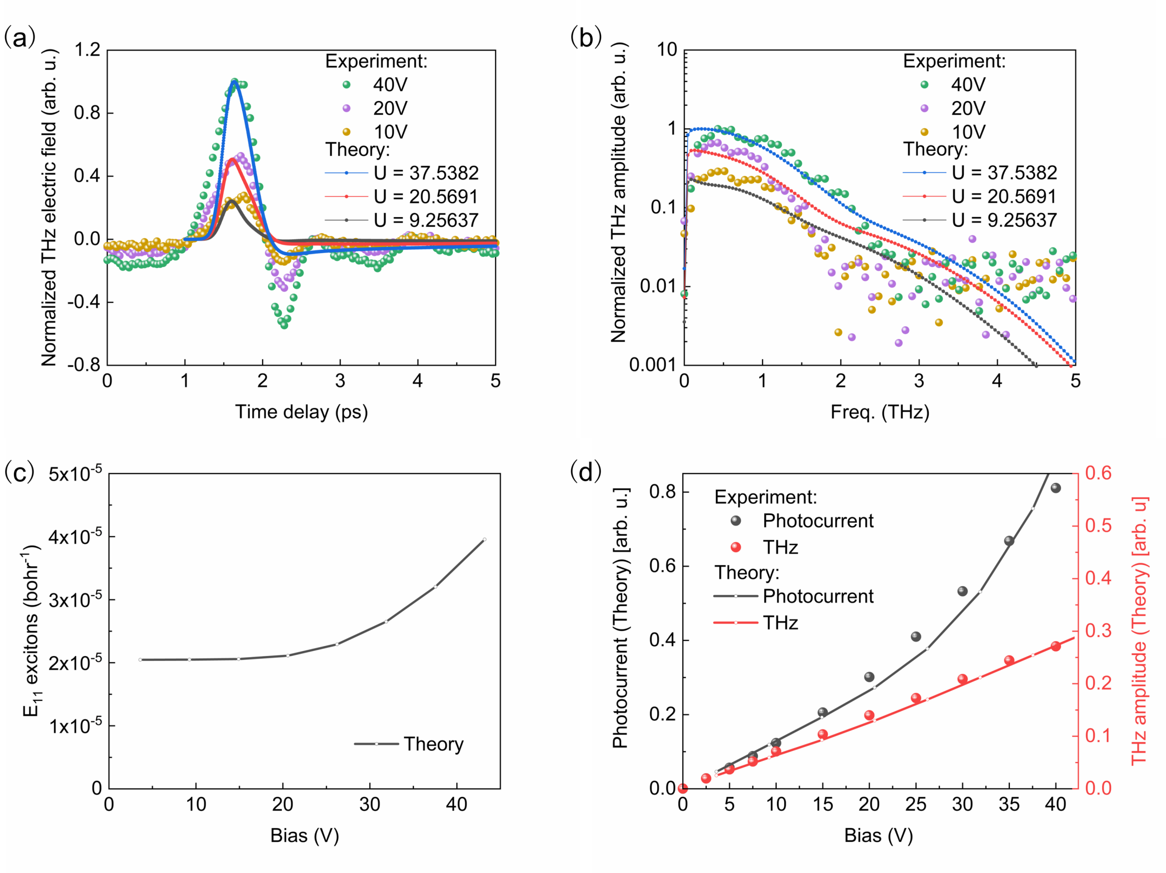
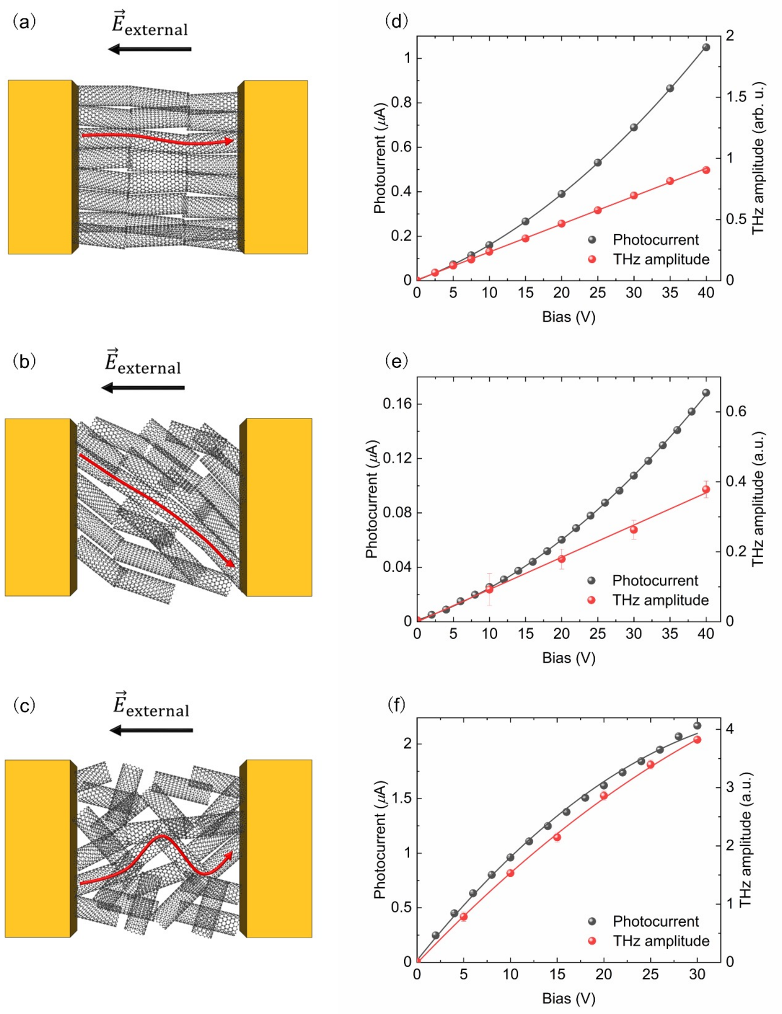


- Understood the unusual THz emission process in CNTs
- Uncovered the role of the "exciton impact generation" scattering
- Produced a very promising CNT-based photoconductive antenna

From ballistic to diffusive in CNTs

Wais*, Bagsican*, Komatsu, Gao, Serita, Murakami, Held, Kawayama, Kono, Battiato and Tonouchi, **Nano Letters** (2023).



