

**HYDRODYNAMIC PHENOMENA IN  
THERMAL TRANSPORT**  
**Universitat Autònoma de Barcelona**  
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**xavier.alvarez@uab.cat**

Purdue, July 2022



Universitat Autònoma de Barcelona



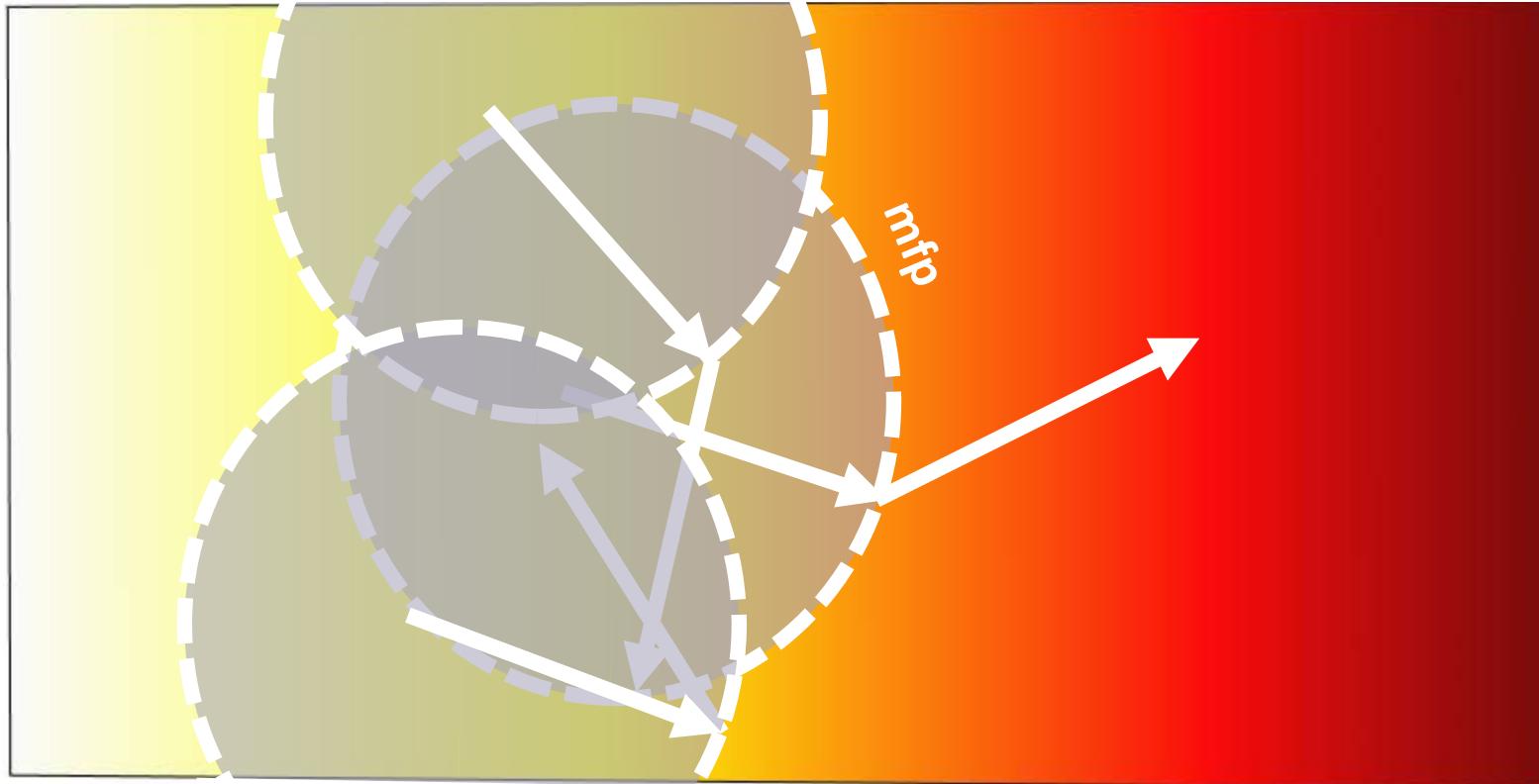
PURDUE, JULY 2022

- Introduction.
- From the phonons to the moments basis
- Hydrodynamic behavior of semiconductors
- BTE calculations for hydrodynamic paràmetres
- New phenomena
- Conclusions

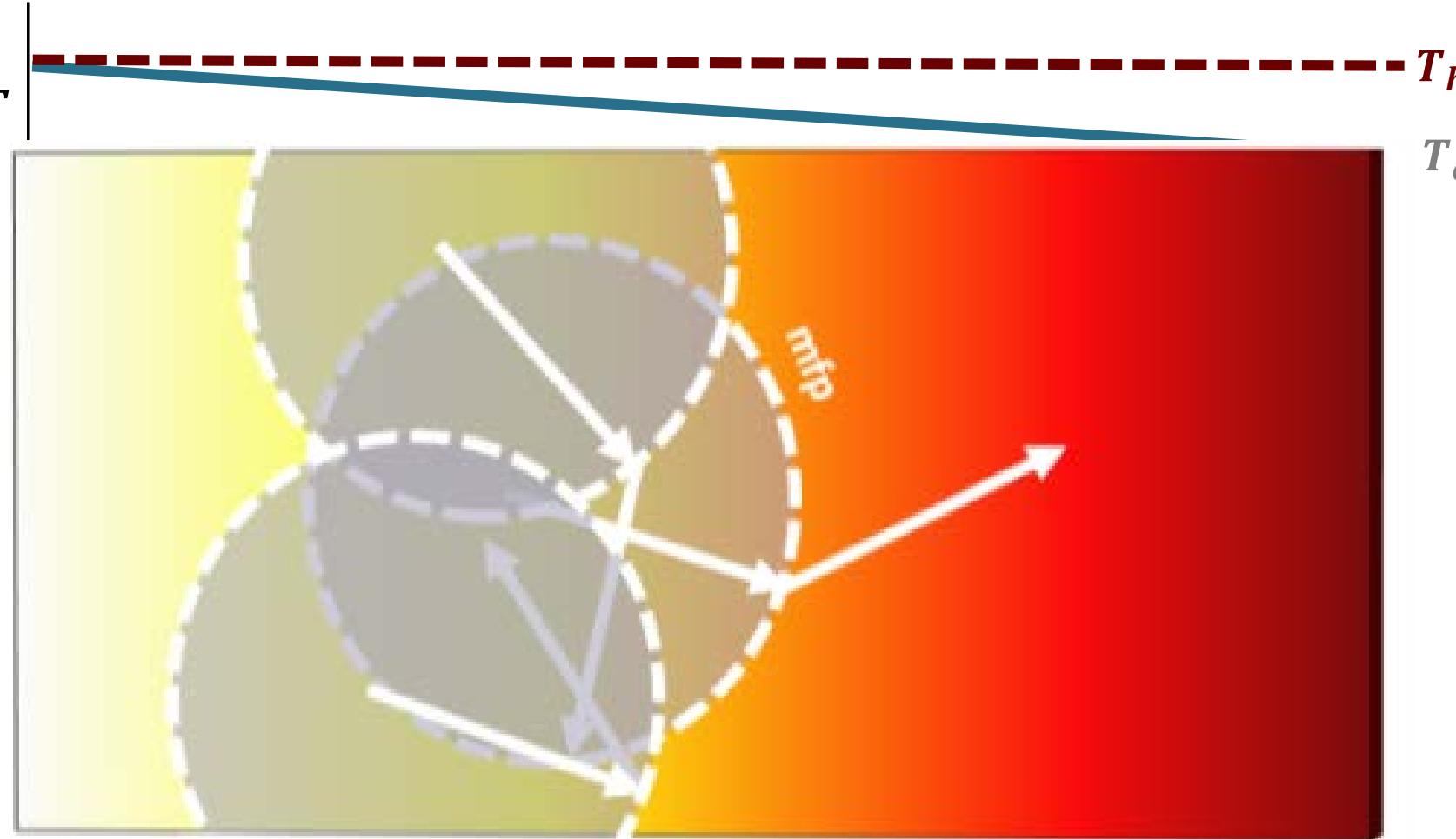
# **INTRODUCTION: THRERMAL TRANSPORT AT THE NANOSCALE**

# Fourier's law

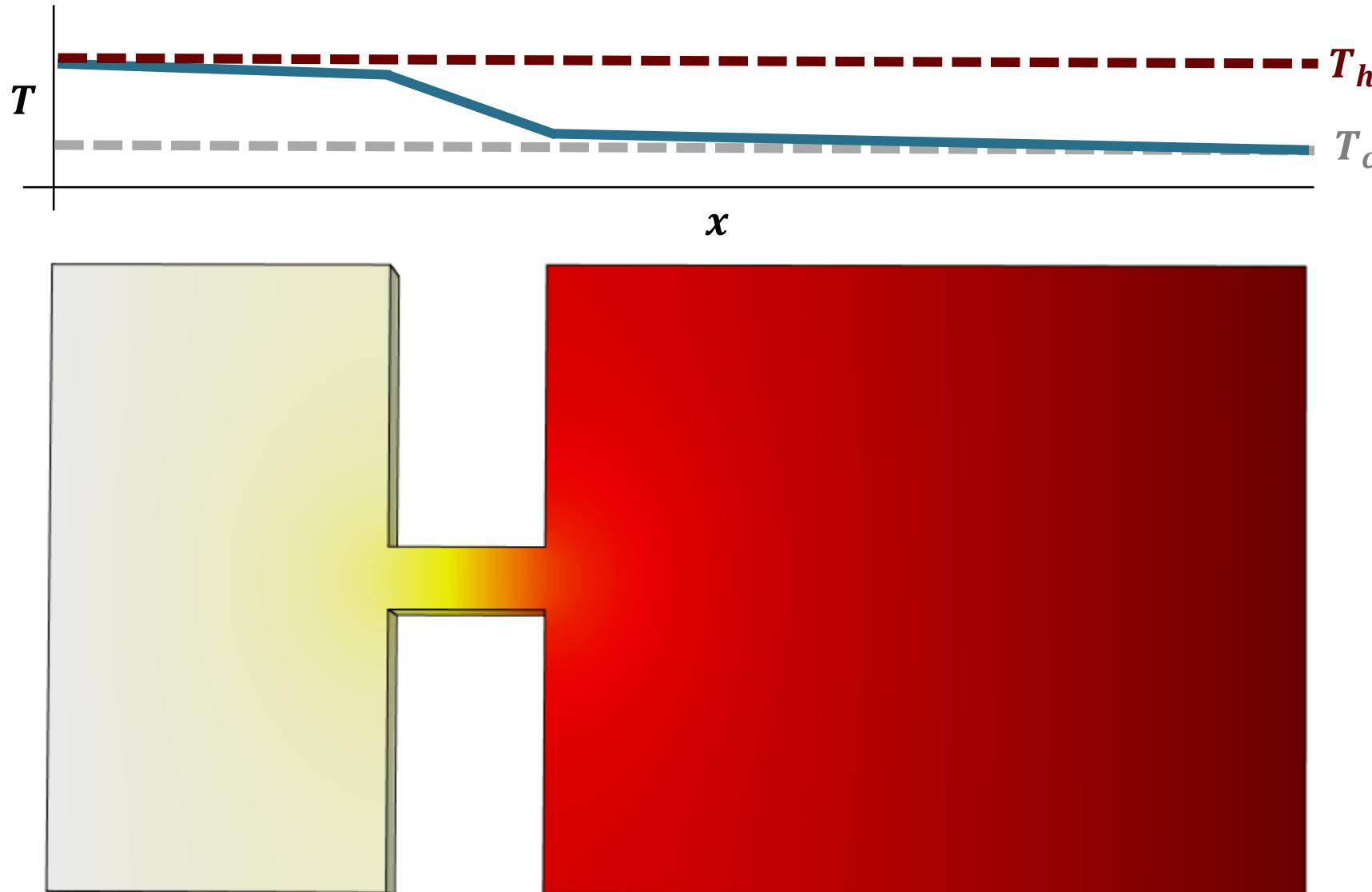
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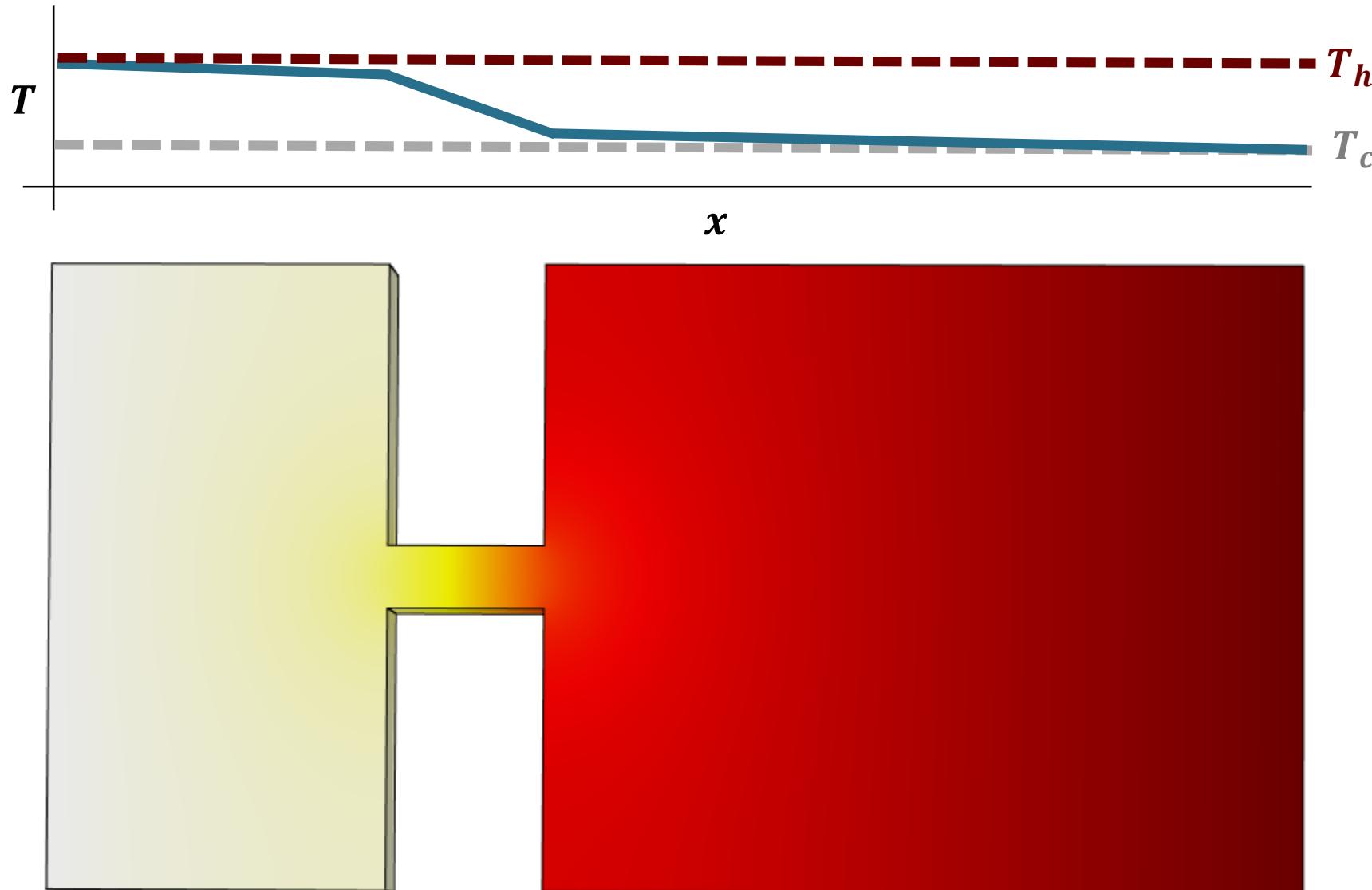
# Fourier's law