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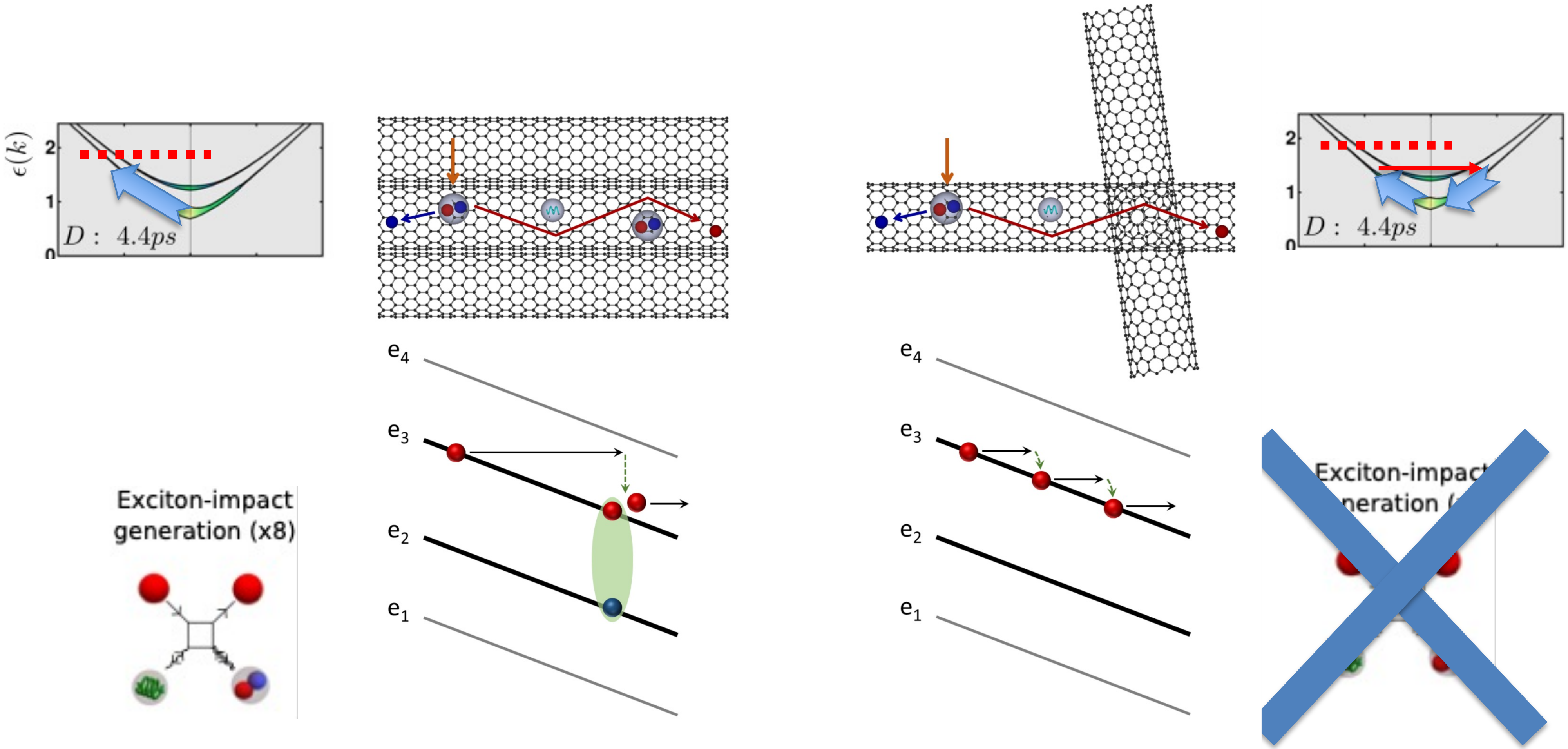

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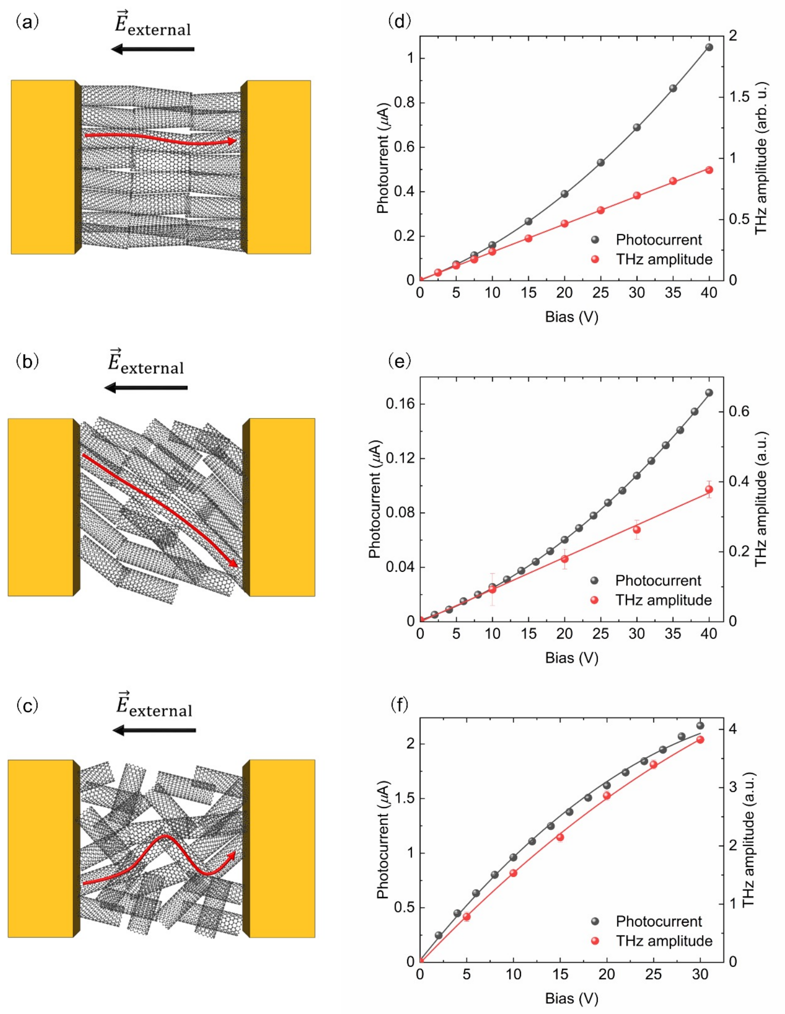
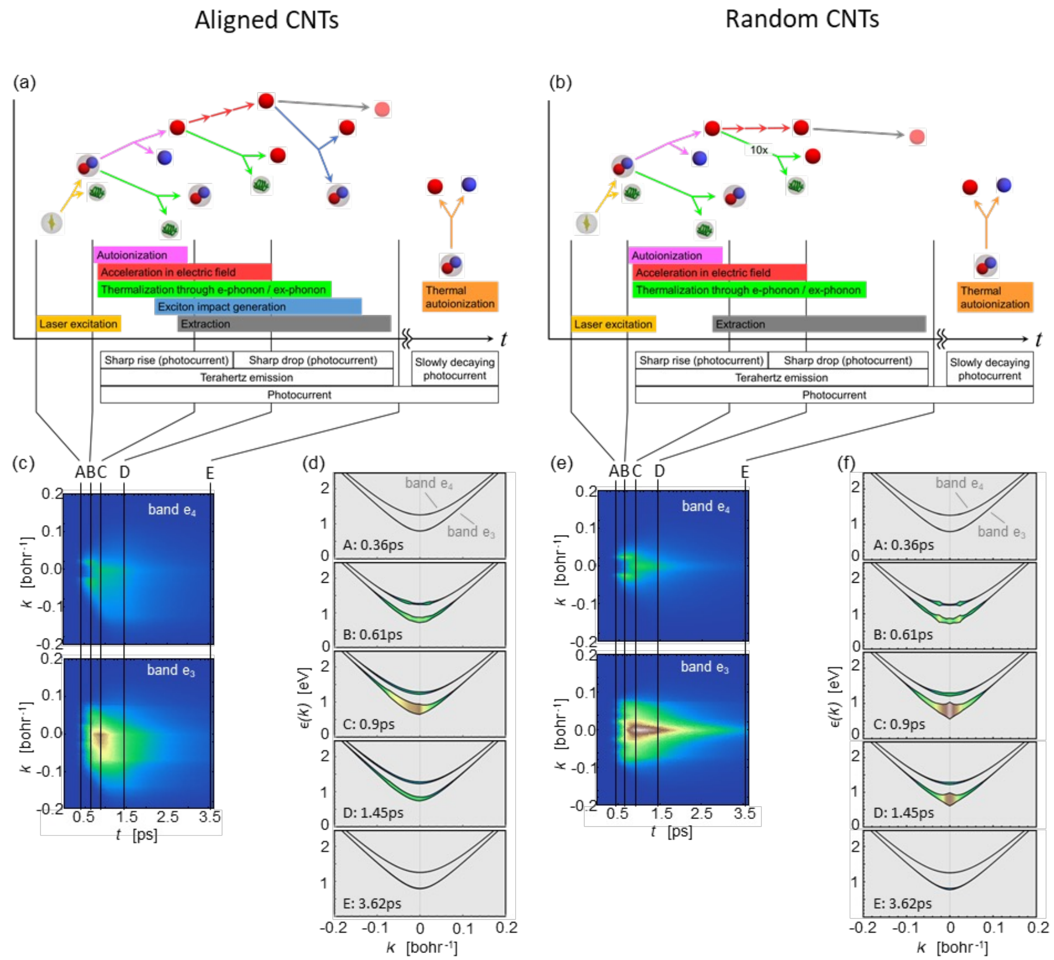
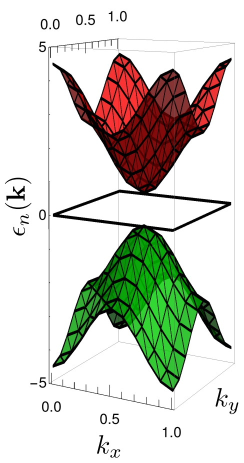
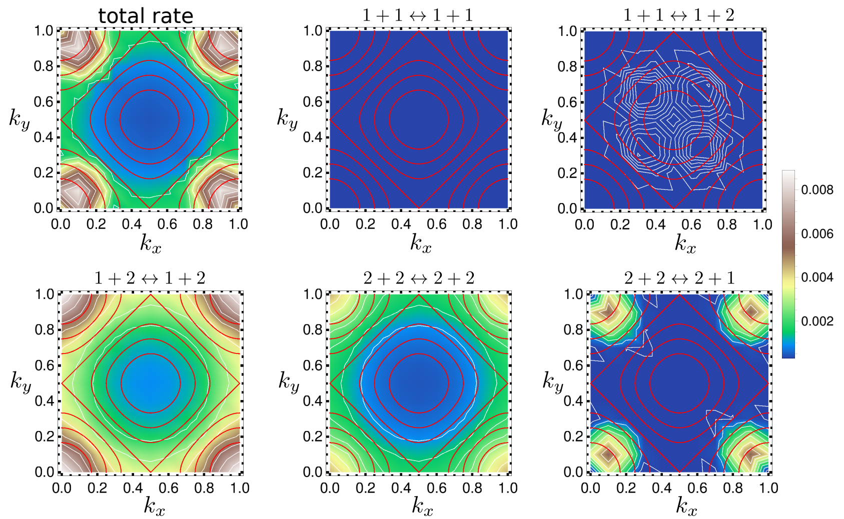