# Geometry effects

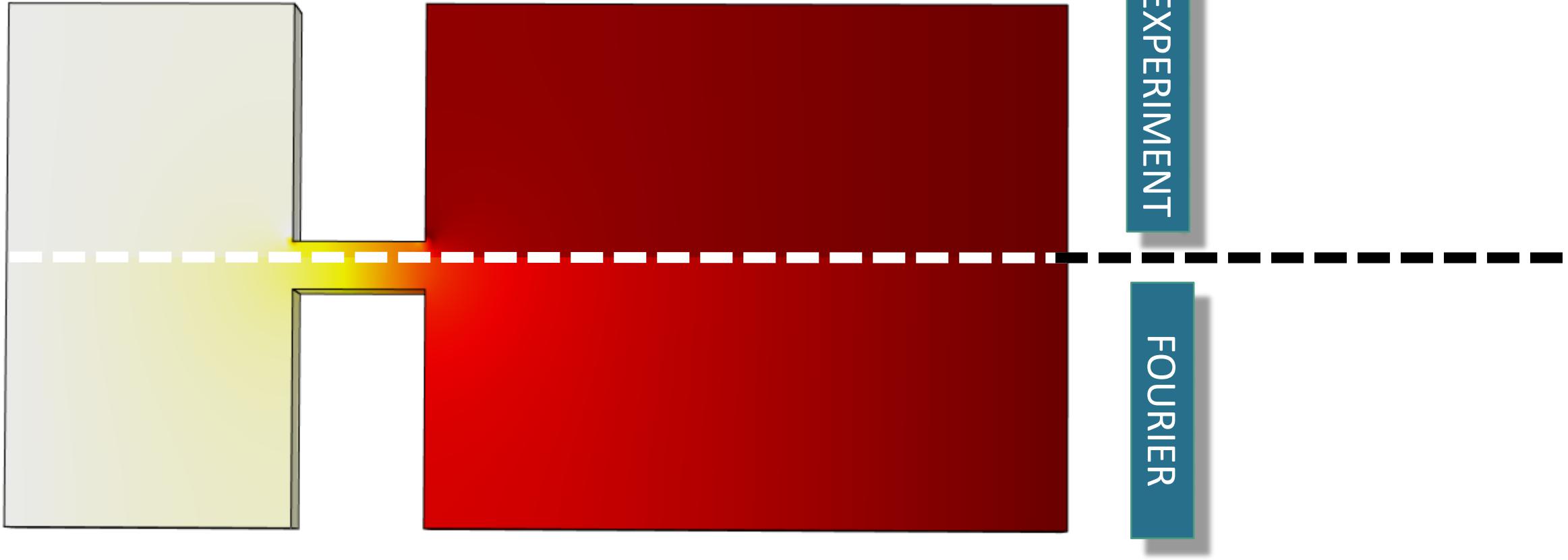


# Geometry effects

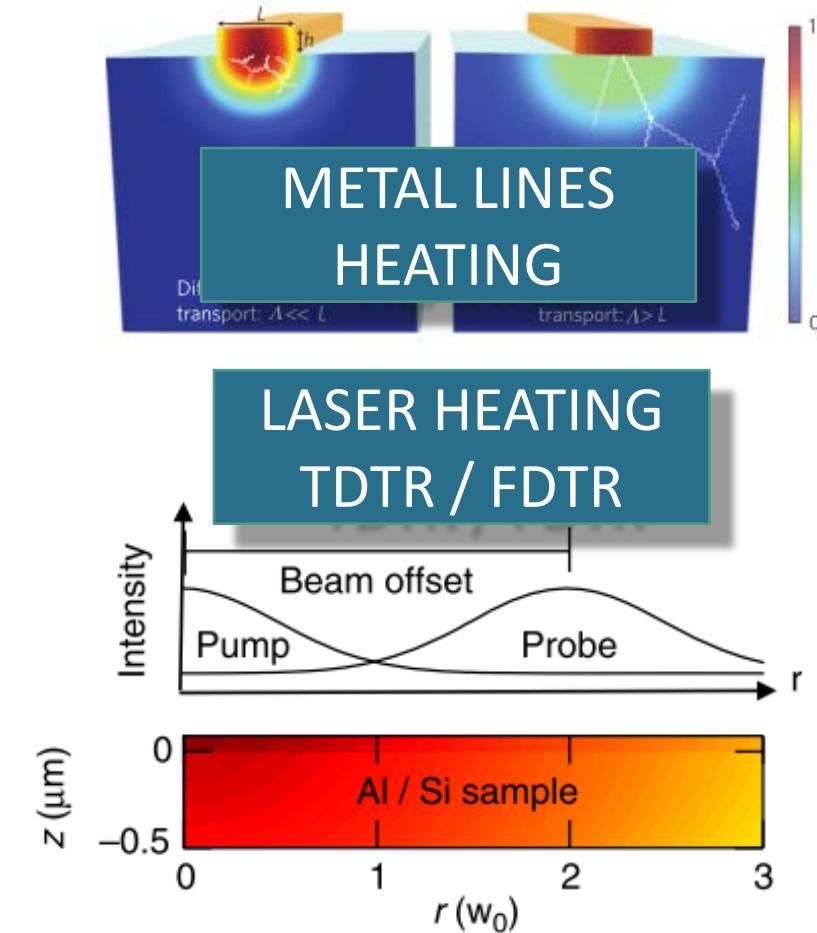
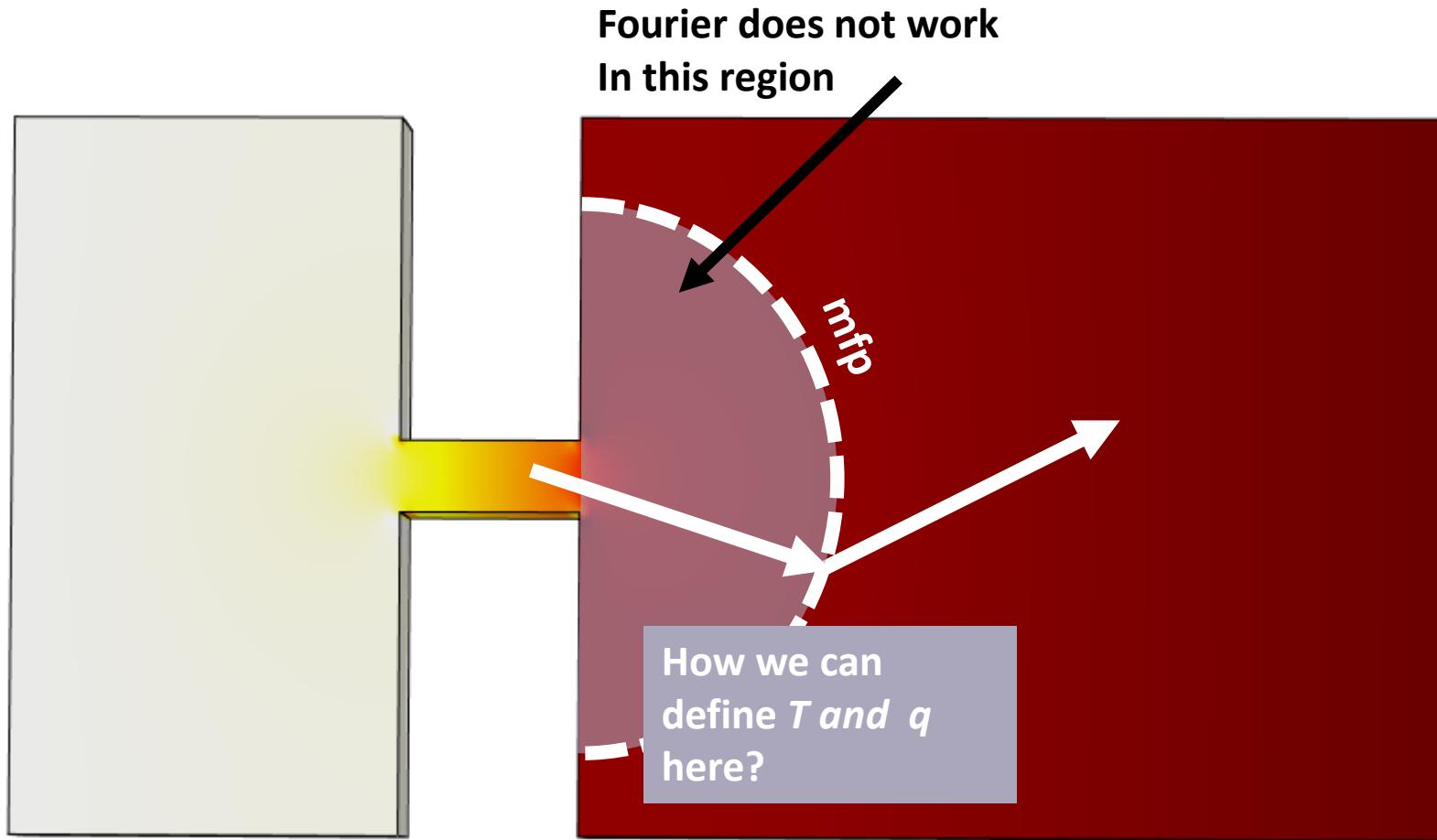


# □ Geometry effects

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# Geometry effects



# Mecanical (Hamiltonian) vs Entropic description



The main goal of  
the talk is to find  
contact points!

# **PHONONS VS MOMENTS BASIS**

# Boltzmann Transport Equation

PHONONS

$$f_k(x, t)$$



BTE

$k$  equations for the  $k$  modes

$$\frac{\partial f_k}{\partial t} + \nu \cdot \frac{d f_k}{dT} \nabla T = C(f_k)$$

# Boltzmann Transport Equation

PHONONS

$$f_k(x, t)$$



BTE

$k$  equations for the  $k$  modes

$$\frac{\partial f_k}{\partial t} + \nu \cdot \frac{df_k}{dT} \nabla T = \frac{f_k - f_k^0}{\tau_k}$$

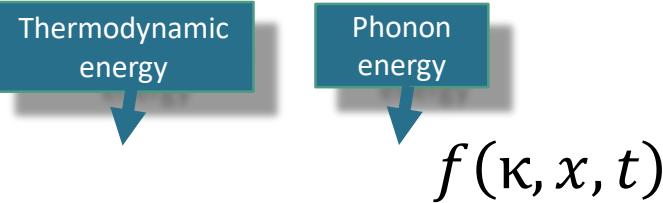
# From phonons $f(\kappa, x, t)$ to moments $Q^{(n)}(x, t)$

0<sup>th</sup> ORDER: Energy

1<sup>st</sup> ORDER: Heat flux

2<sup>nd</sup> ORDER: Flux of the flux

n<sup>th</sup> ORDER



$$q(x, t) = \int \hbar \omega_k \vec{v}_k f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

$$Q^{(2)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdot \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

$$Q^{(n)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdots \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

# From phonons $f(\kappa, x, t)$ to moments $Q^{(n)}(x, t)$

0<sup>th</sup> ORDER: Energy

1<sup>st</sup> ORDER: Heat flux

2<sup>nd</sup> ORDER: Flux of the flux

n<sup>th</sup> ORDER

$$c(x, t) = \int \hbar \omega_k f(\kappa, x, t)$$

Thermodynamic energy

Thermodynamic Heat flux

Phonon energy

Phonon Heat flux

$$q(x, t) = \int \hbar \omega_k \vec{v}_k f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

$$Q^{(2)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdot \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

$$Q^{(n)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdots \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

# From phonons $f(\kappa, x, t)$ to moments $Q^{(n)}(x, t)$

0<sup>th</sup> ORDER: Energy

1<sup>st</sup> ORDER: Heat flux

2<sup>nd</sup> ORDER: Flux of the flux

n<sup>th</sup> ORDER

$$c(x, t) = \int \hbar \omega_k f(\kappa, x, t)$$

Thermodynamic Heat flux

$$a(x, t) = \int \hbar \omega_k \vec{v}_k f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

Phonon Heat flux

$$Q^{(2)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdot \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

Thermodynamic Flux of the flux

Phonon Stress T

$$Q^{(n)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdots \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

# From phonons $f(\kappa, x, t)$ to moments $Q^{(n)}(x, t)$

0<sup>th</sup> ORDER: Energy

$$\epsilon(x, t) = \int \hbar \omega_k f(\kappa, x, t) d^3 k / (2\pi)^3$$

1<sup>st</sup> ORDER: Heat flux

$$a(x, t) = \int \hbar \omega_k \vec{v}_k f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

Thermodynamic Flux of the flux

Phonon Stress T

2<sup>nd</sup> ORDER: Flux of the flux

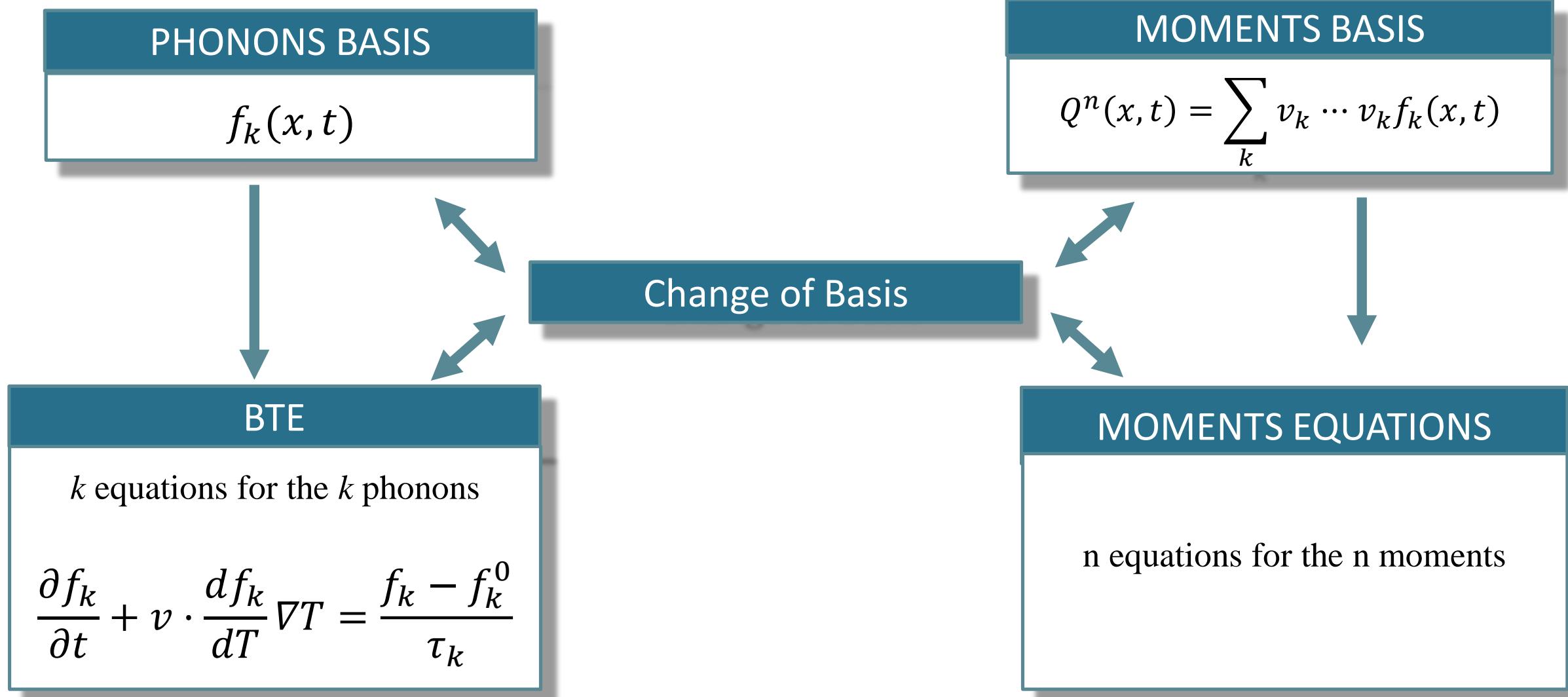
$$Q^{(2)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdot \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

n<sup>th</sup> ORDER

$$Q^{(n)}(x, t) = \int \hbar \omega_k (\vec{v}_k \cdots \vec{v}_k) f(\kappa, x, t) \frac{d^3 k}{(2\pi)^3}$$

Moments are more easily to measure experimentally than phonon abundances: Temperature, fluxes, etc...

# From phonons $f(k, x, t)$ to moments $Q^{(n)}(x, t)$



## From phonons $f(k, x, t)$ to moments $Q^{(n)}(x, t)$

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$$\frac{\partial f}{\partial t} + \nu \cdot \nabla f = - \frac{f - f_0}{\tau}$$

$$c_V \frac{\partial T}{\partial t} - \nabla \cdot q = 0$$

0<sup>th</sup> ORDER: Energy conservation

## From phonons $f(k, x, t)$ to moments $Q^{(n)}(x, t)$

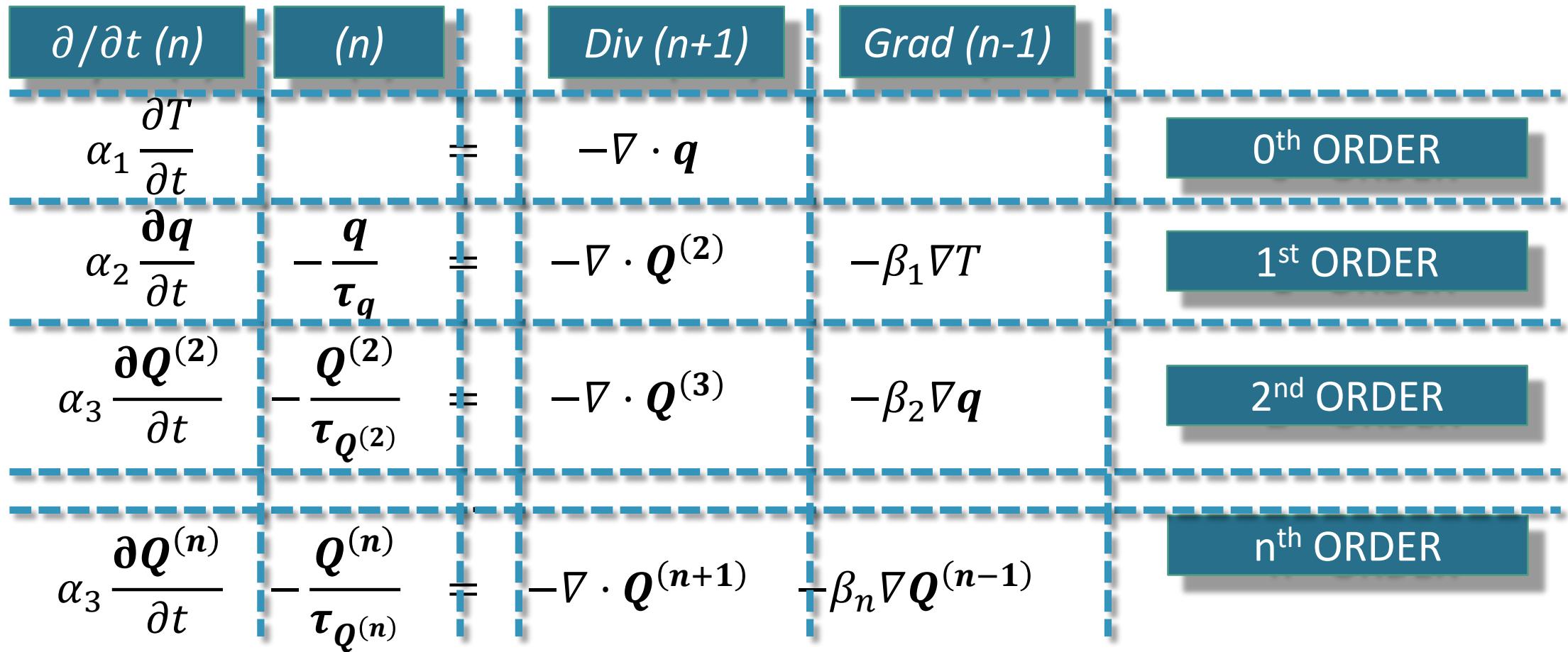
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$$\int \frac{\partial f}{\partial t} + v \cdot \nabla f = - \frac{f - f_0}{\tau}$$

$$\frac{\partial q}{\partial t} - \nabla \cdot Q = \frac{q}{\tau_q}$$

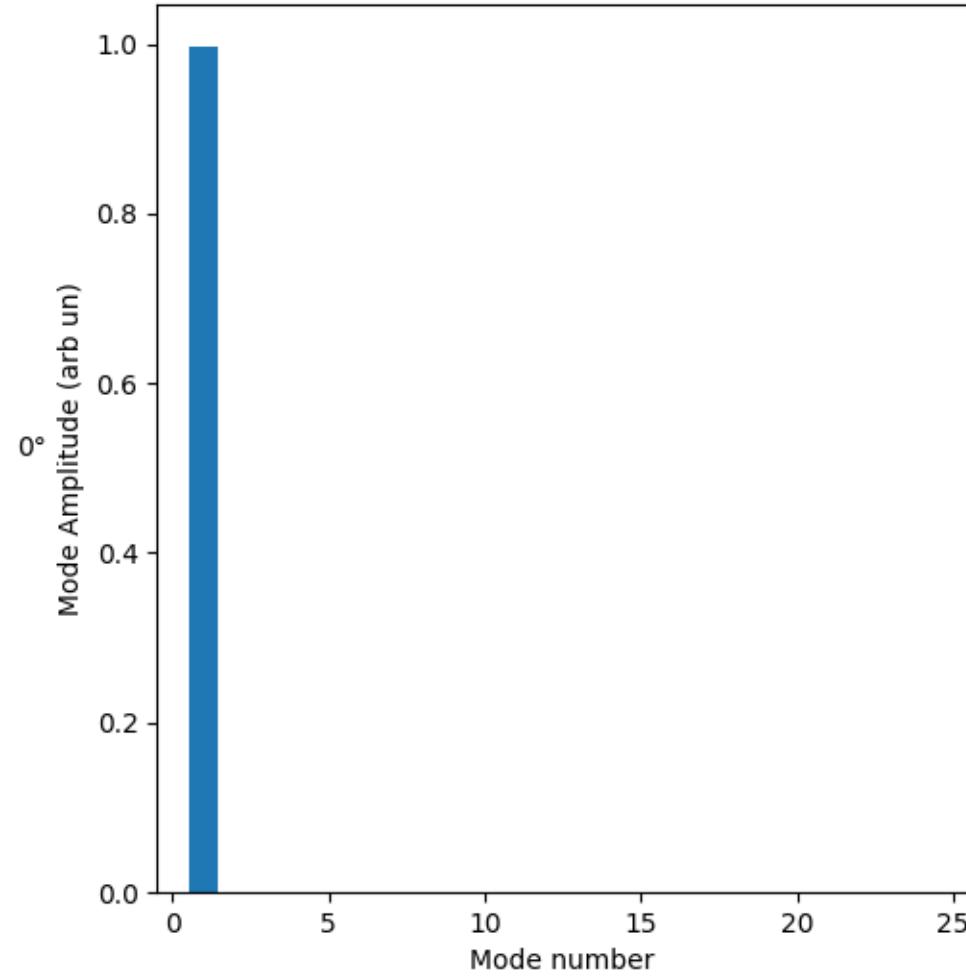
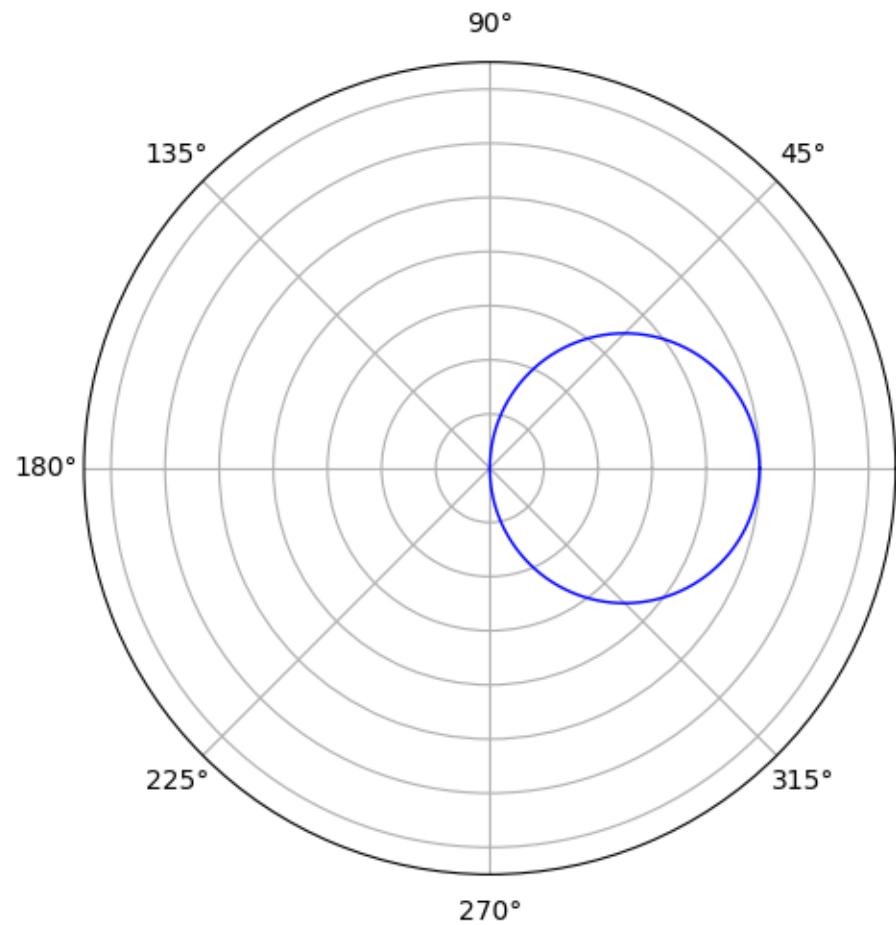
1<sup>st</sup> ORDER: Energy conservation