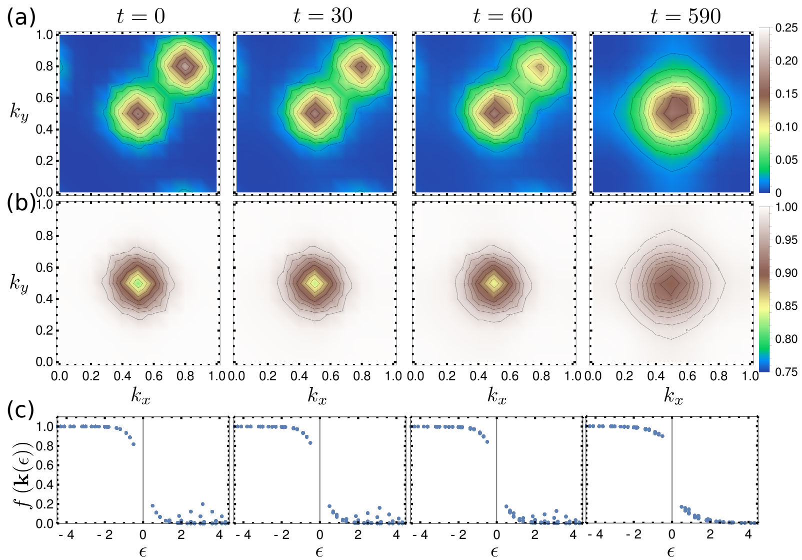


Strongly out-of-equilibrium thermalisation and transport

Wais, Held, Battiato, Comput. Phys. Commun. 264, 107877 (2021)
Wadgaonkar, Jain, Battiato, Comput. Phys. Commun 263, 107863 (2021)
Wadgaonkar, Wais, Battiato, Comput. Phys. Commun 271, 108207 (2021)







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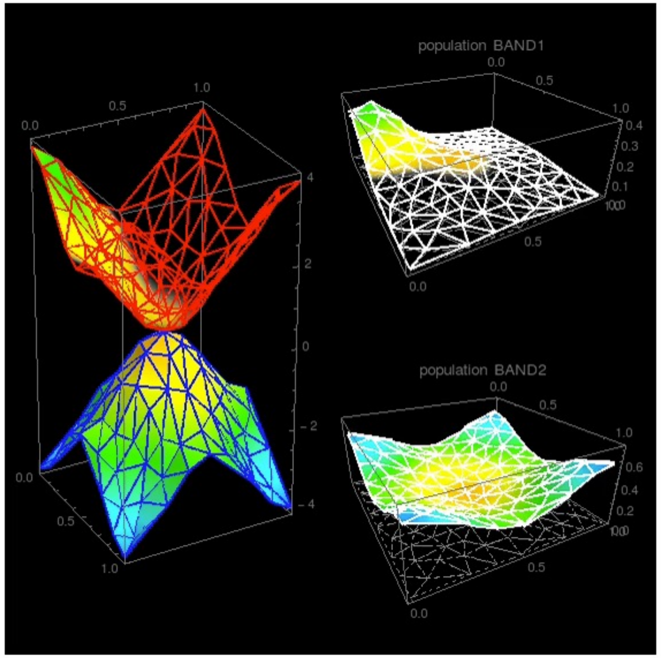
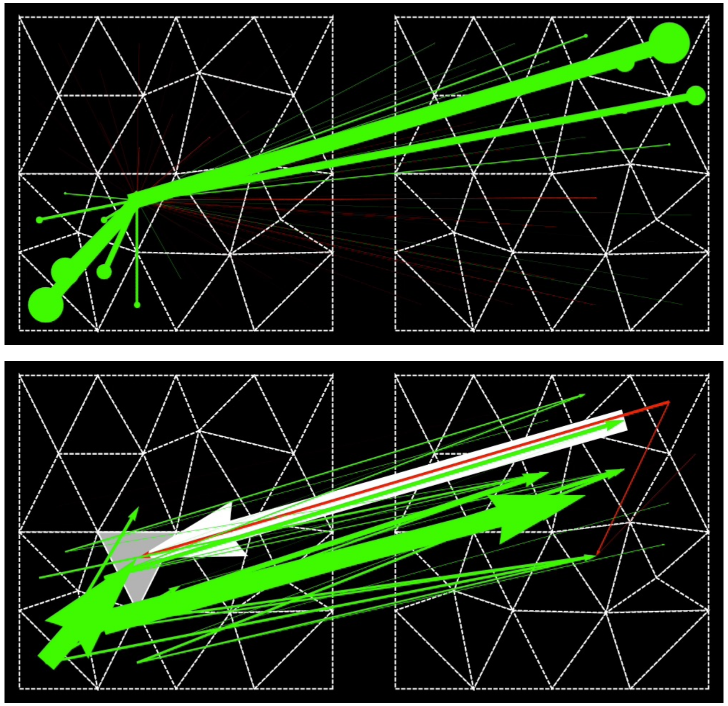
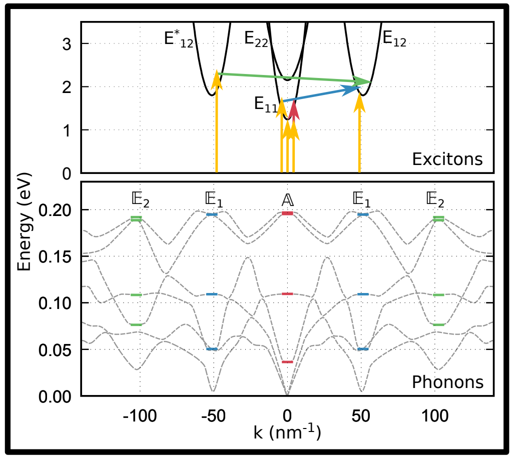
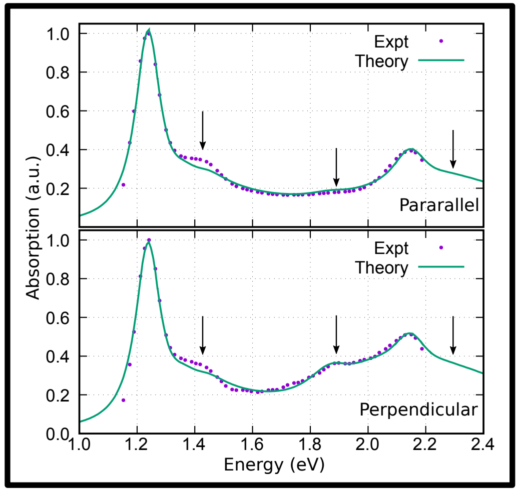