# From phonons $f(k, x, t)$ to moments $Q^{(n)}(x, t)$



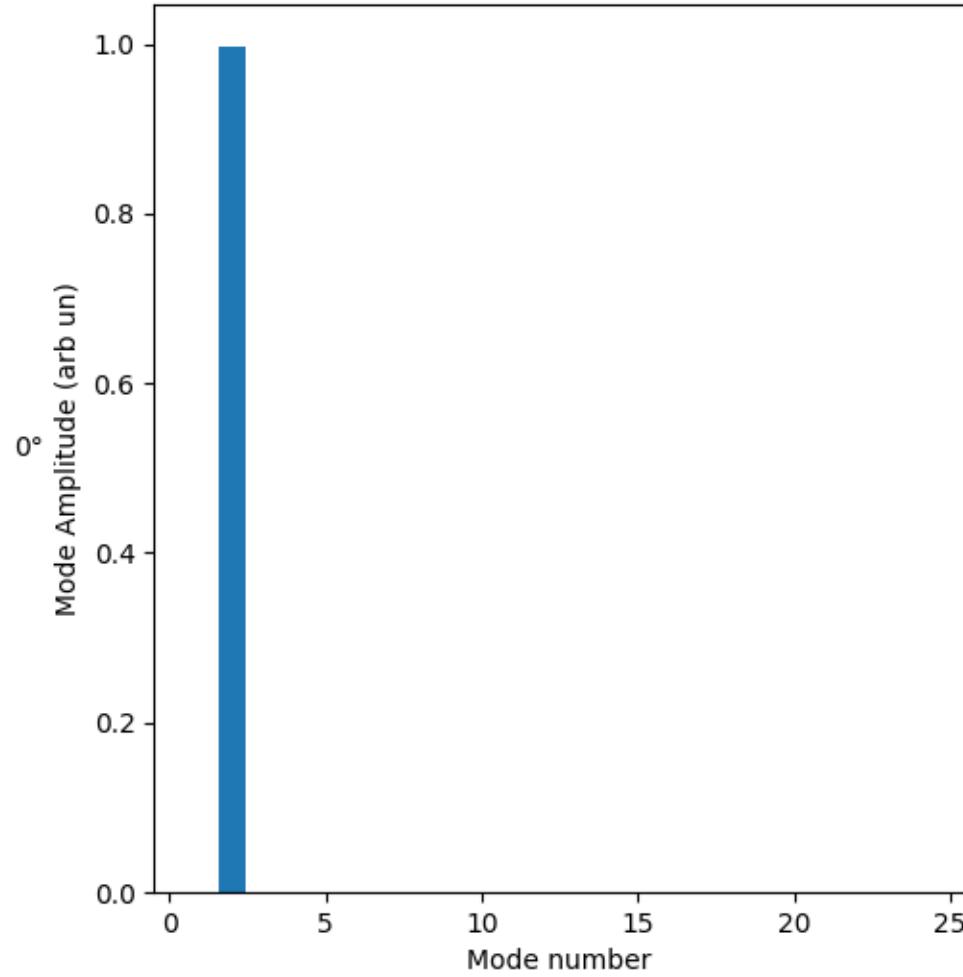
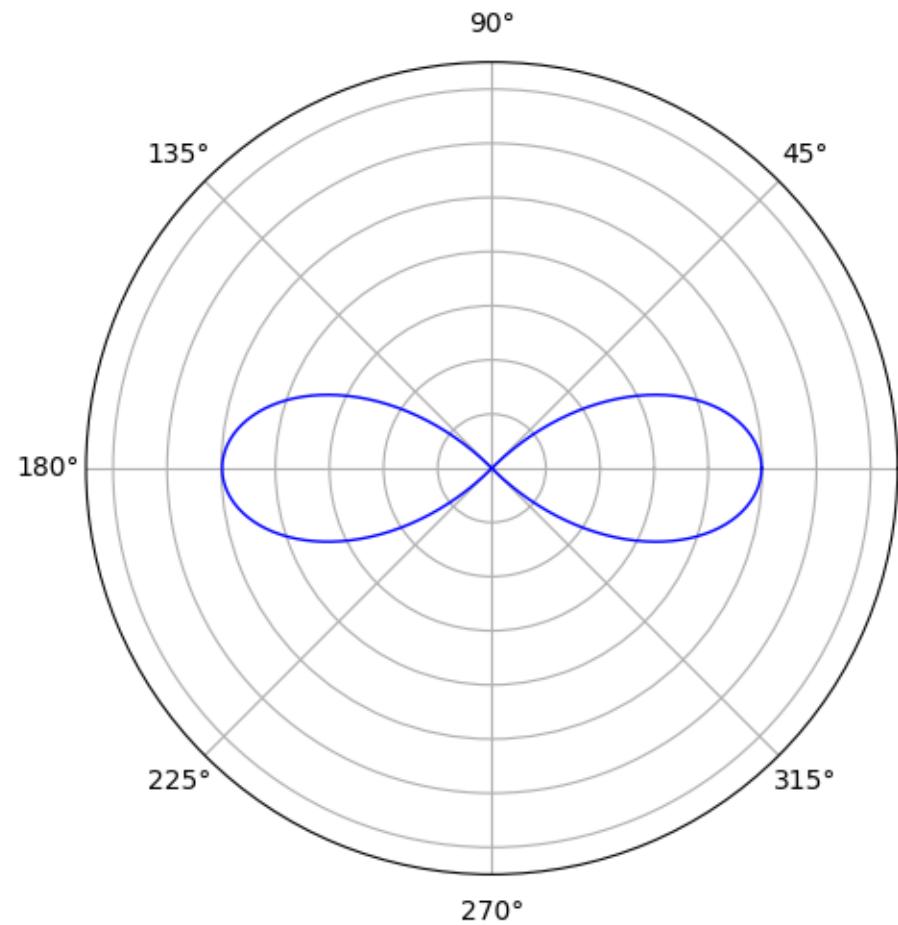
# Moments of the distribution

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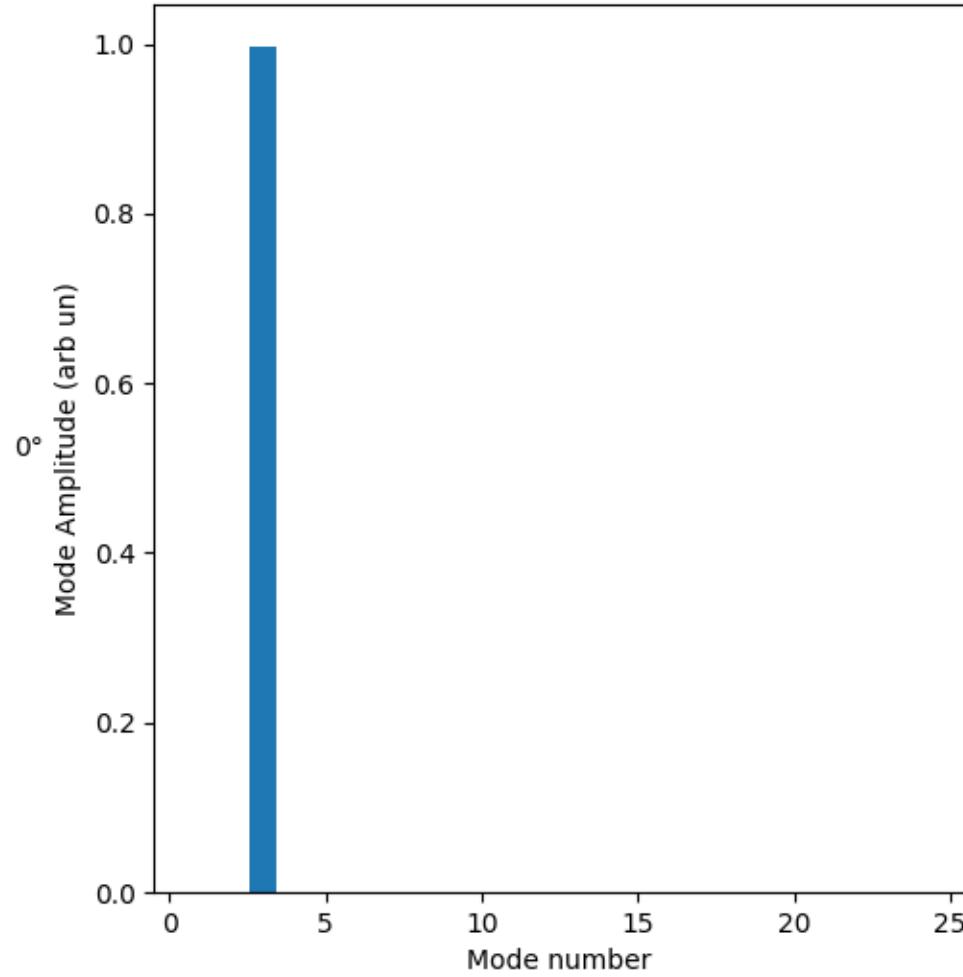
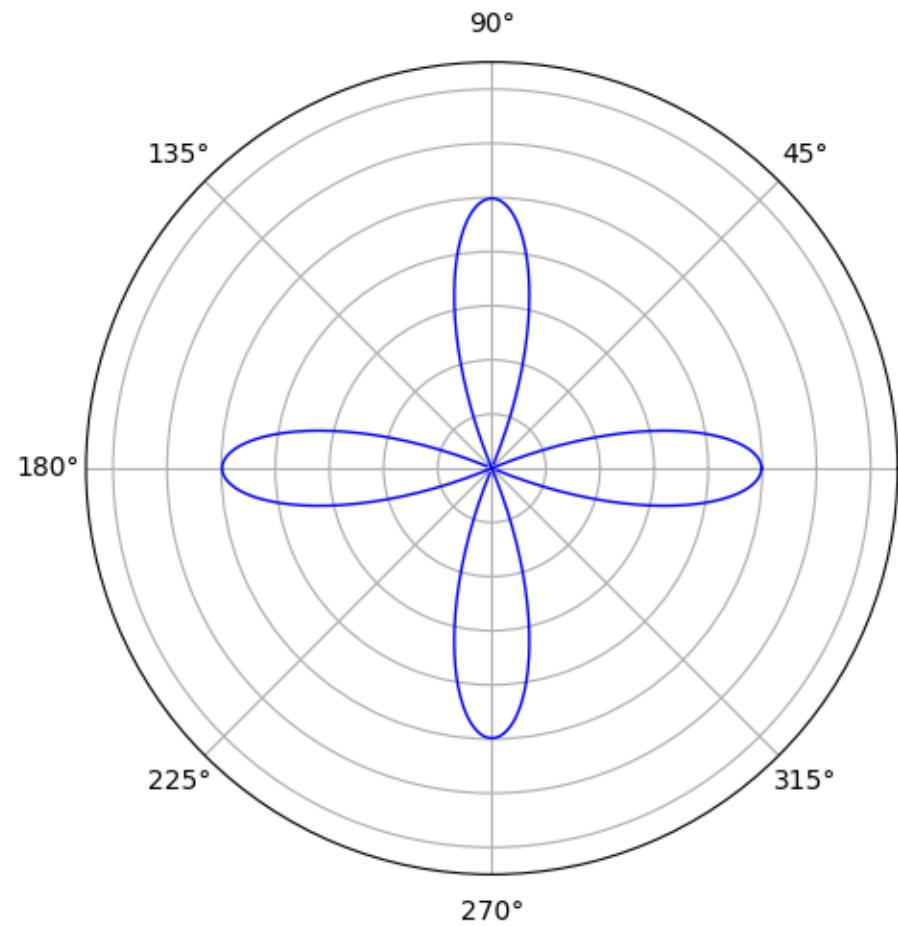
# Moments of the distribution

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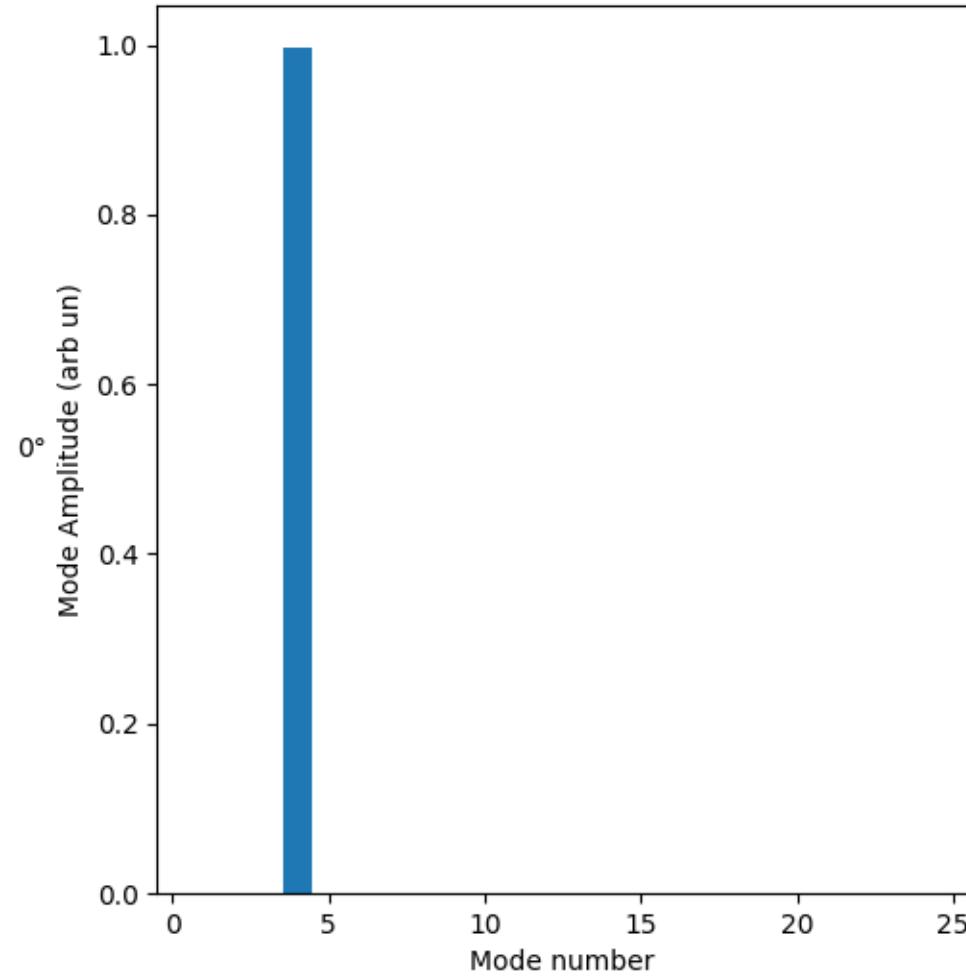
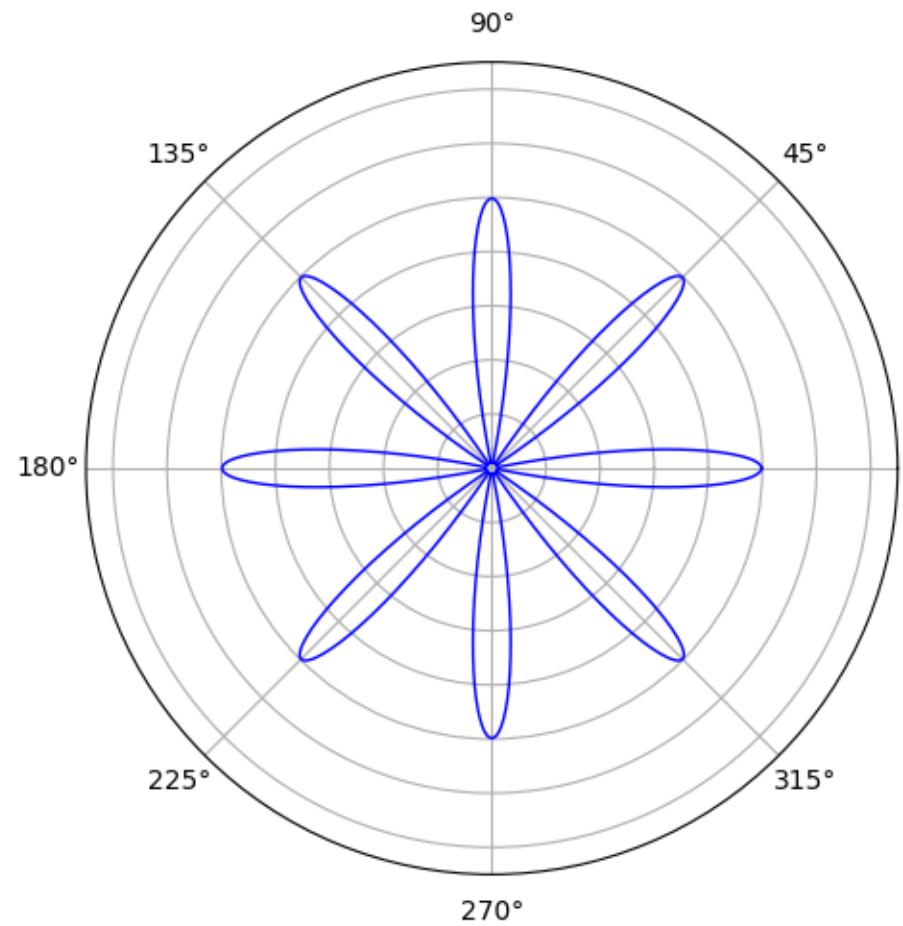
# Moments of the distribution

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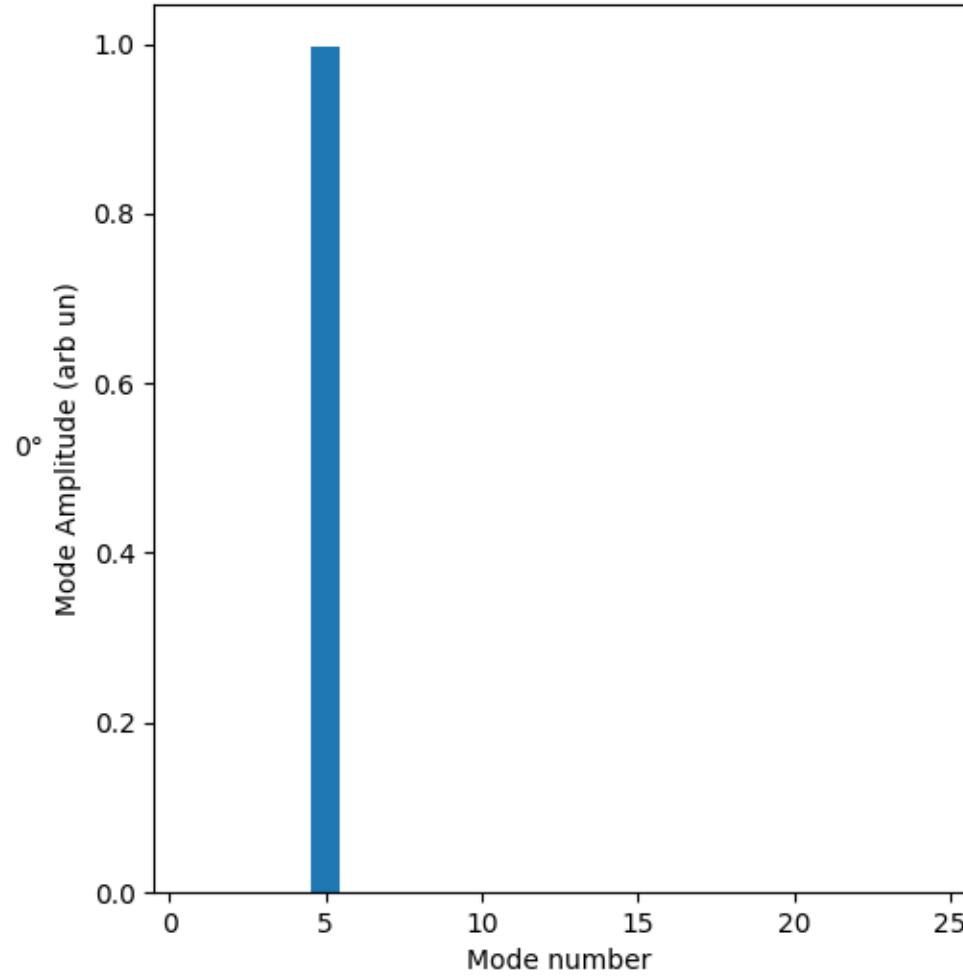
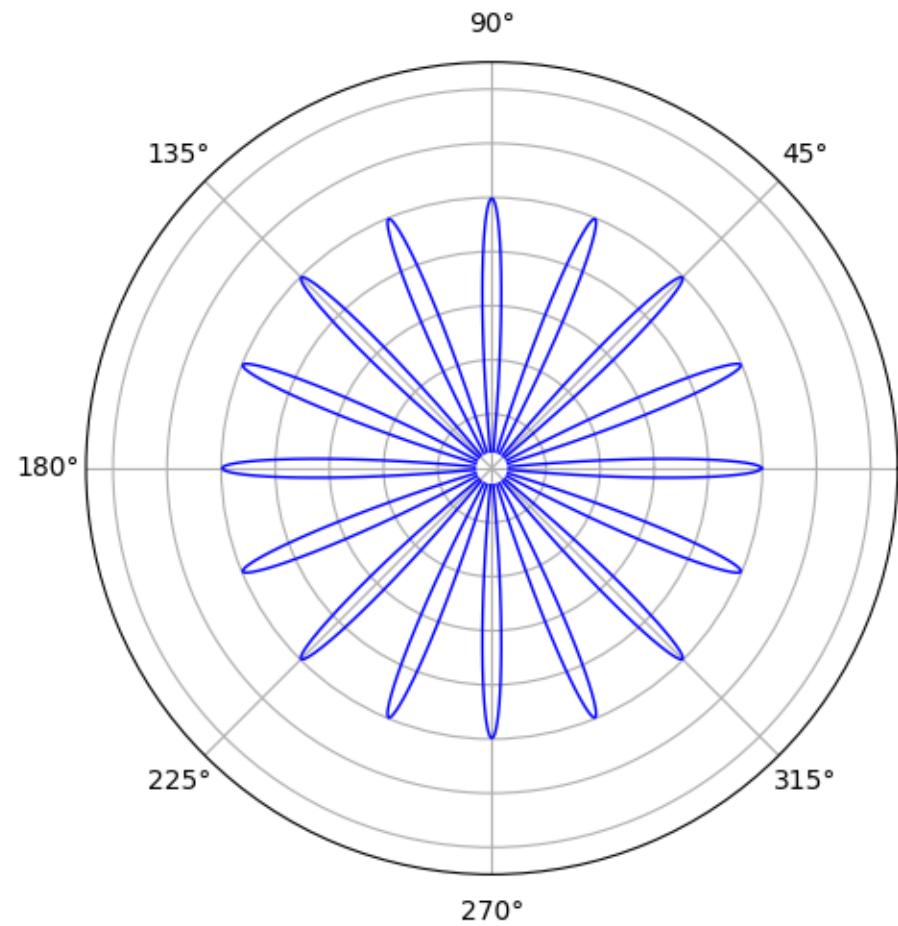


# Moments of the distribution

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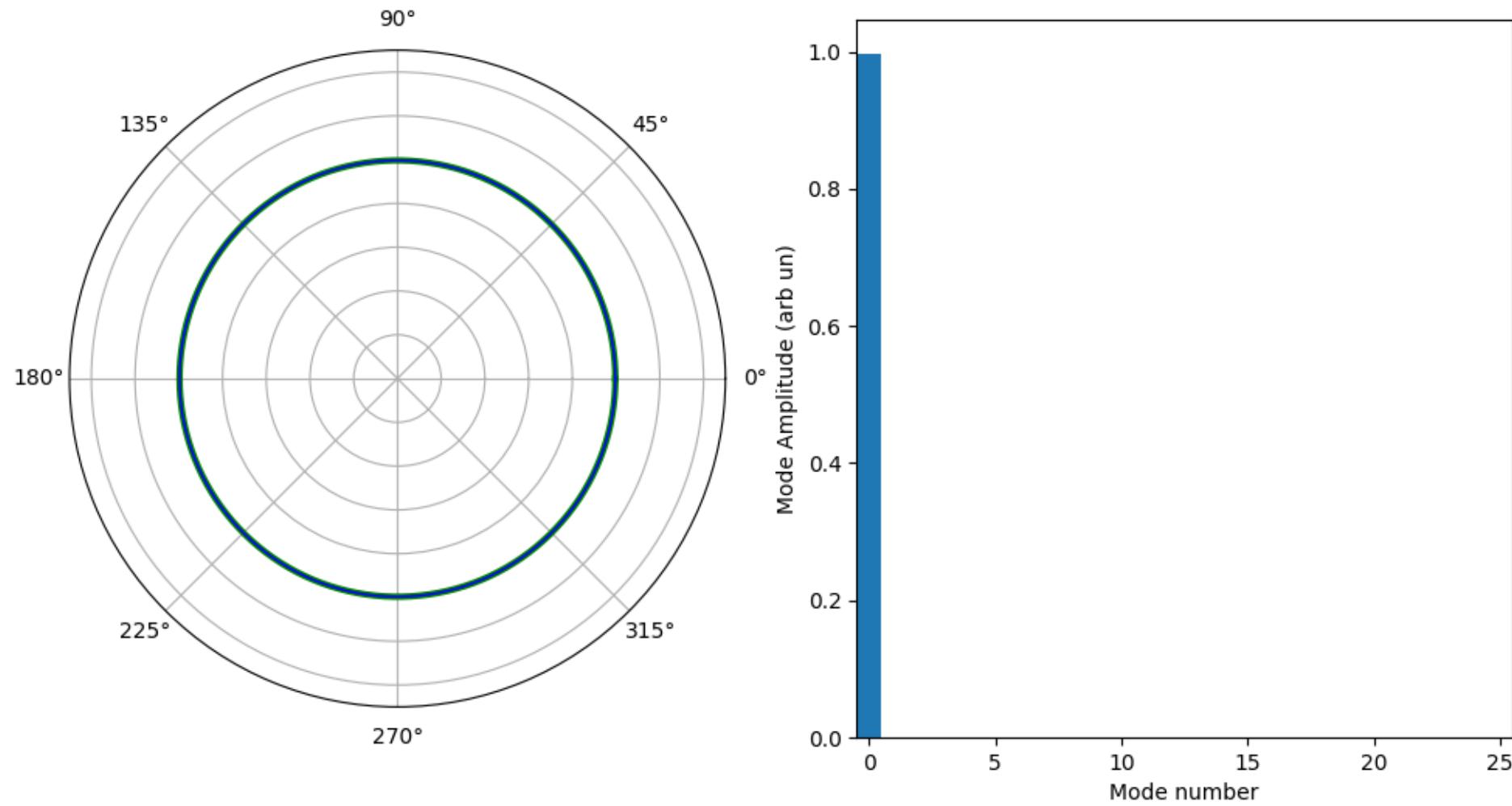


# Moments of the distribution



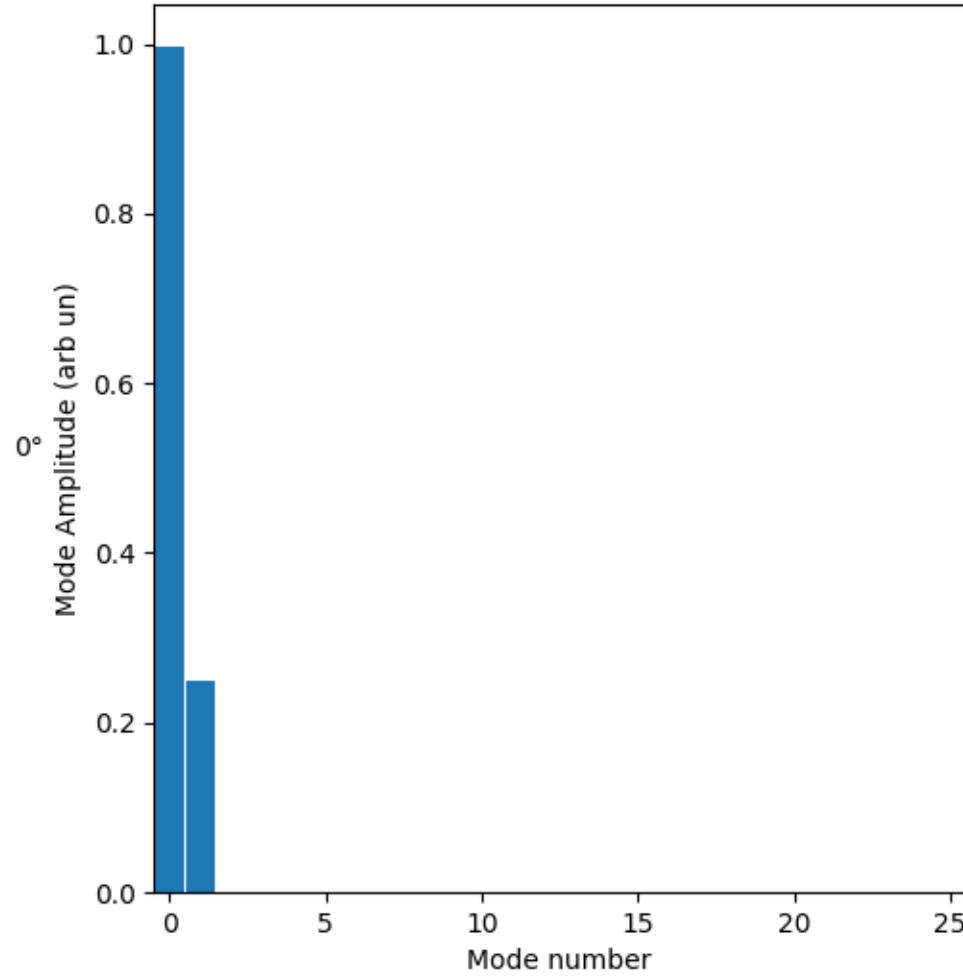
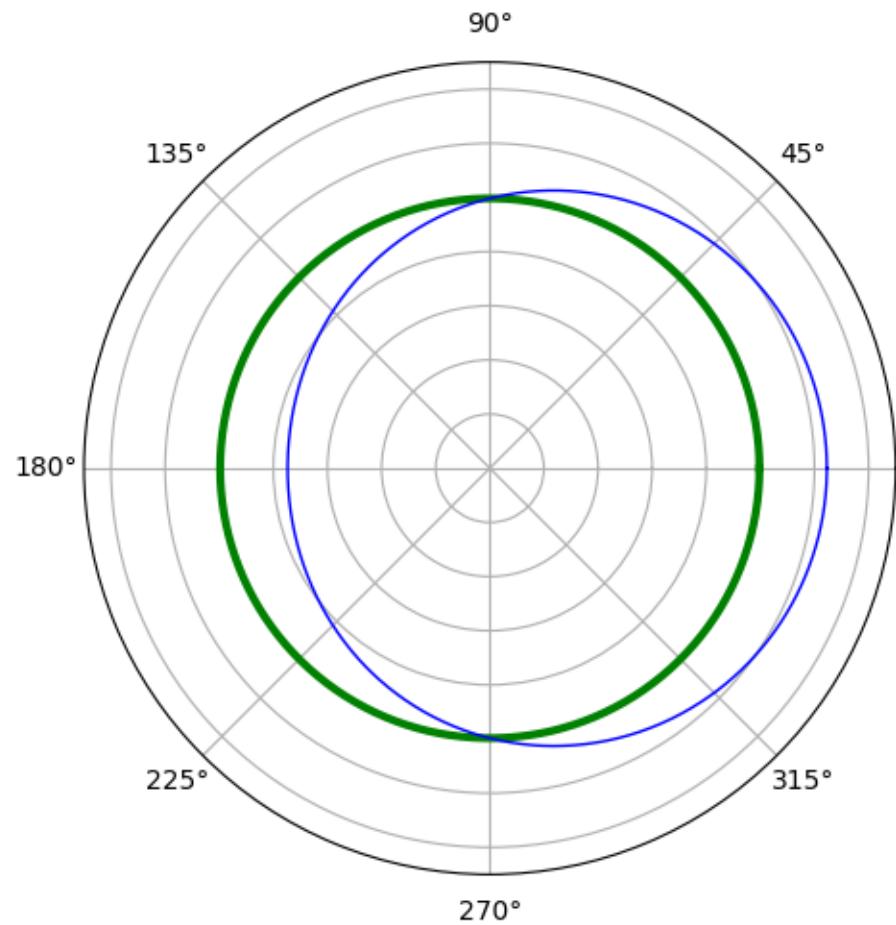
# Moments of the distribution

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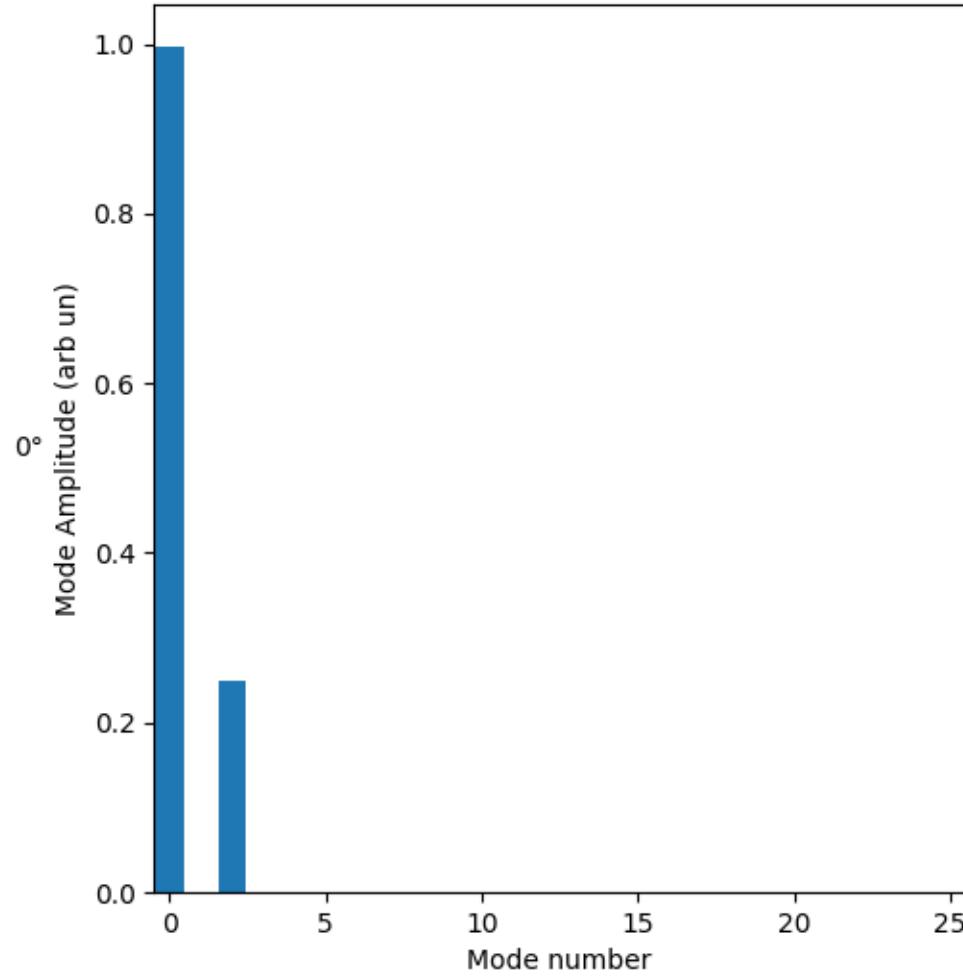
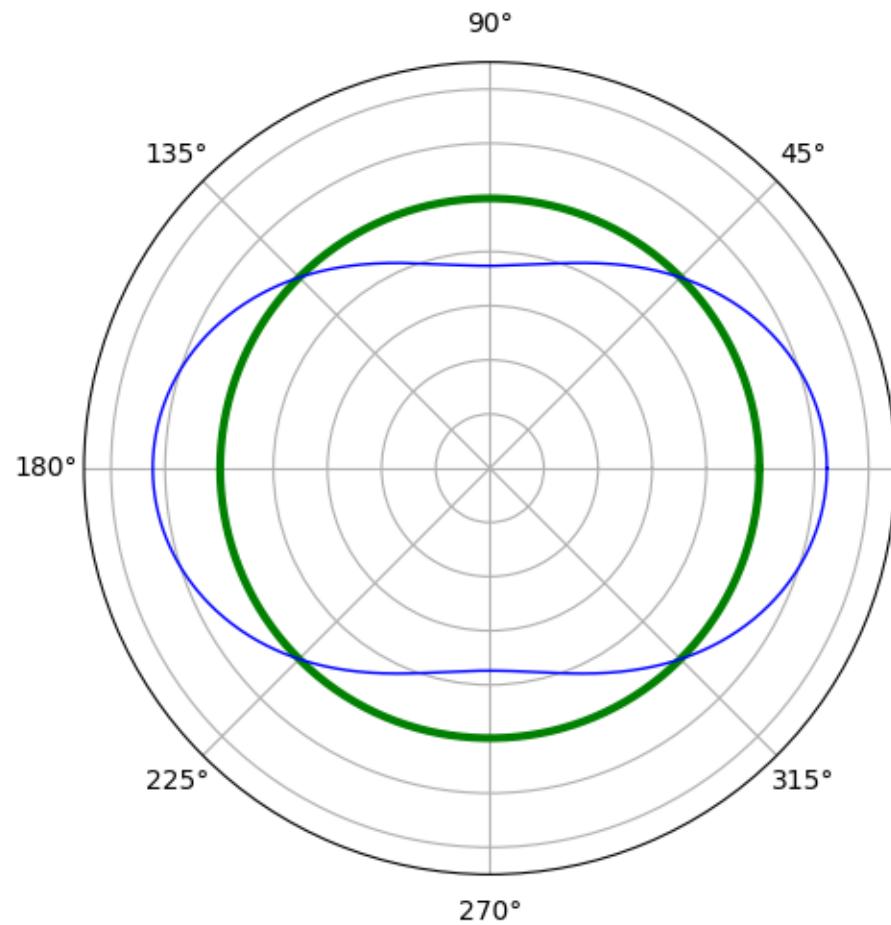
# Moments of the distribution