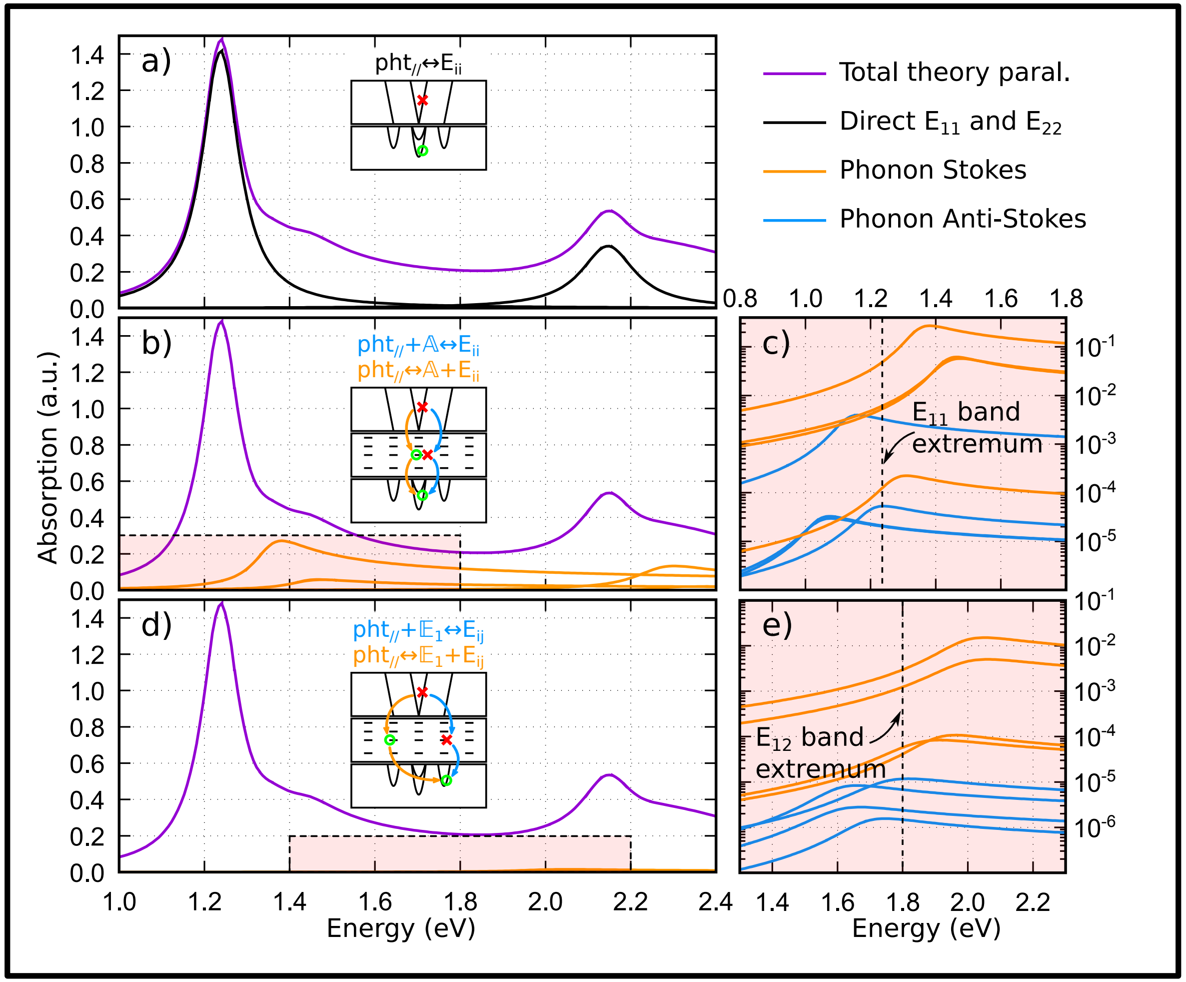


Time-resolved absorption spectra

Dal Forno, Komatsu, Wais, Mojibpour, Wadgaonkar, Ghosh, Yomogida, Yanagi, Held, Kono, Battiato, **Carbon** 186, 465 (2021)

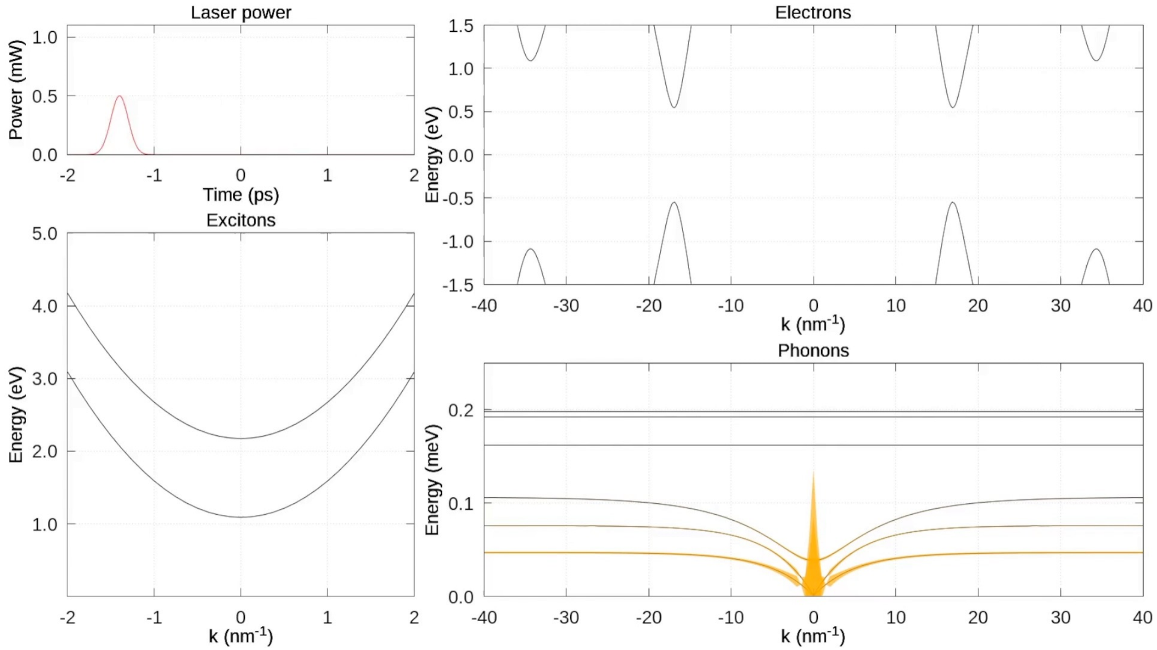


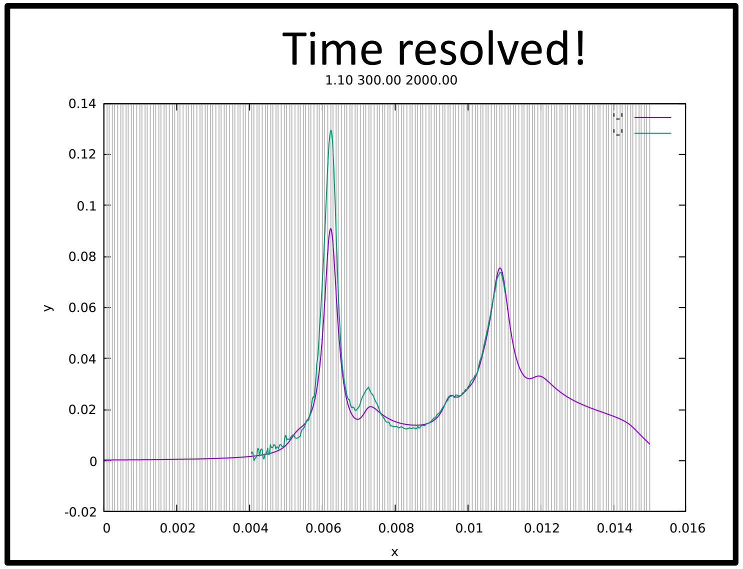




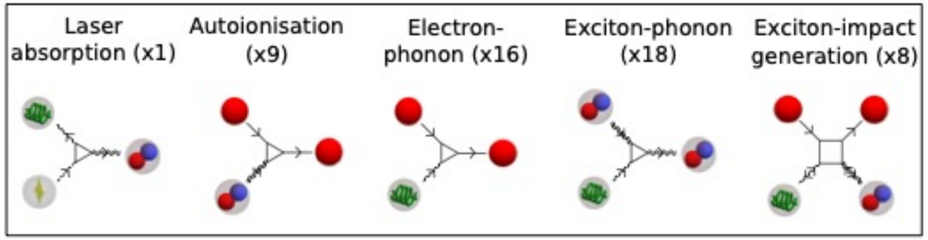
Time-resolved absorption spectra

Dal Forno, Komatsu, Wais, Wadgaonkar, Held, Kono, Battiato, **manuscript**.



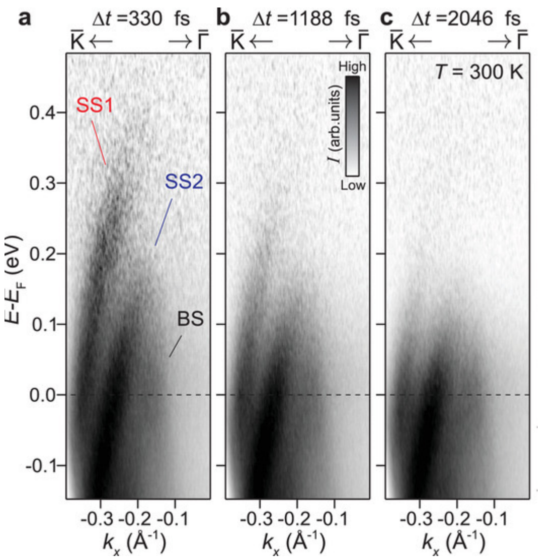


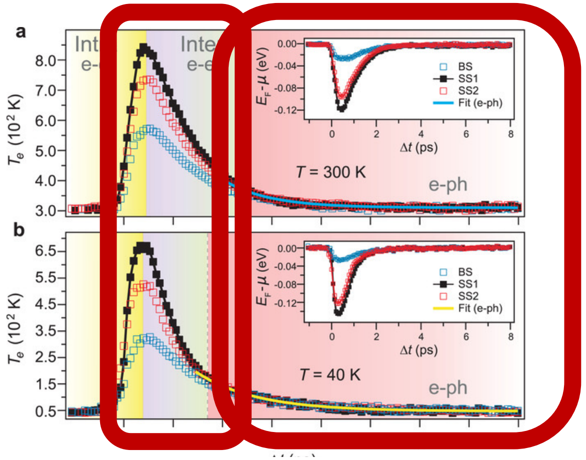
Work in progress

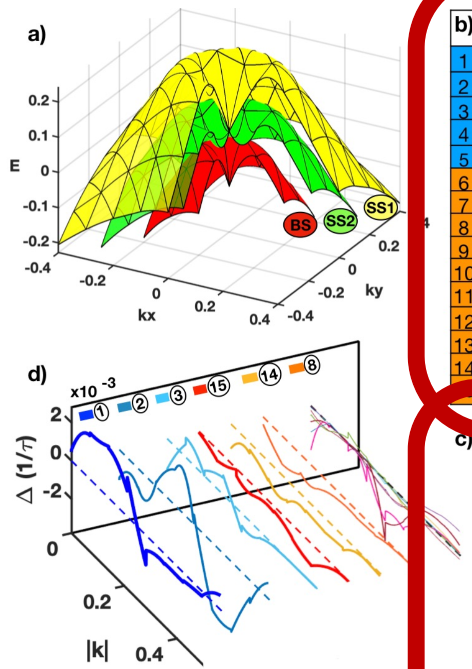


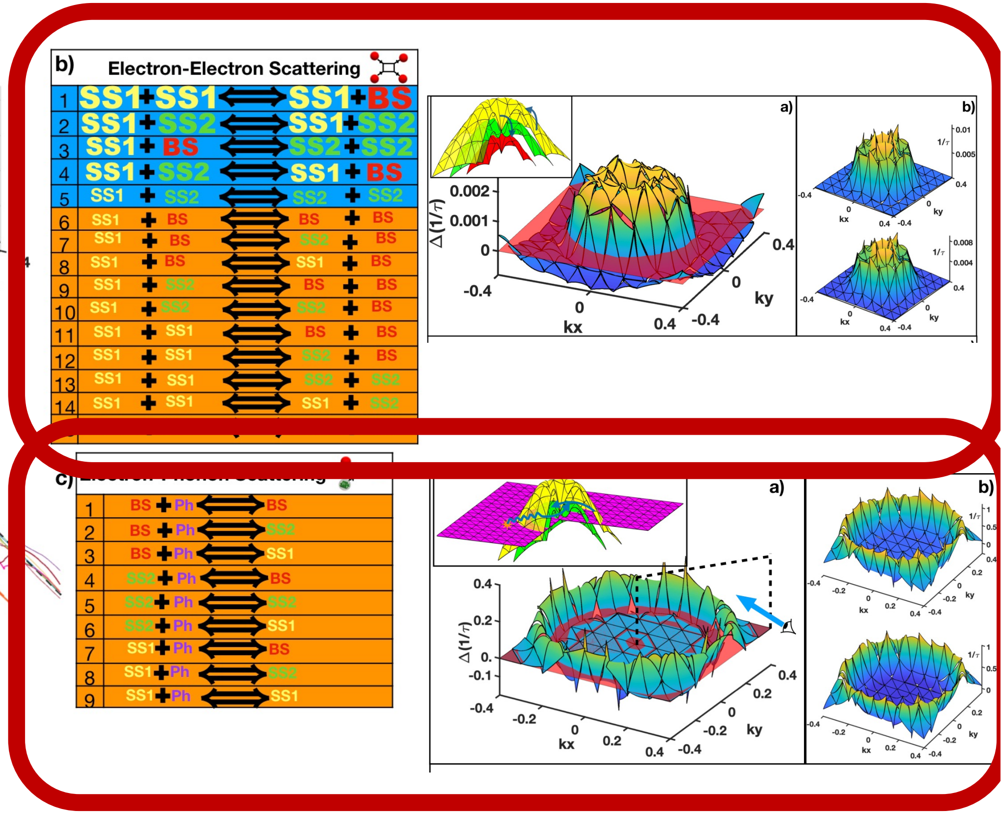
Ultrafast thermalisation pathways in GeTe

Clark, Wadgaonkar, Freyse, Springholz, Battiato, Sanchez-Barriga **Advanced Materials** 34, 2200323 (2022).