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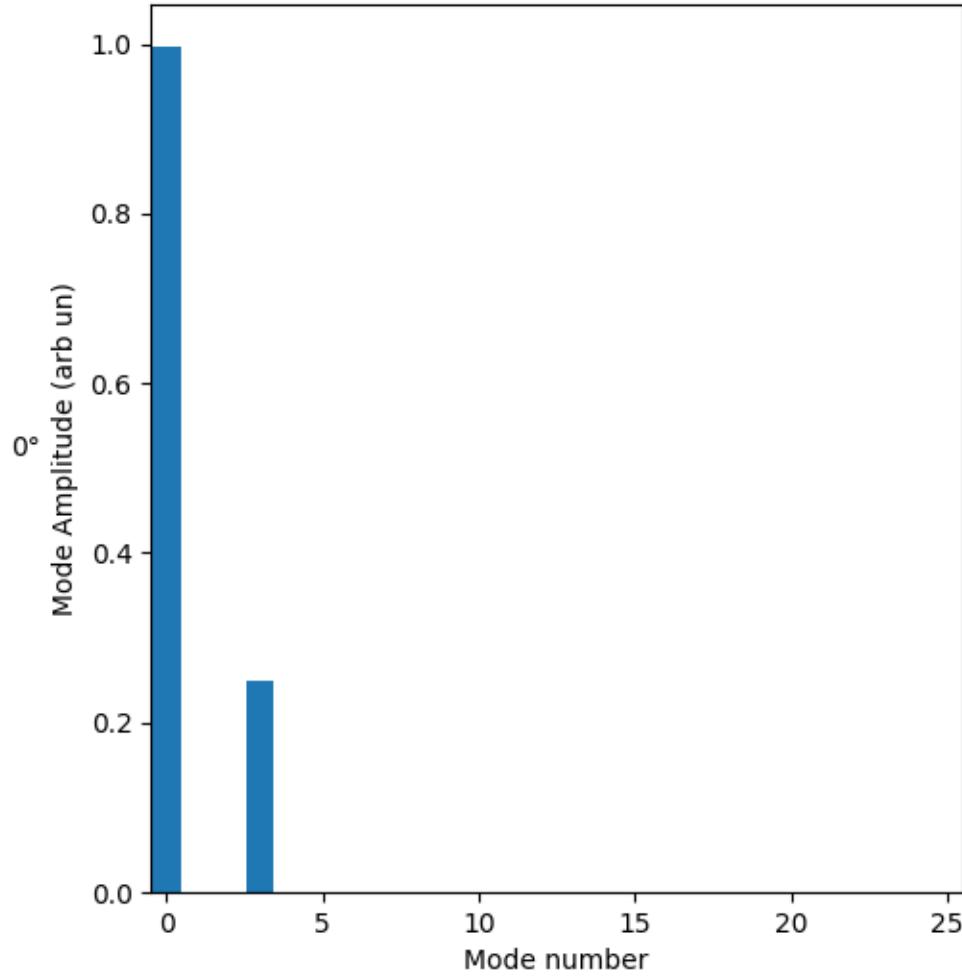
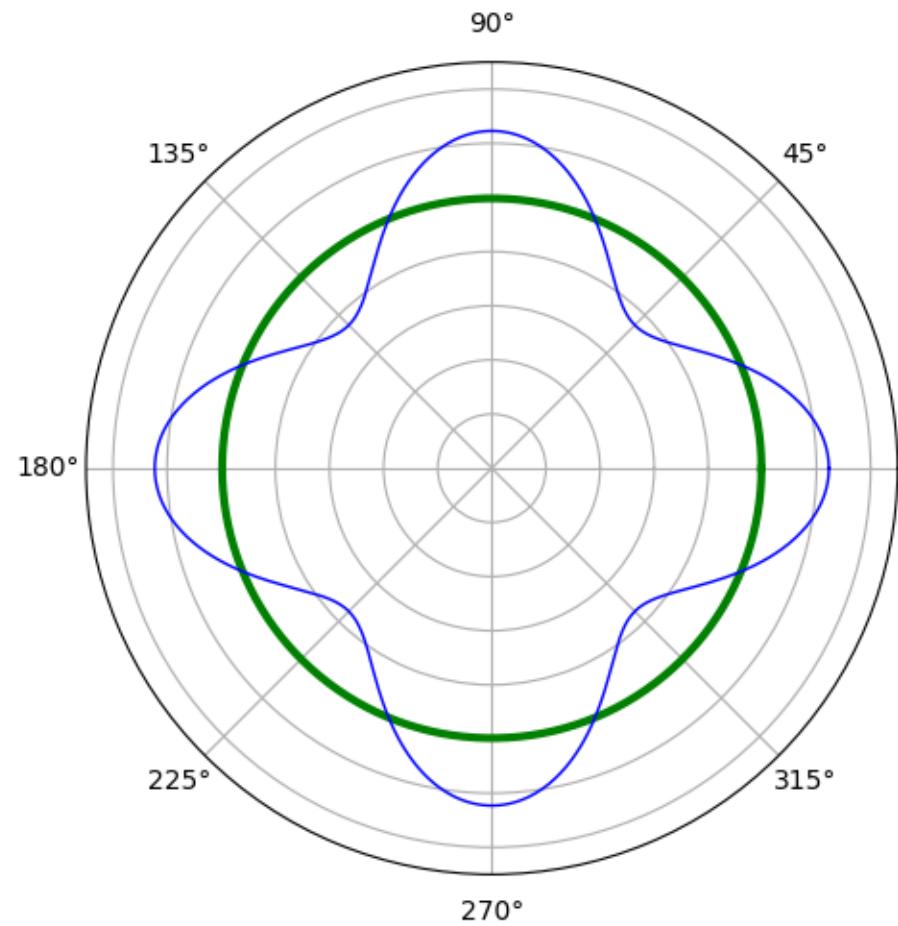
# Moments of the distribution

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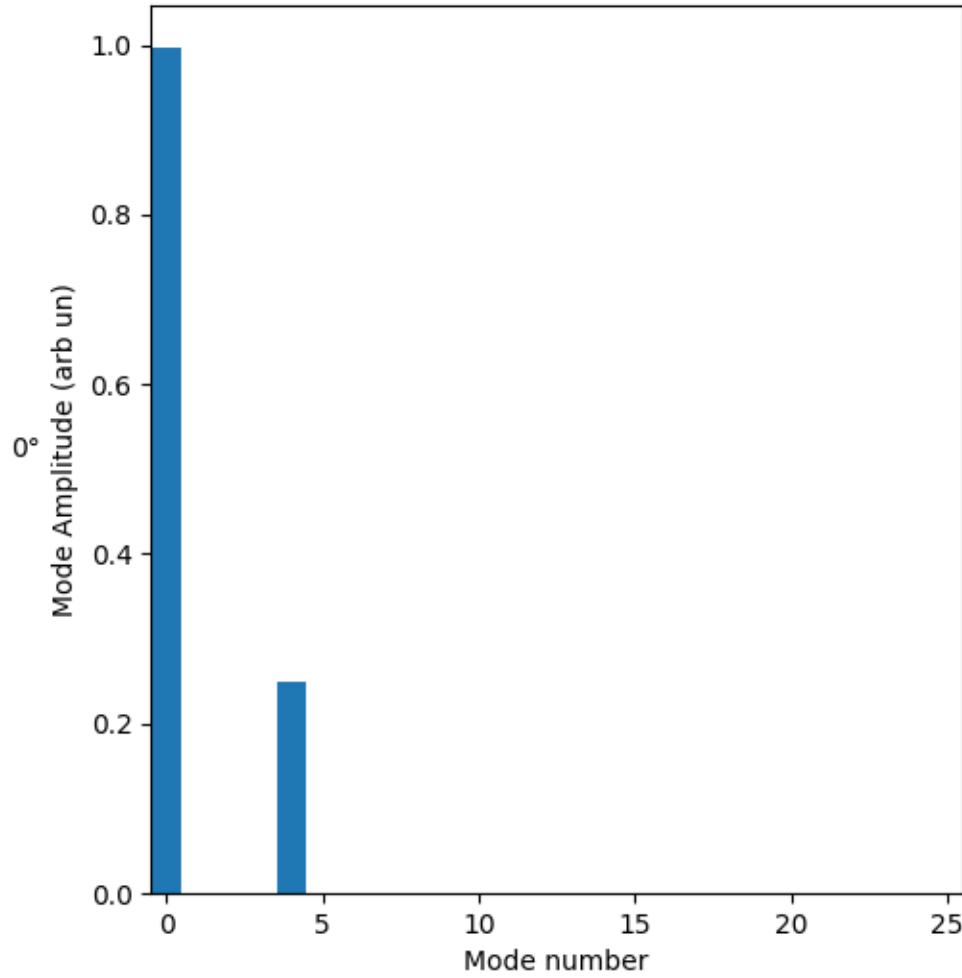
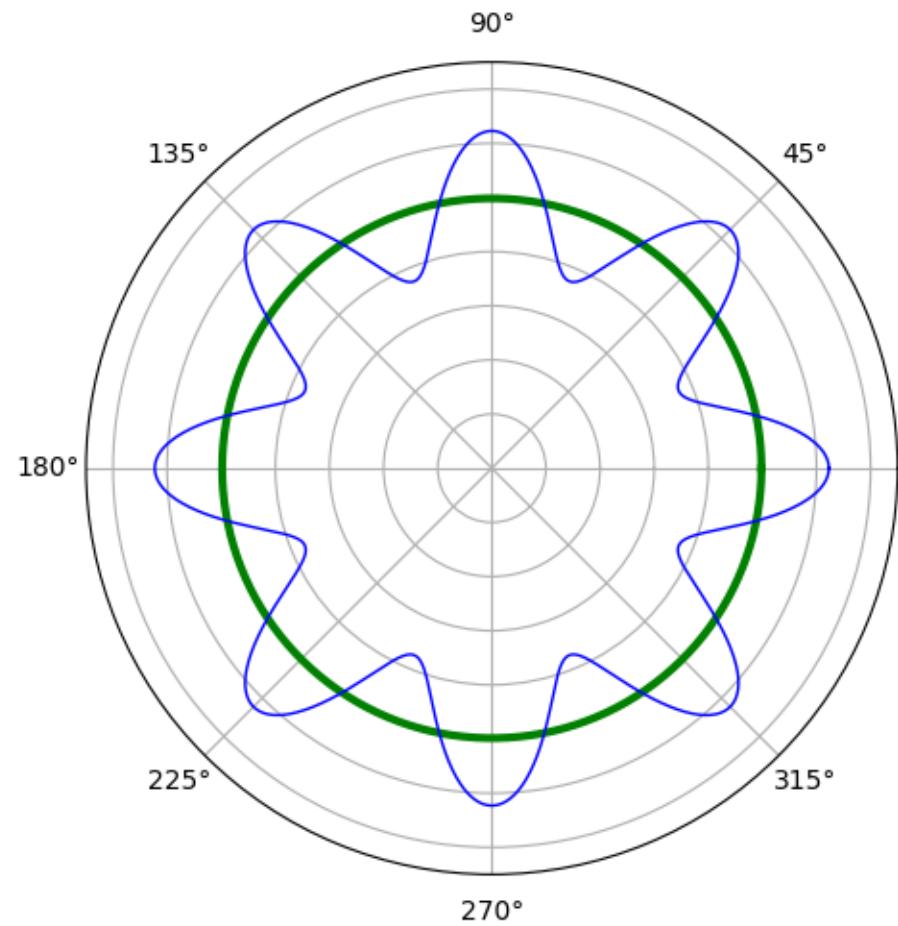


# Moments of the distribution

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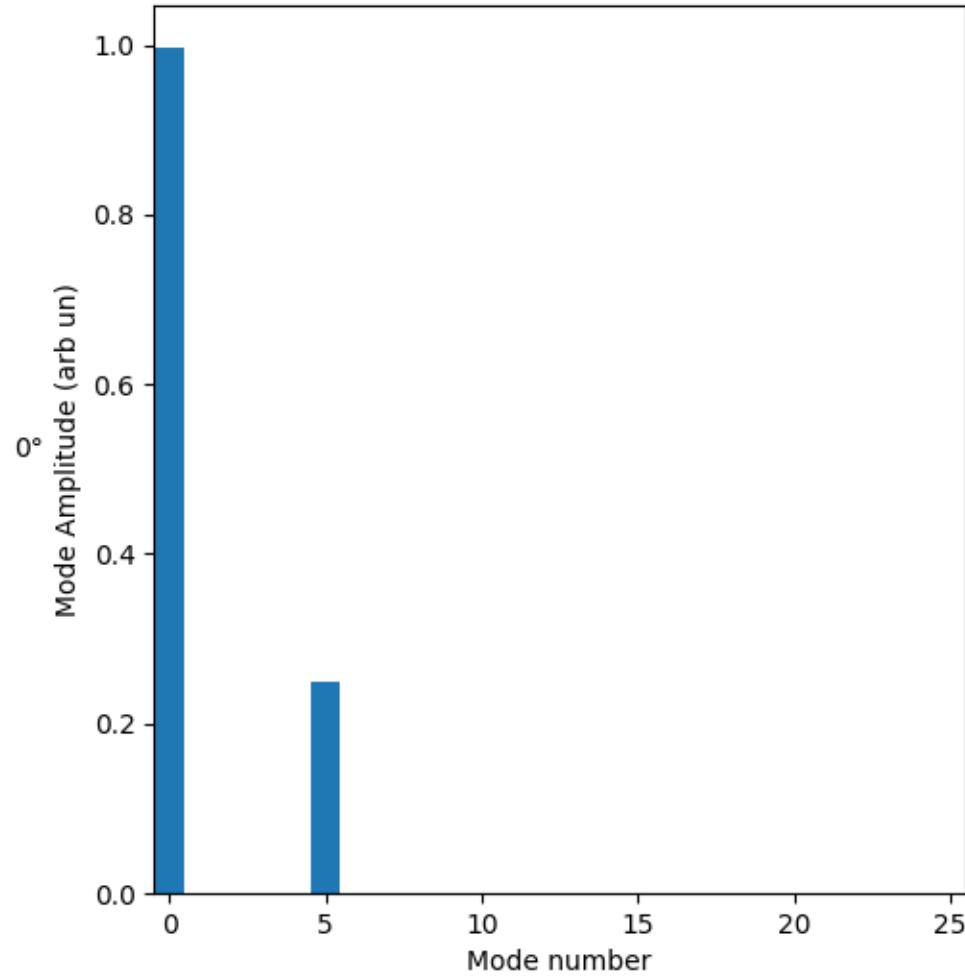
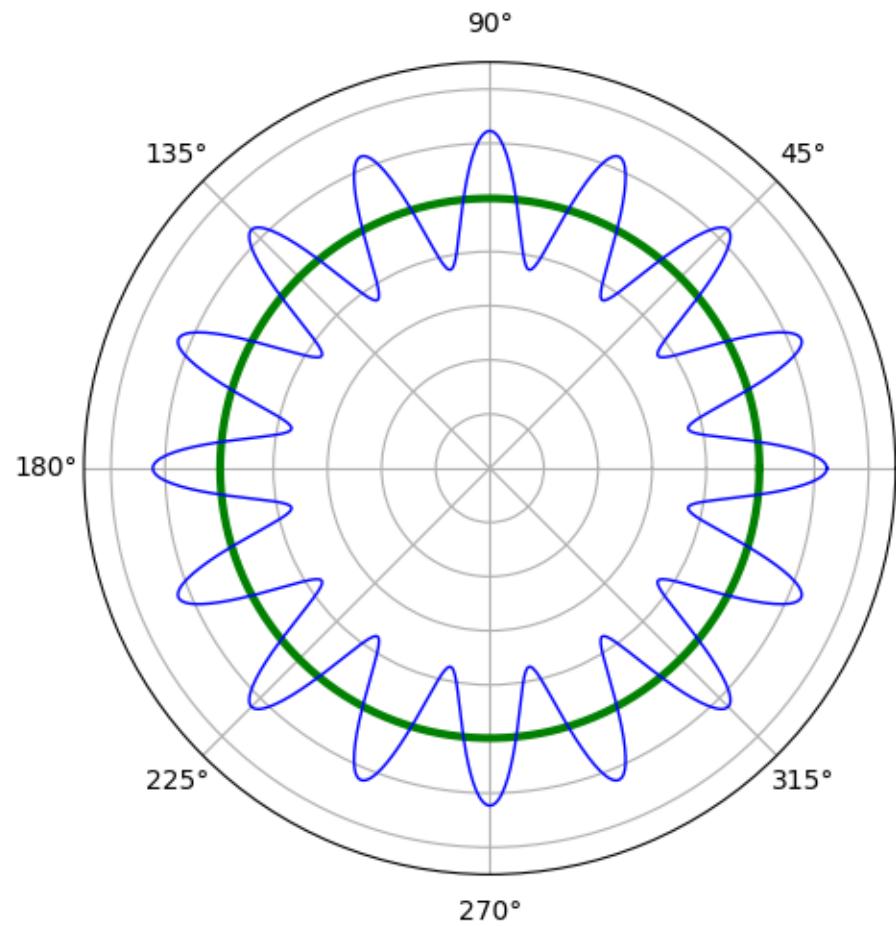