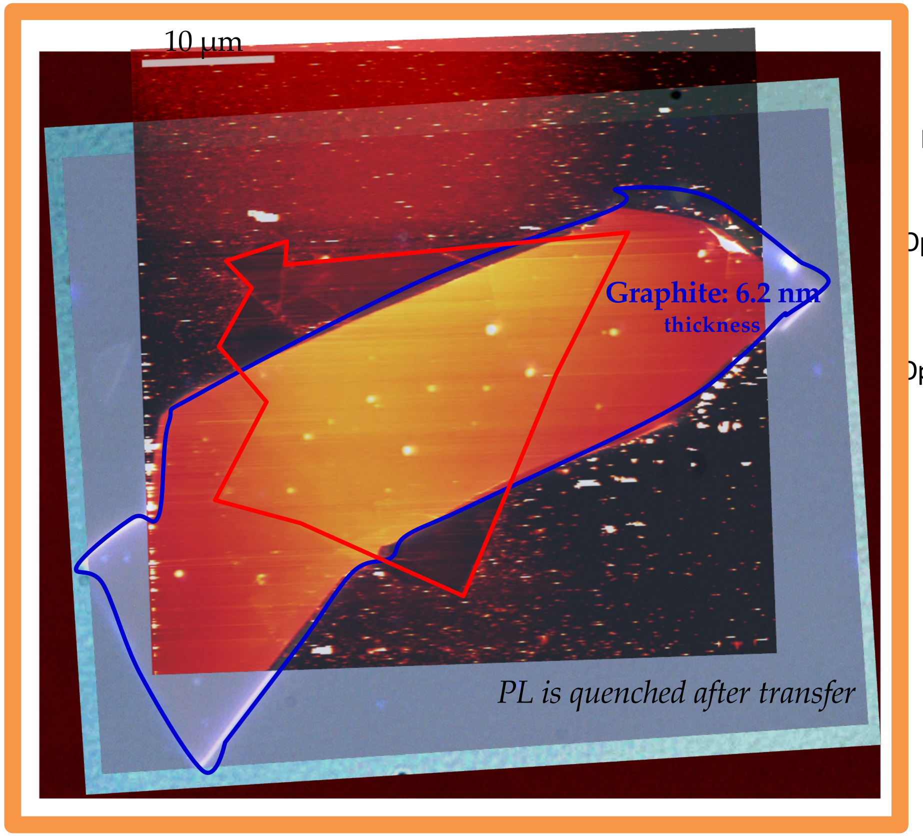




WSe_2 exciton decay

Woo, Wadgaonkar, Xiang, Battiato, Loh, work in progress

Samples we have: **1L-WSe_2 / Si** with different supports

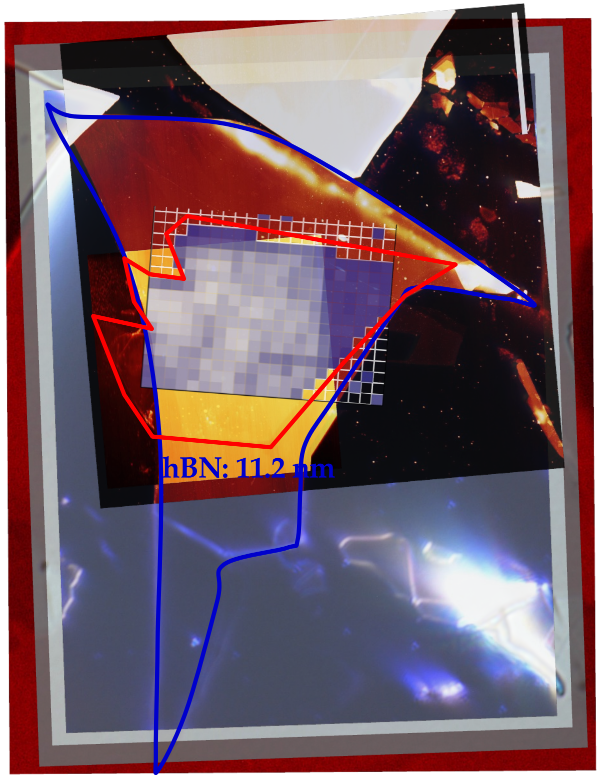


PL (before transfer)

Optical Microscope (bright field)

Optical Microscope (dark field)

AFM



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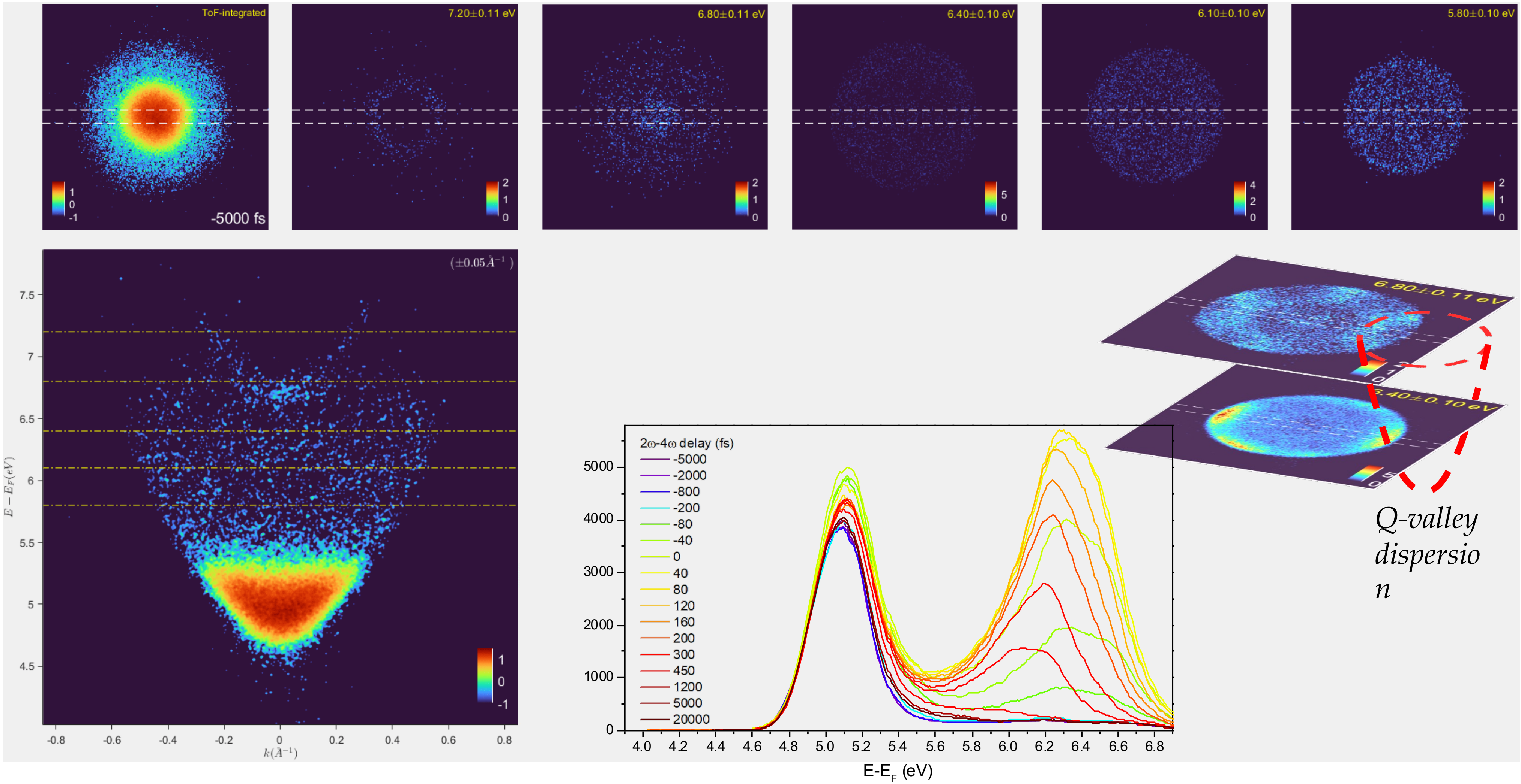

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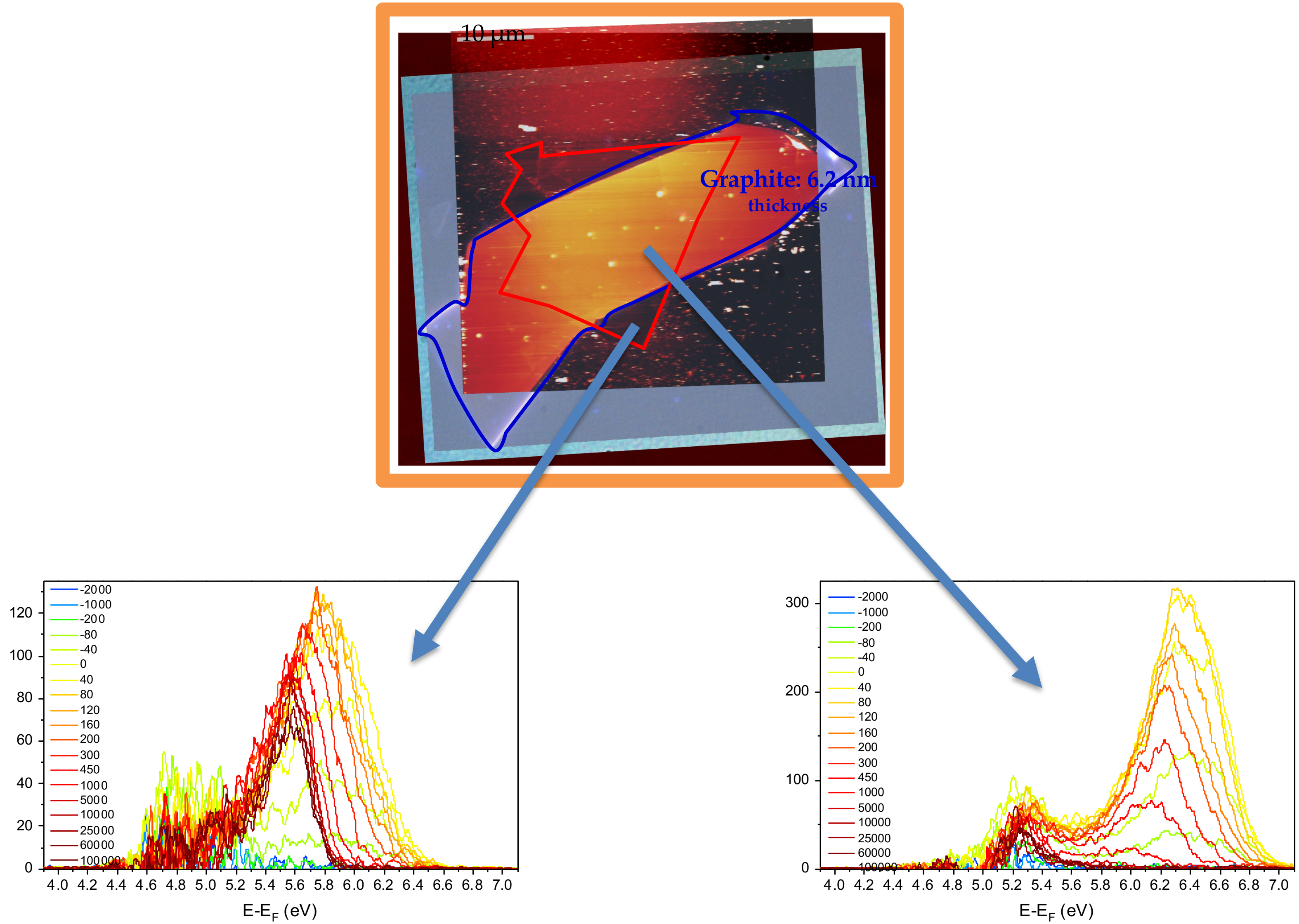

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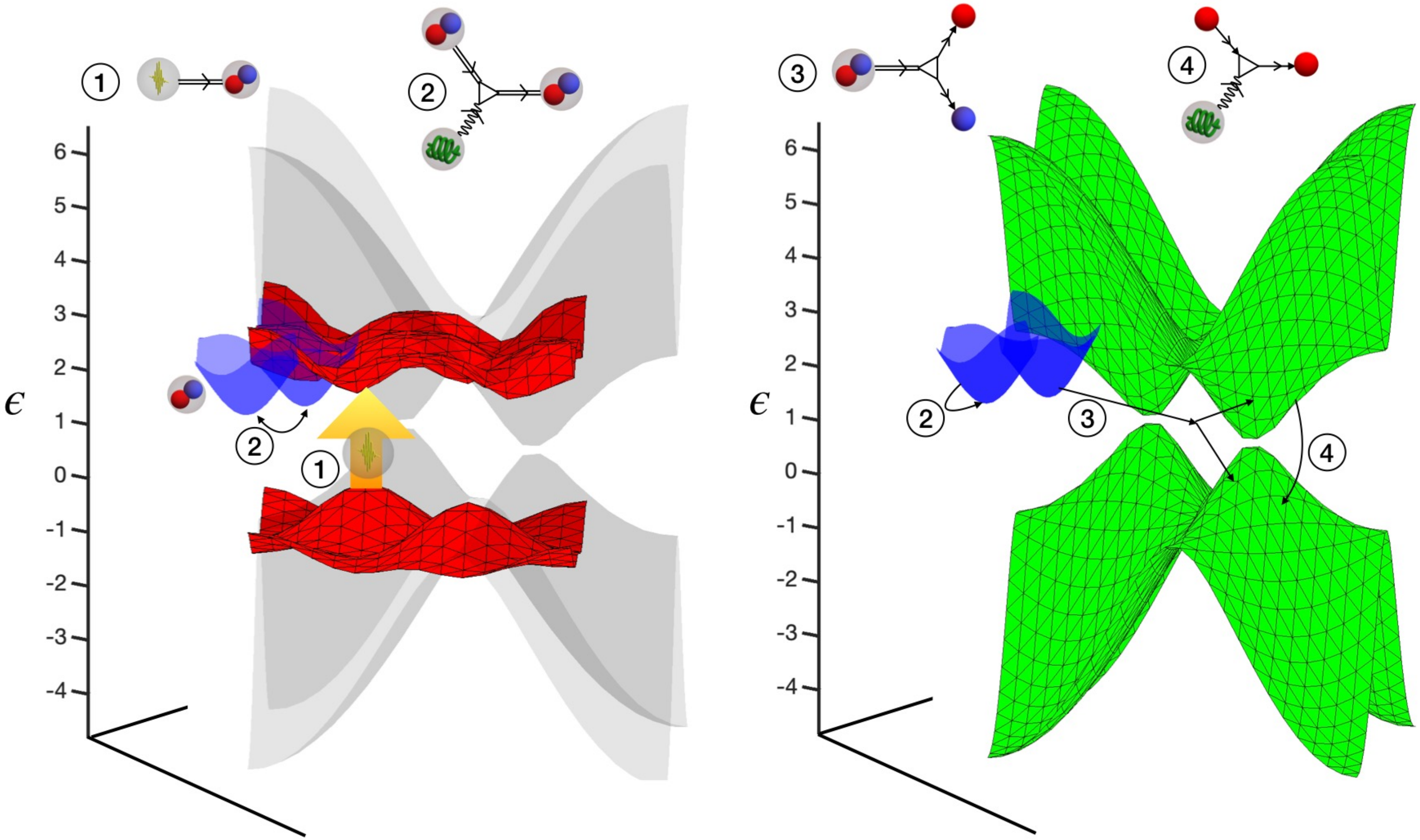

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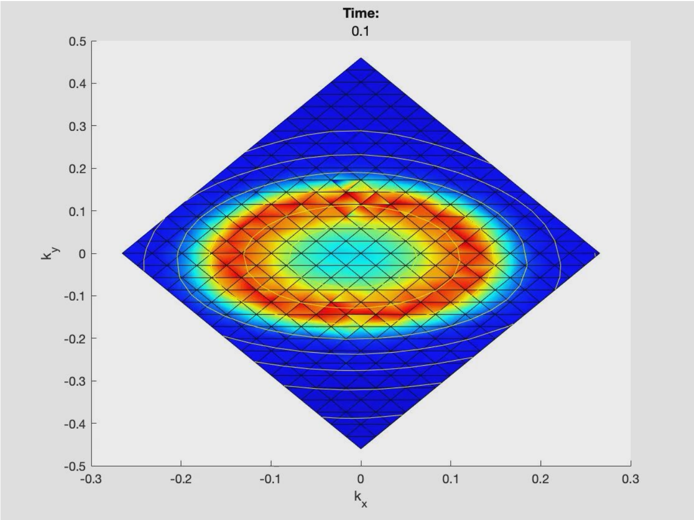