# Moments of the distribution

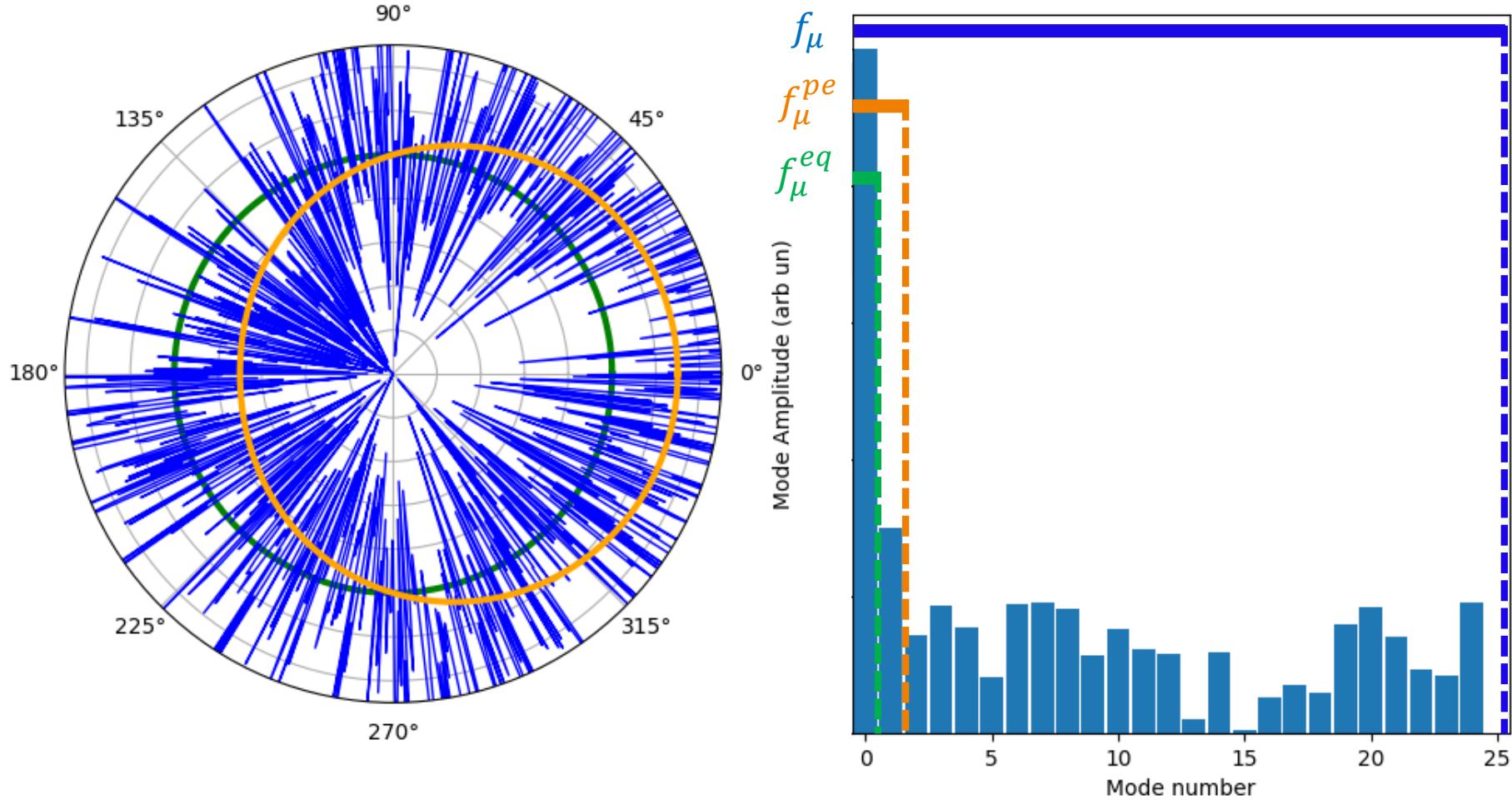


# Moments of the distribution

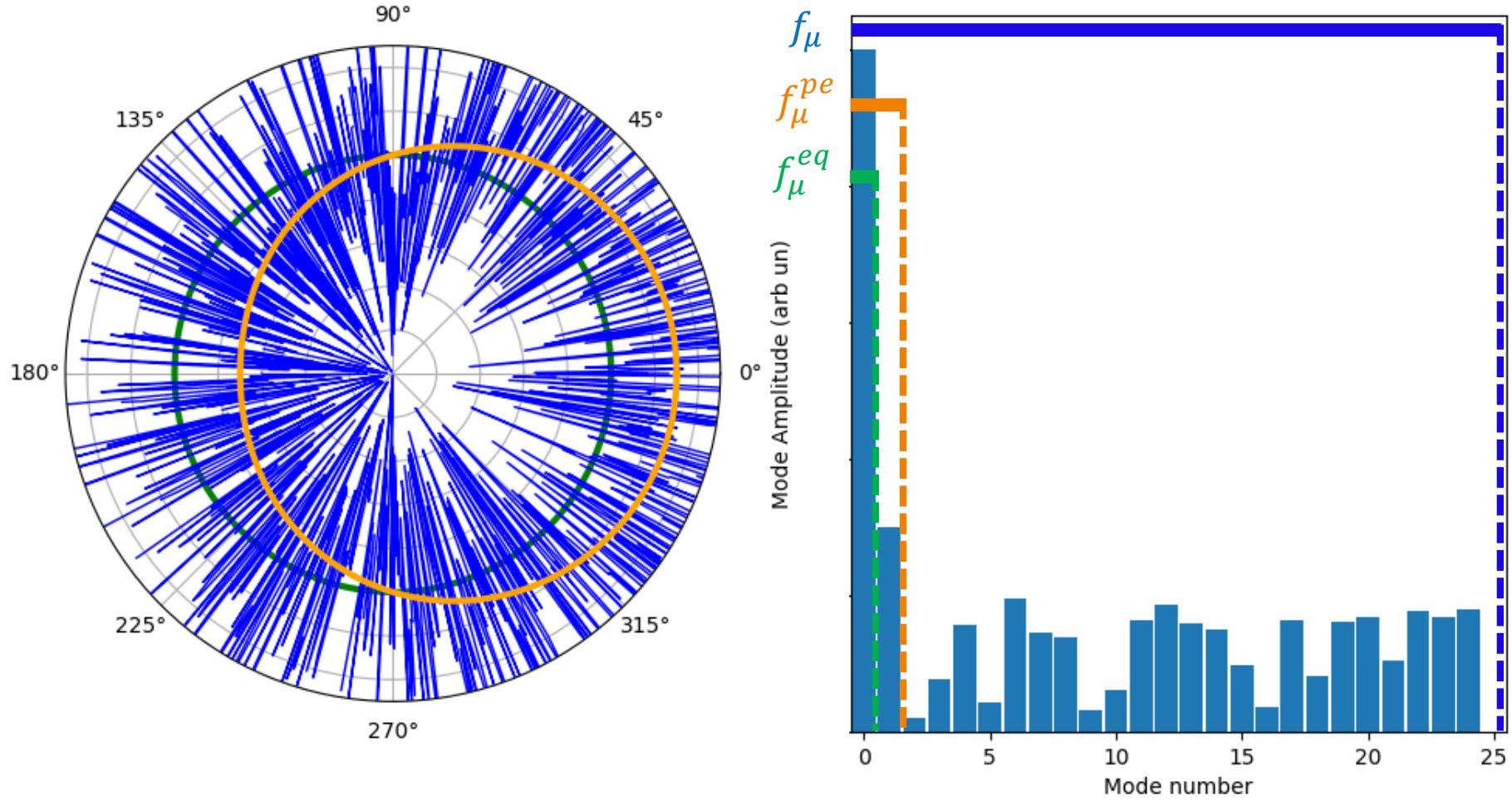
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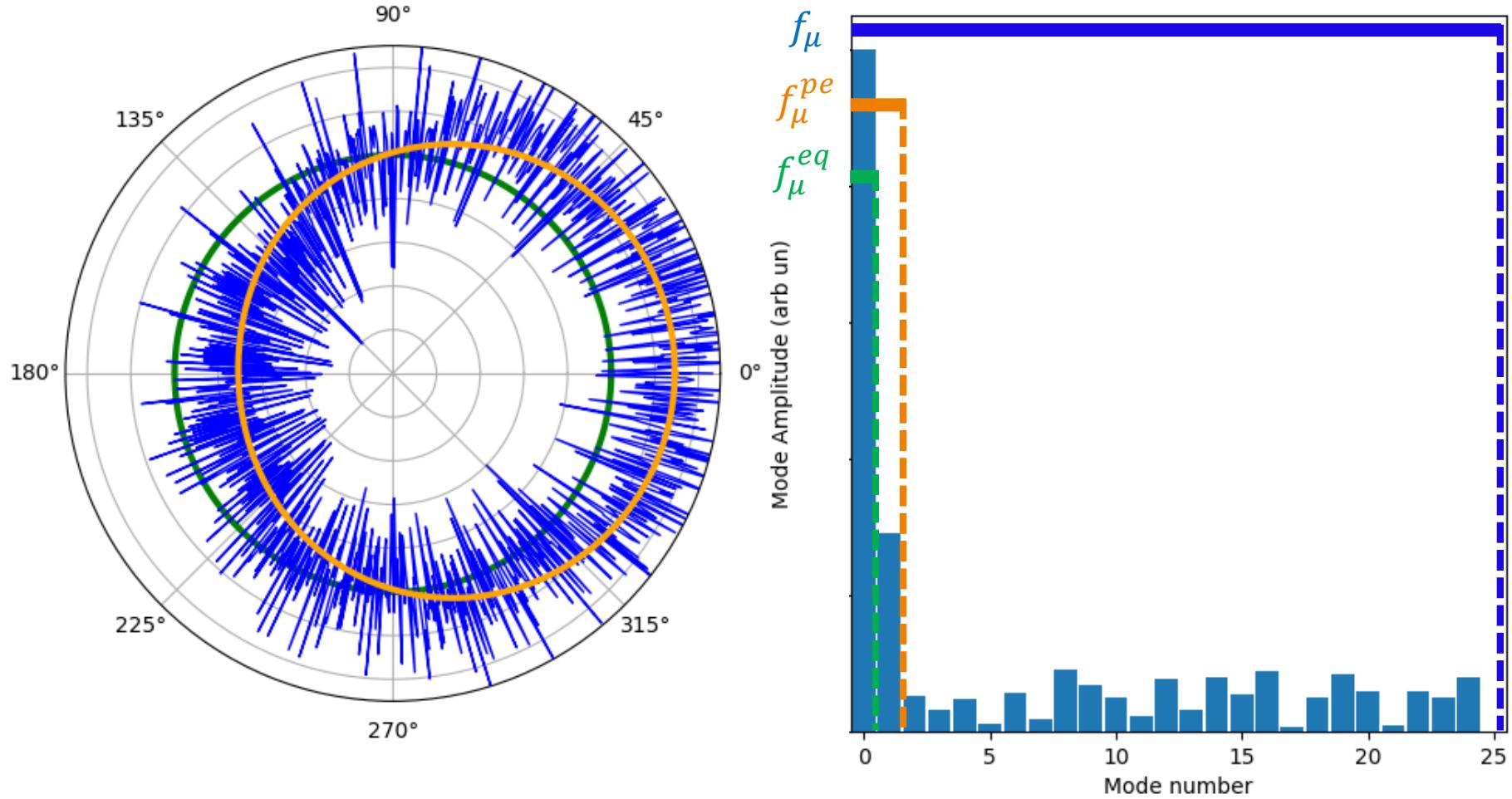
# □ (Pseudo)conserved magnitudes



# □ (Pseudo)conserved magnitudes



# □ (Pseudo)conserved magnitudes



# Fourier's law

$$\alpha_1 \frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{q}$$

$$\alpha_2 \frac{\partial \mathbf{q}}{\partial t} - \frac{\mathbf{q}}{\tau_q} = -\nabla \cdot \mathbf{Q}^{(2)} - \beta_1 \nabla T$$

$$\alpha_3 \frac{\partial \mathbf{Q}^{(2)}}{\partial t} - \frac{\mathbf{Q}^{(2)}}{\tau_{eq}} = -\nabla \cdot \mathbf{Q}^{(3)} - \beta_2 \nabla q$$

## THERMODYNAMIC EQUATIONS

$$c_v \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0$$

$$\mathbf{q} = -\lambda \nabla T$$

$$\nabla \cdot \mathbf{Q}^{(n+1)}$$

## BTE DISTRIBUTION FUNCT.

$$f = f_{eq} - \frac{3}{c_v v^2} \mathbf{q} \cdot \mathbf{v}_g \frac{\partial f_{eq}}{\partial T}$$

# Guyer and Krumhansl equation

$$\alpha_1 \frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{q}$$

$$\alpha_2 \frac{\partial \mathbf{q}}{\partial t} - \frac{\mathbf{q}}{\tau_q} = -\nabla \cdot \mathbf{Q}^{(2)} - \beta_1 \nabla T$$

$$\alpha_3 \frac{\partial \mathbf{Q}^{(2)}}{\partial t} - \frac{\mathbf{Q}^{(2)}}{\tau_{\mathbf{Q}^{(2)}}} = -\nabla \cdot \mathbf{Q}^{(3)} - \beta_2 \nabla \mathbf{q}$$

## THERMODYNAMIC EQUATIONS

$$c_v \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0$$

$$\mathbf{q} = -\lambda \nabla T - A_1 \nabla \cdot \mathbf{Q}^{(2)}$$

$$\mathbf{Q}^{(2)} = A_2 \nabla \mathbf{q}$$

$$S = -\nabla \cdot \mathbf{Q}^{(n+1)} - \beta \nabla \mathbf{Q}^{(n-1)}$$

## BTE DISTRIBUTION FUNCT.

$$f \simeq f_{eq} - \frac{3}{c_v v_g^2} \frac{\partial f_{eq}}{\partial T} q_i v_{gi} + \frac{\tau}{c_V} \frac{\partial q_i}{\partial x_i} \frac{\partial f_{eq}}{\partial T}$$

# Guyer and Krumhansl equation

$$\begin{aligned}\alpha_1 \frac{\partial T}{\partial t} &= -\nabla \cdot q \\ \alpha_2 \frac{\partial q}{\partial t} - \frac{q}{\tau_q} &= -\nabla \cdot Q^{(2)} \\ \alpha_3 \frac{\partial Q^{(2)}}{\partial t} - \frac{Q^{(2)}}{\tau_{Q^{(2)}}} &= -\nabla \cdot Q^{(3)}\end{aligned}$$

NEW BOUNDARY CONDITION

GK is a second order PDE, a new boundary condition is needed in order to be solvable

## THERMODYNAMIC EQUATIONS

$$c_v \frac{\partial T}{\partial t} + \nabla \cdot q = 0$$

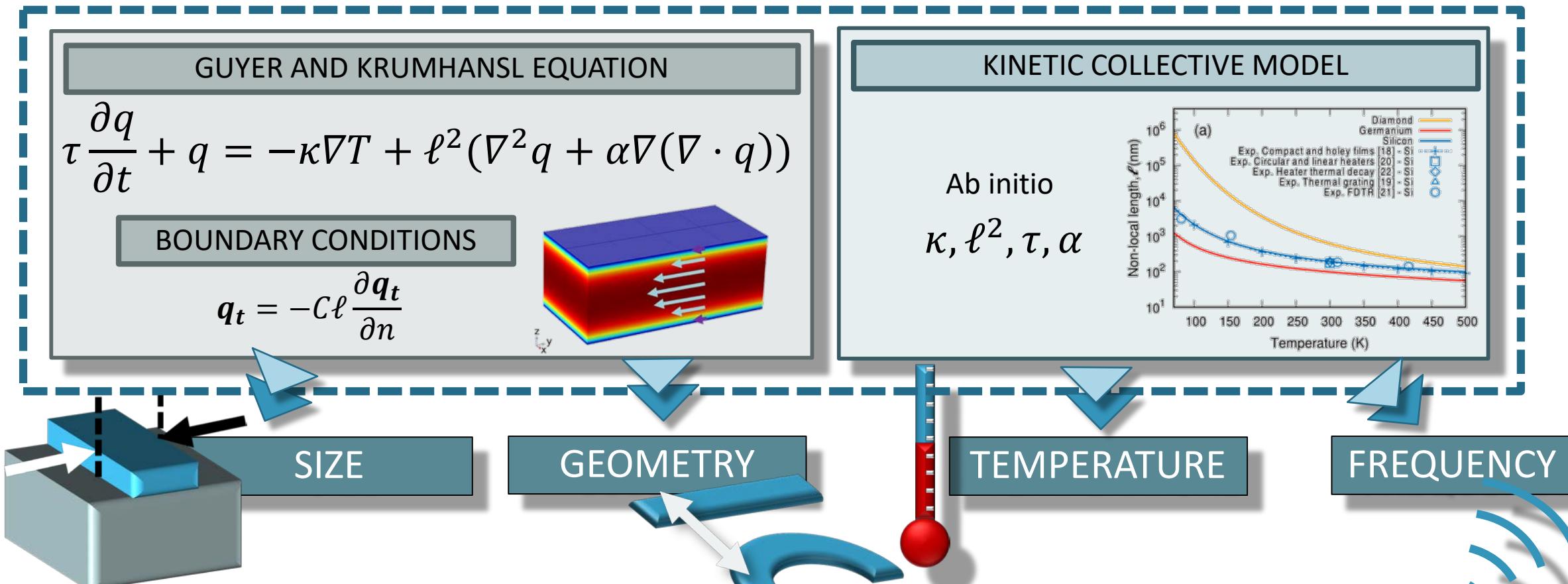
$$q = -\lambda \nabla T - \ell^2 (\nabla^2 q + 2 \nabla \nabla \cdot q)$$

## BTE DISTRIBUTION FUNCT.

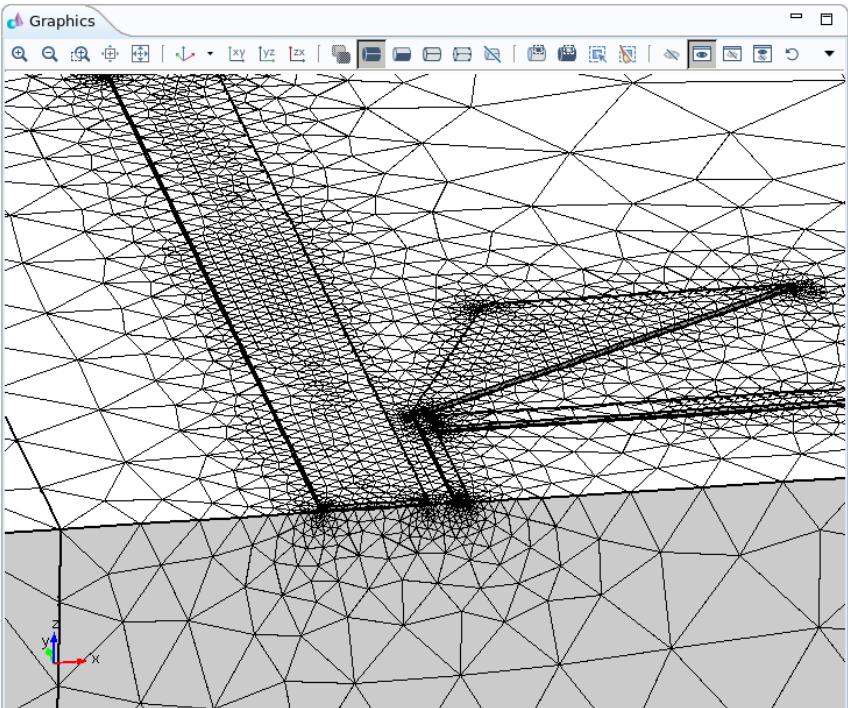
$$f \simeq f_{eq} - \frac{3}{c_v v_g^2} \frac{\partial f_{eq}}{\partial T} q_i v_{gi} + \frac{\tau}{c_V} \frac{\partial q_i}{\partial x_i} \frac{\partial f_{eq}}{\partial T}$$

# GK-ab initio formalism

Combination of the **Guyer and Krumhansl** equation with ab initio calculations for the parameters in the framework of **Kinetic Collective Model** offers a **full predictive model** for materials like silicon



# COMSOL module



graph\_phon\_crys4.mph (root)

- Global Definitions
  - Parameters
  - Materials
- Component 1 (comp1)
  - Definitions
  - Geometry 1
  - Materials
- Nanoscale Heat Transfer - Kinetic Collective Model (kcm)
  - Initial Values 1
    - Hydrodynamic Heat Transfer 1
  - Slip Boundary Condition 1
  - Periodic Heat Flux Condition 1
  - Pointwise Constraint 1
  - Temperature BC 1
  - Energy Source 1
    - Equation View
  - Heat Transfer in Solids (ht)
  - Mesh 1
- Study KCM
- Study Fourier

- Results
- Data Sets
- Derived Values
- Tables
- Temperature (ht)
- Isothermal Contours (ht)

Label: Hydrodynamic Heat Transfer 1

Domain Selection

Selection: Manual

Active

Override and Contribution

Equation

Show equation assuming:

Study KCM, Time Dependent

$$C_v \frac{\partial T}{\partial t} + \nabla \cdot q = Q$$
$$q + \tau \frac{\partial q}{\partial t} + k \nabla T = l^2 (\nabla^2 q + 2 \nabla \nabla \cdot q)$$

Heat Transfer Parameters

Volumetric heat capacity:  $C_v$  J/(m<sup>3</sup>·K)

Thermal conductivity:  $k$  W/(m·K)

Hydrodynamic Length:  $l$  m

Hydrodynamic Time:  $\tau$  s

# EFFECTS OF THE GUYER AND KRUMHANSL TERMS

## TRANSPORT EQUATIONS

$$c_v \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0$$

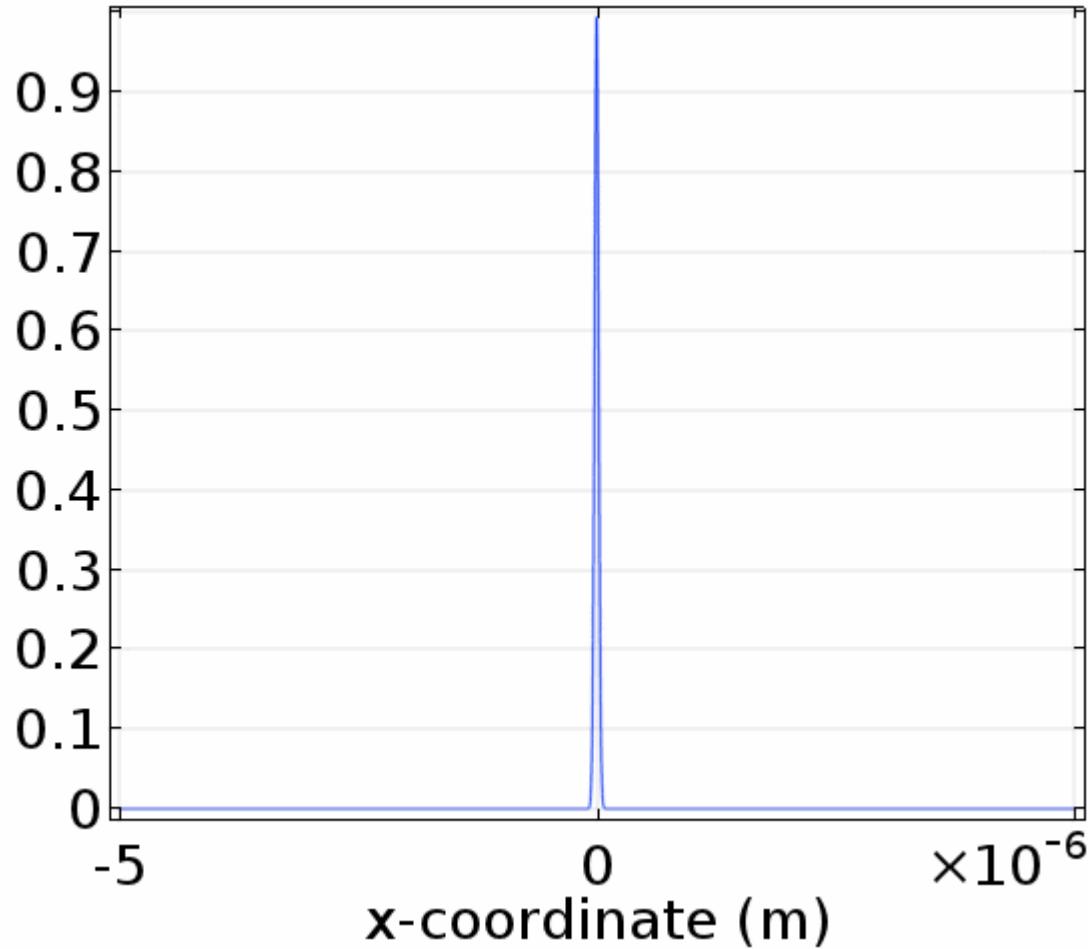
$$\mathbf{q} = -\lambda \nabla T$$

## HEAT-DIFFUSION EQUATION

$$\frac{\partial T}{\partial t} = \chi \nabla^2 T$$

# Fourier's law

Temperature (K)