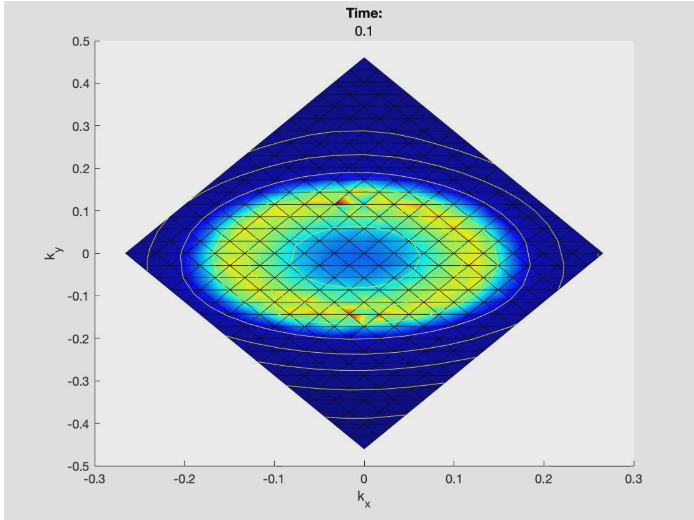

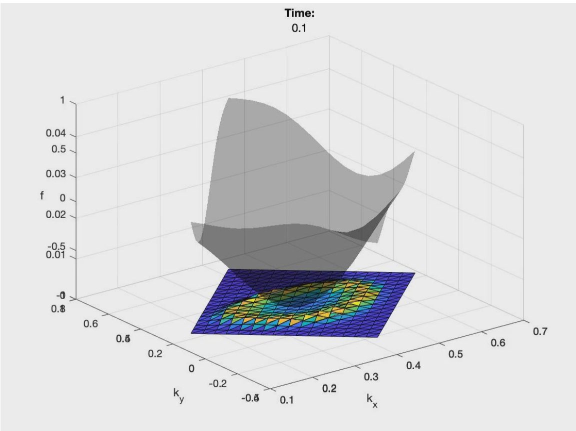

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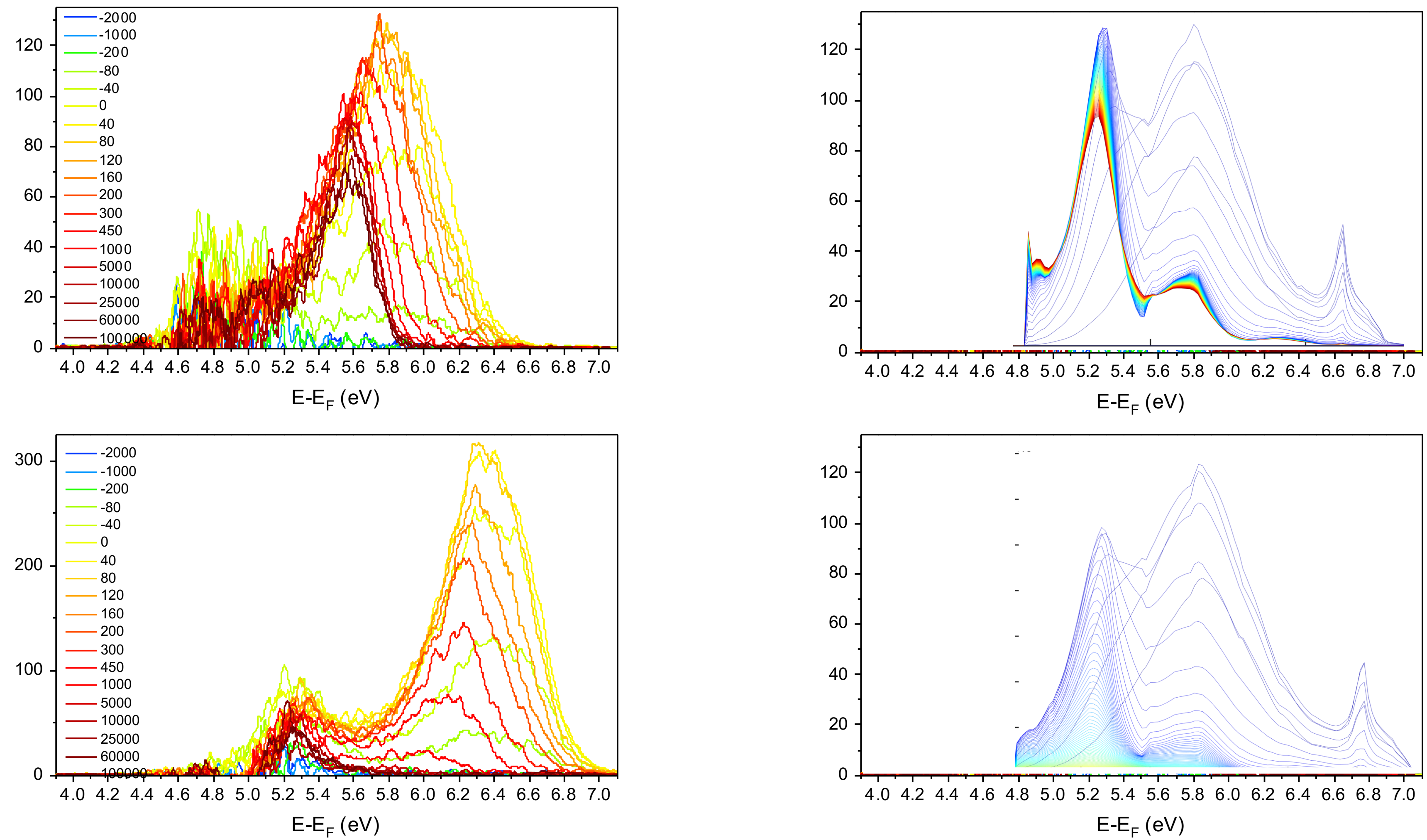

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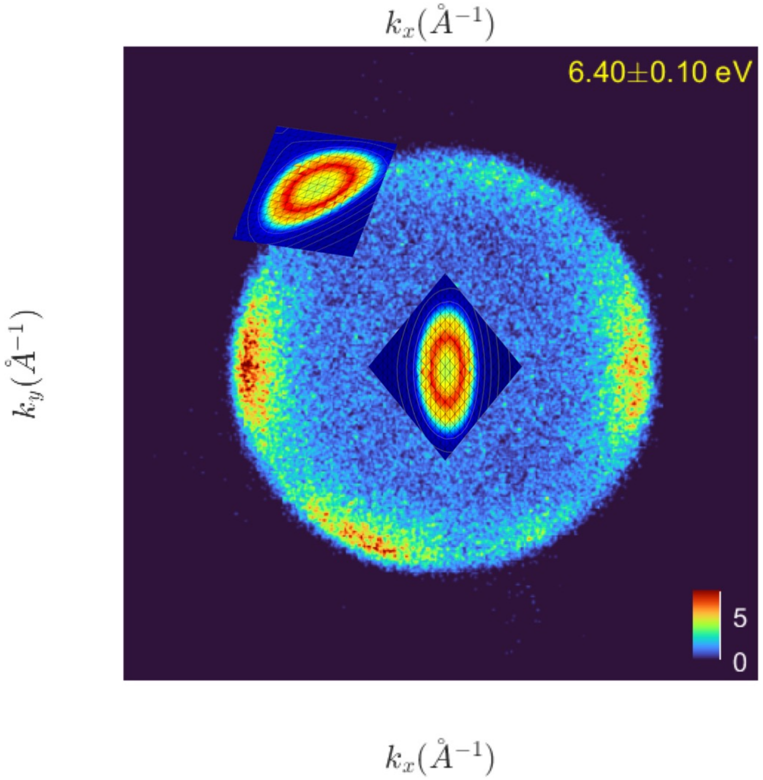

Movie: work in progress