HEAT-DIFFUSION  
EQUATION

$$\frac{\partial T}{\partial t} = \chi \nabla^2 T$$

## TRANSPORT EQUATIONS

$$c_v \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0$$

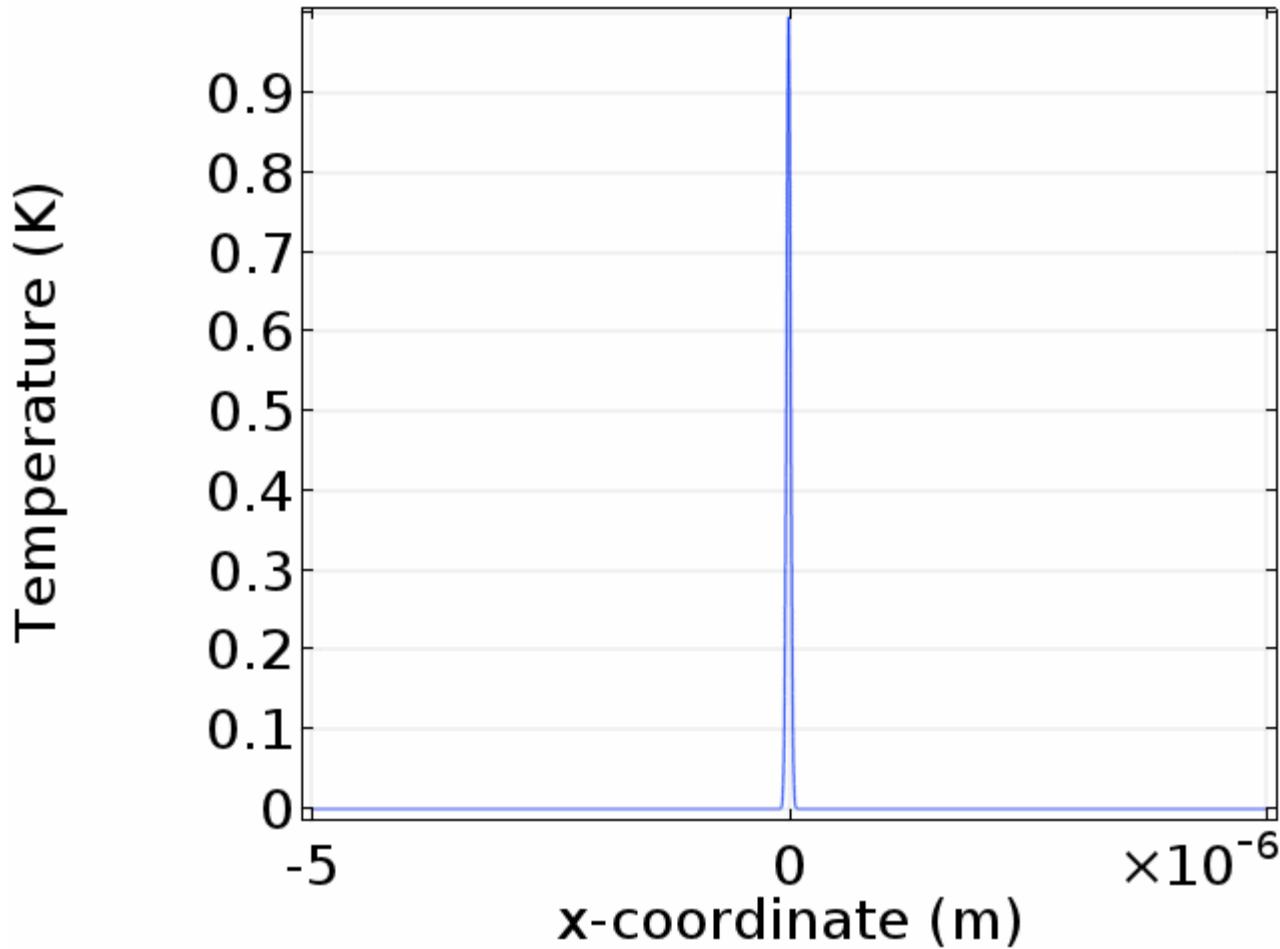
$$\tau \frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -\lambda \nabla T$$

Fast excitation changes  $T \ll \tau$

## MAXWELL-CATTANEO EQUATION

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \chi \nabla^2 T$$

# Memory term



MAXWELL-CATTANEO  
EQUATION

$$\tau \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = \chi \nabla^2 T$$

Steep spatial variations  $L \ll \ell$

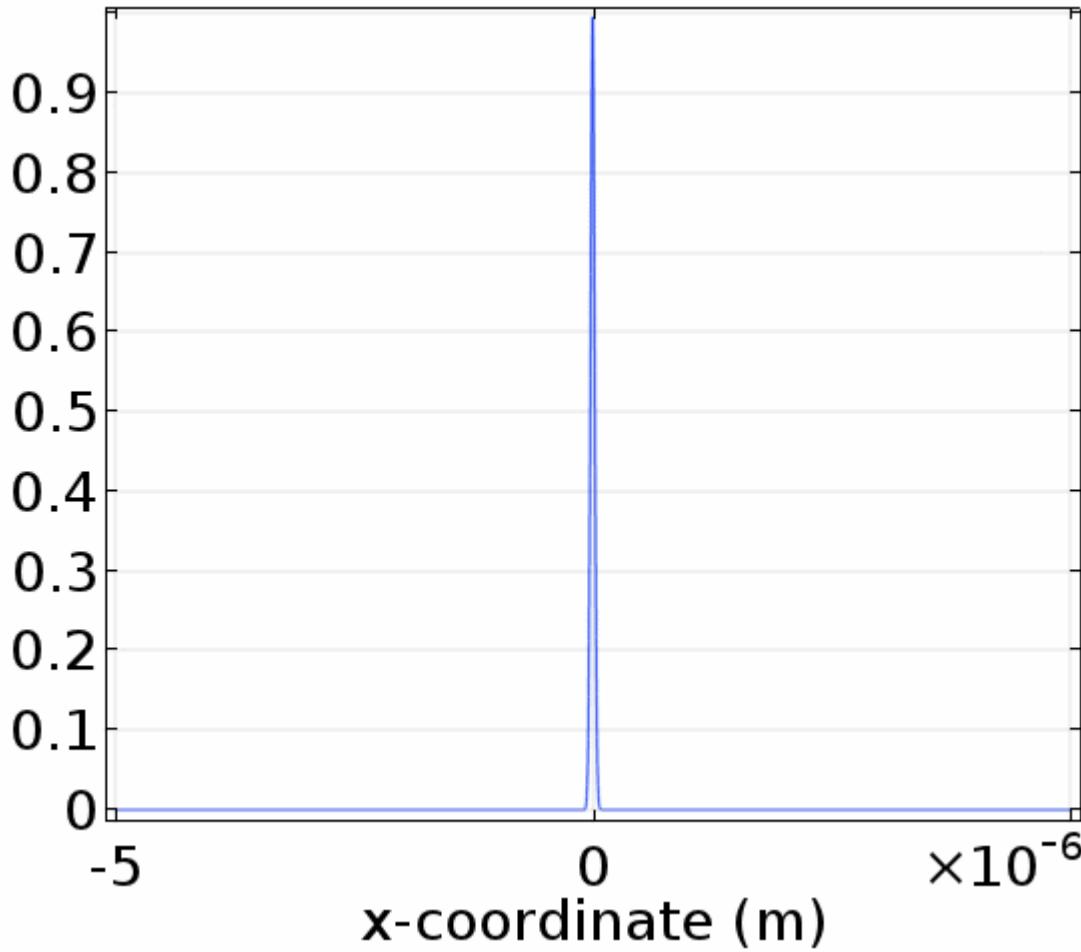
## TRANSPORT EQUATIONS

$$c_v \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0$$

$$\mathbf{q} = -\lambda \nabla T + \ell \nabla^2 \mathbf{q}$$

# Nonlocal term

Temperature (K)



## TRANSPORT EQUATIONS

$$c_v \frac{\partial T}{\partial t} + \nabla \cdot q = 0$$

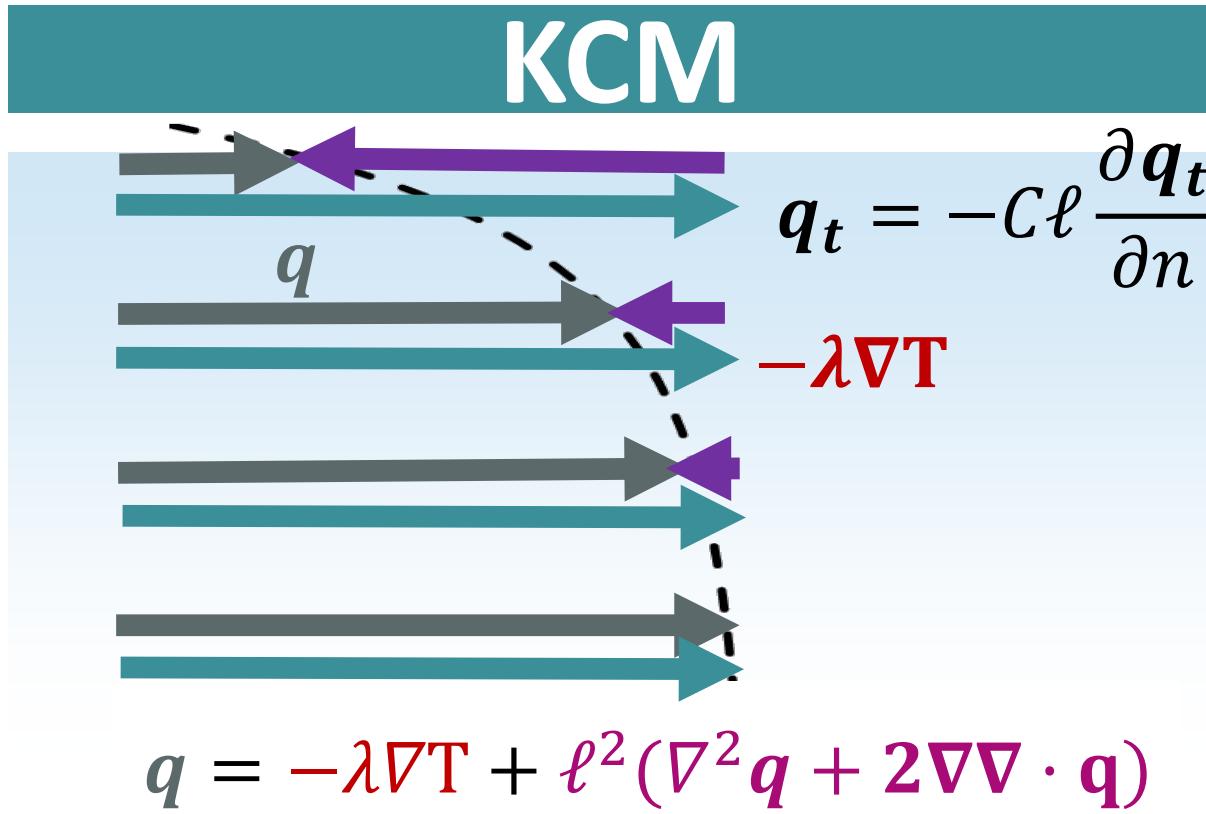
$$q = -\lambda \nabla T + \ell \nabla^2 q$$

# APPLICATIONS

# **KCM VS KINETIC FORMALISM 1:**

## **SIZE EFFECTS**

# Hydrodynamic effects I: Boundaries



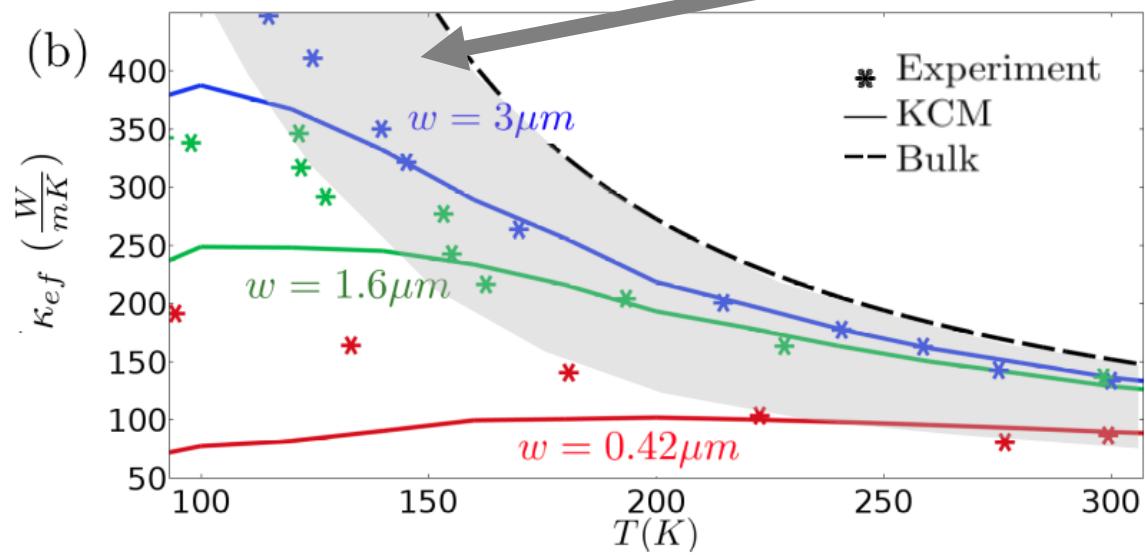
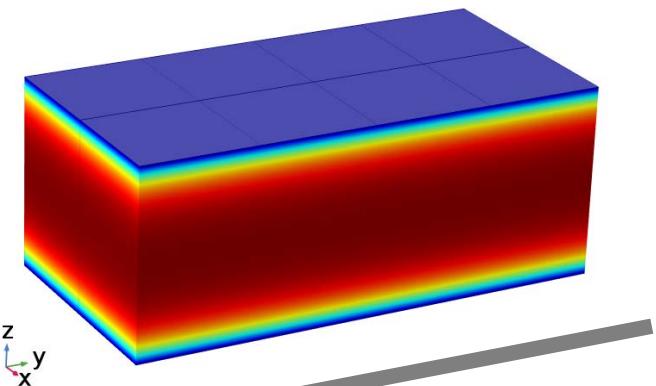
The boundary condition is applied directly to the heat flux in a consistent way with respect to the transport equation

# Applicability of hydrodynamic ab initio model

Beardo et al.  
*Phys. Rev. Appl.*,  
11, 034003

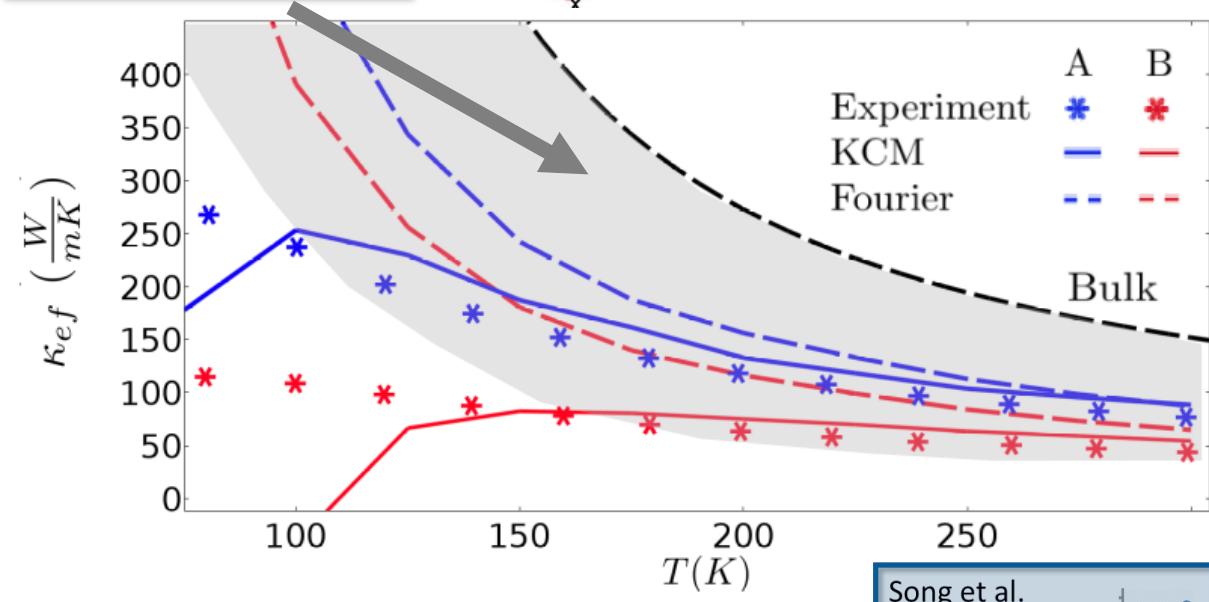
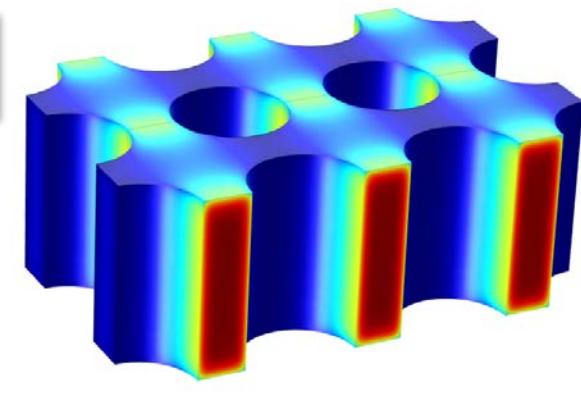
## Thin films

Asheghi et al.  
*J. Appl. Phys.*,  
91, 5079 (2002)



## Holey films

Region of predictability  
 $L < 2\ell$



Silicon  $\ell = 180$  nm

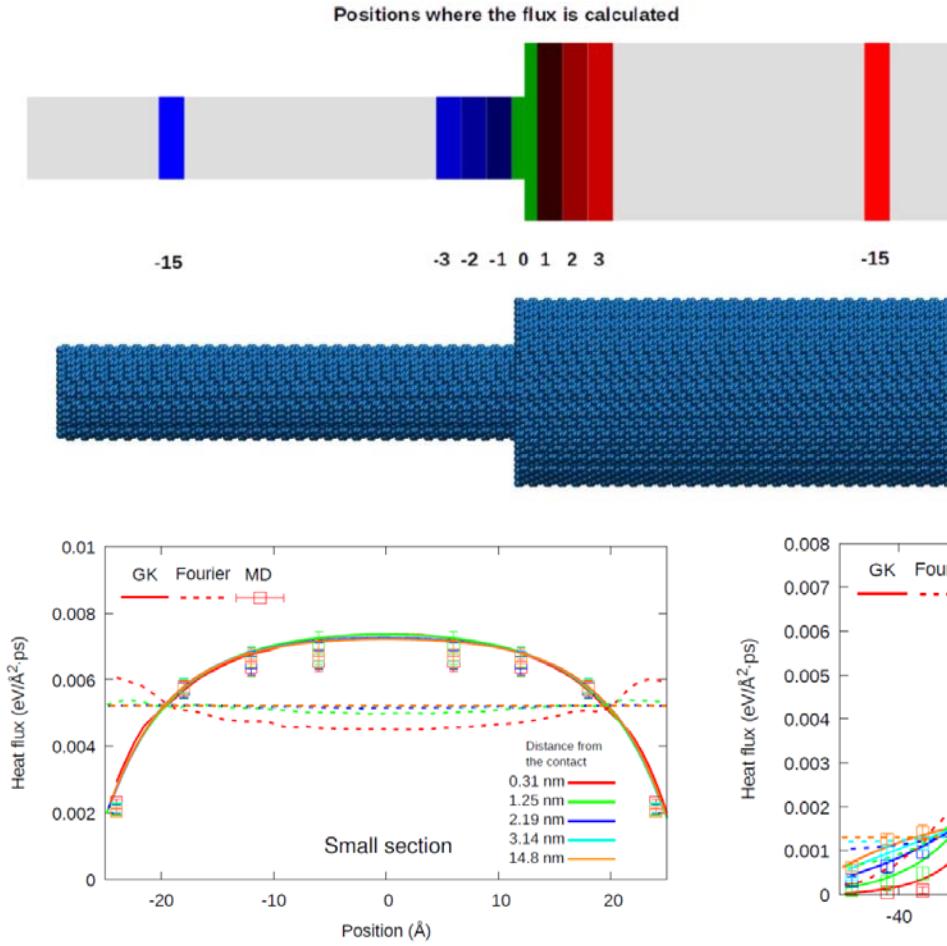
Song et al.  
*Appl. Phys. Lett.*,  
84, 687 (2004)

# Curved heat flow in MC, MD and FE



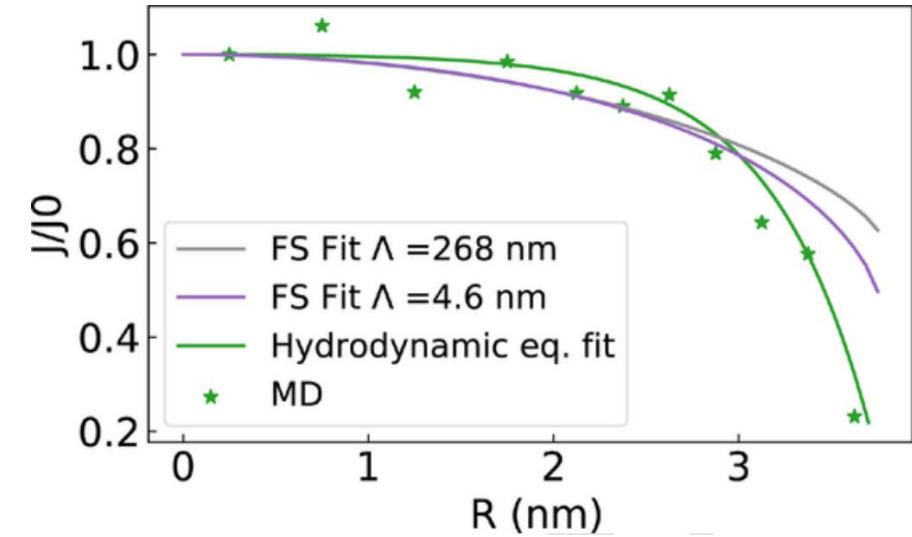
Melis et al.

*Phys. Rev. Appl.*, **11**, 054059 (2019)



Desmarchelier et al.

*IJHMT*, **194** 123003 (2022)

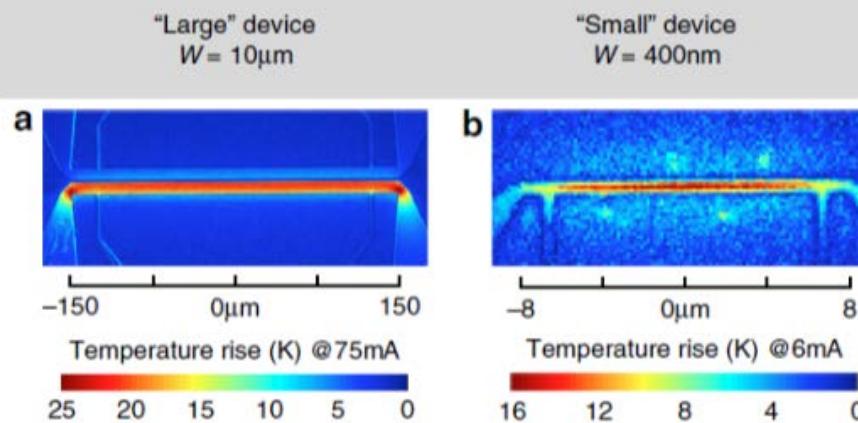


# **KCM VS KINETIC FORMALISM 2: THERMAL BOUNDARY RESISTANCE**

# Thermoreflectance Imaging (TRI)



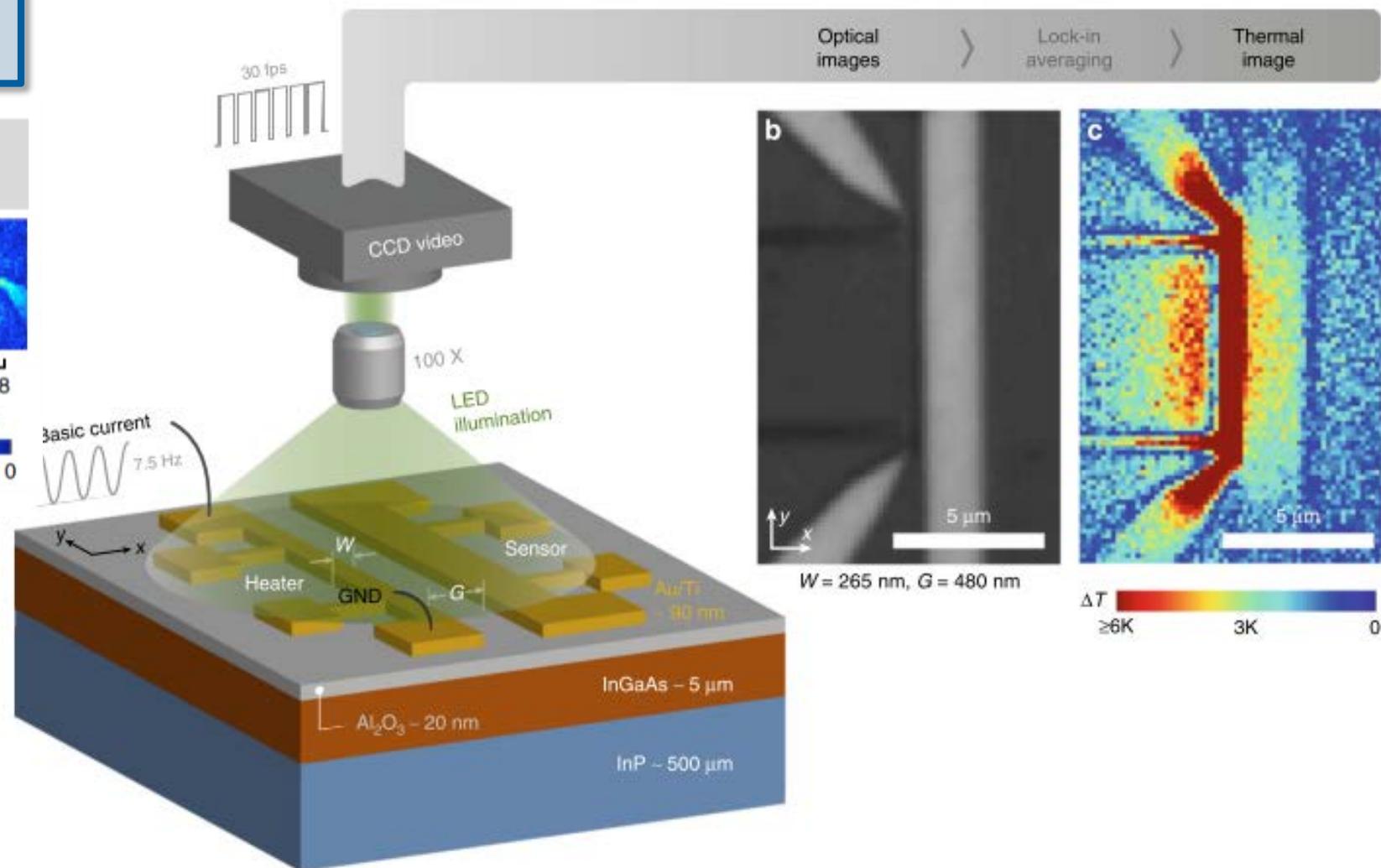
Ziabari et al.  
Nat. Commun. 9, 255 (2018)



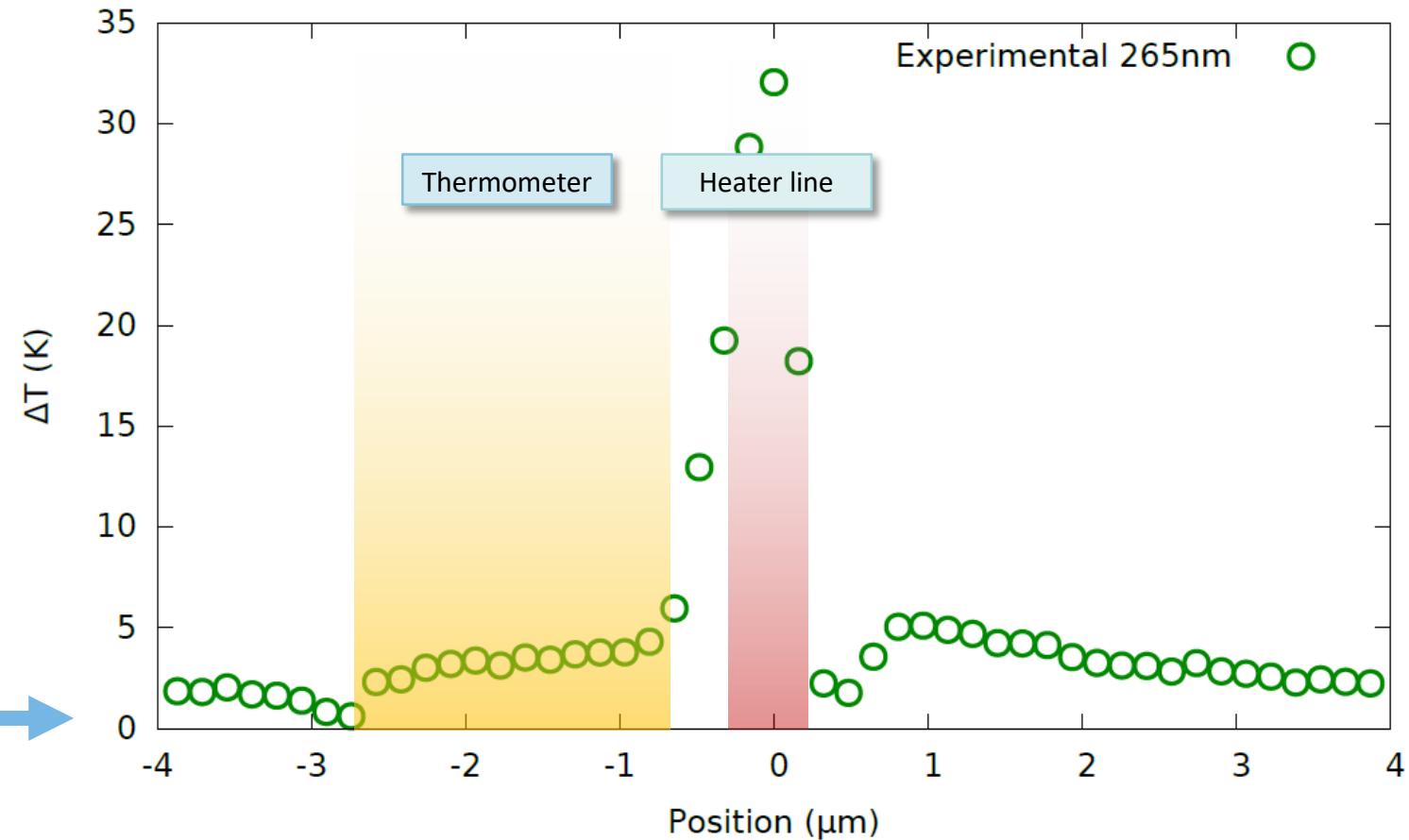
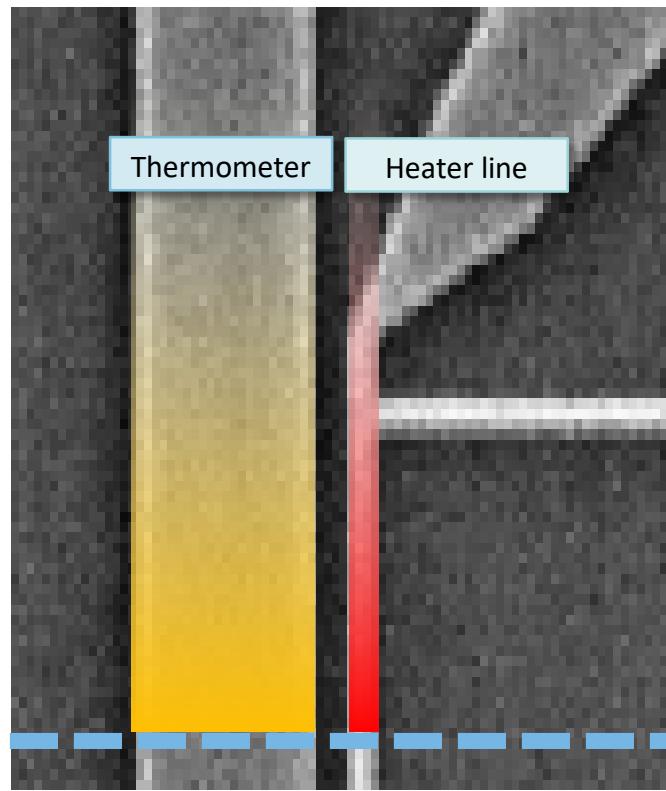
PURDUE  
UNIVERSITY®



Ali  
Shakouri



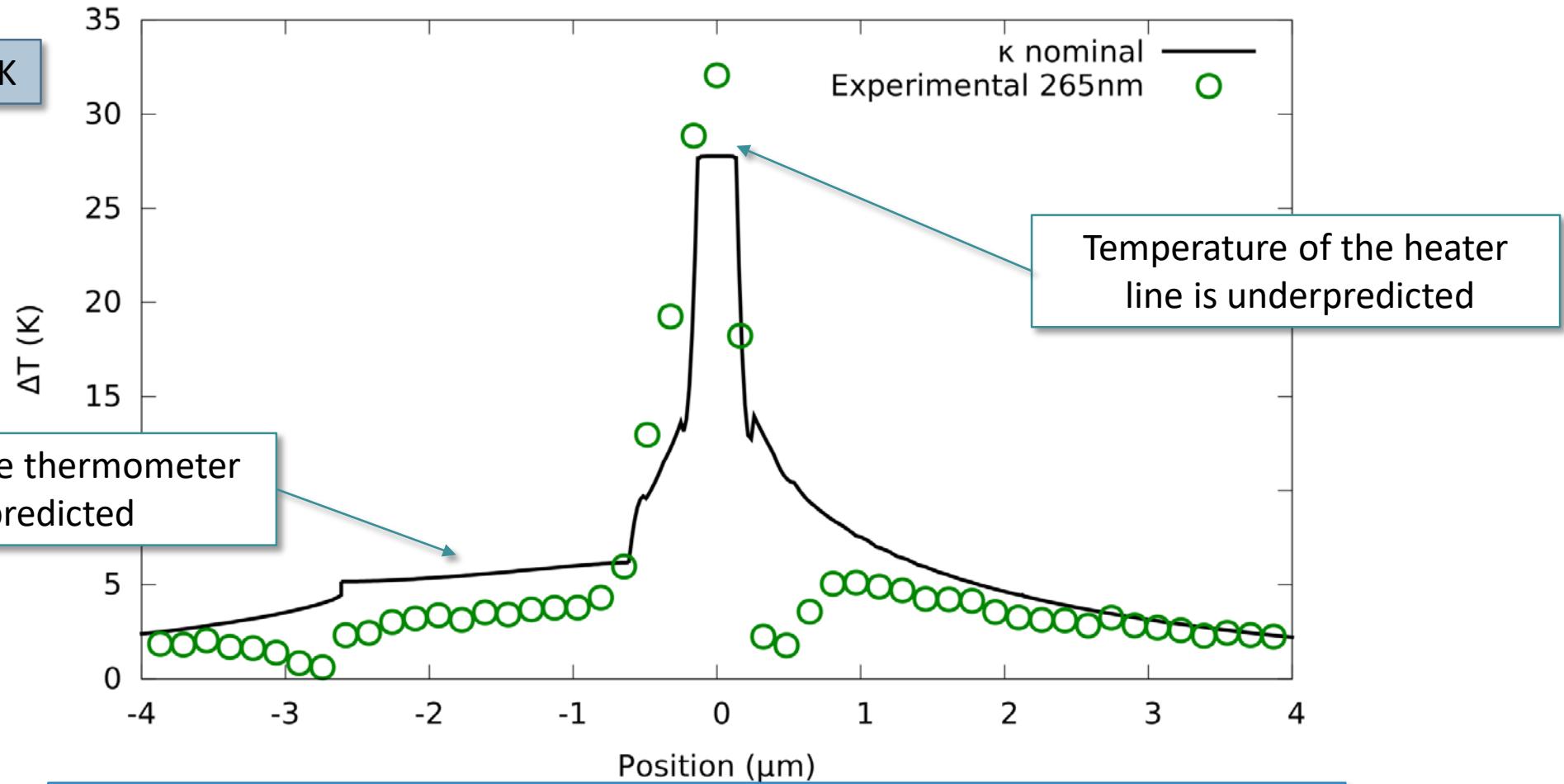
# Experimental Data



We obtain a thermal map of the surface of the sample using the optical setup. Heater line and thermometer are also obtained using electrical measurements.

# Fourier's law test (I)

$$\kappa_{\text{InGaAs}} = 5.4 \text{ W/m}\cdot\text{K}$$

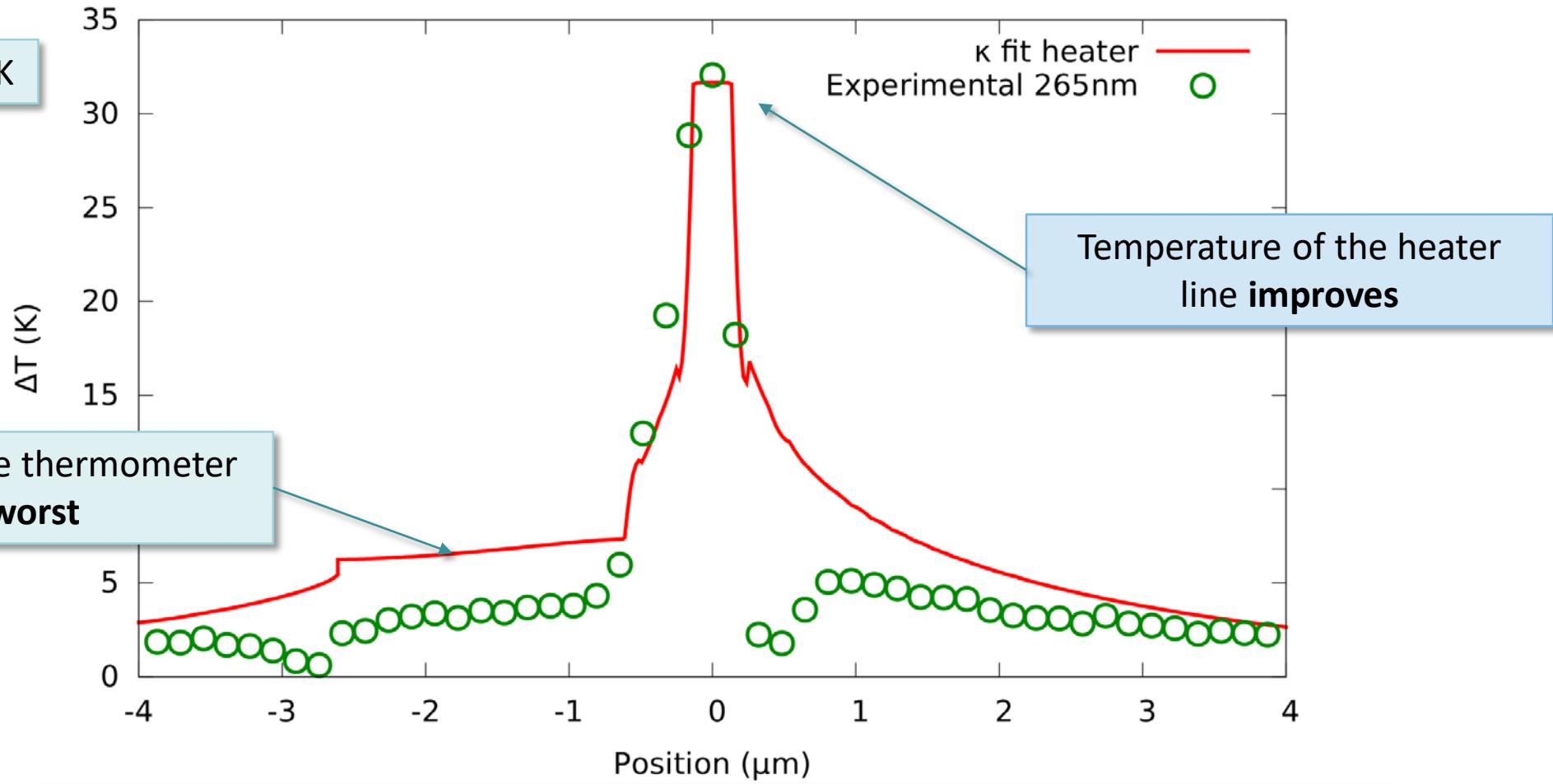


Using a finite element software (COMSOL) we test the validity of the Fourier's law using the nominal value of the thermal conductivity of InGaAs

# Fourier's law test (II)

$$\kappa_{\text{InGaAs}} = 4.4 \text{ W/m}\cdot\text{K}$$

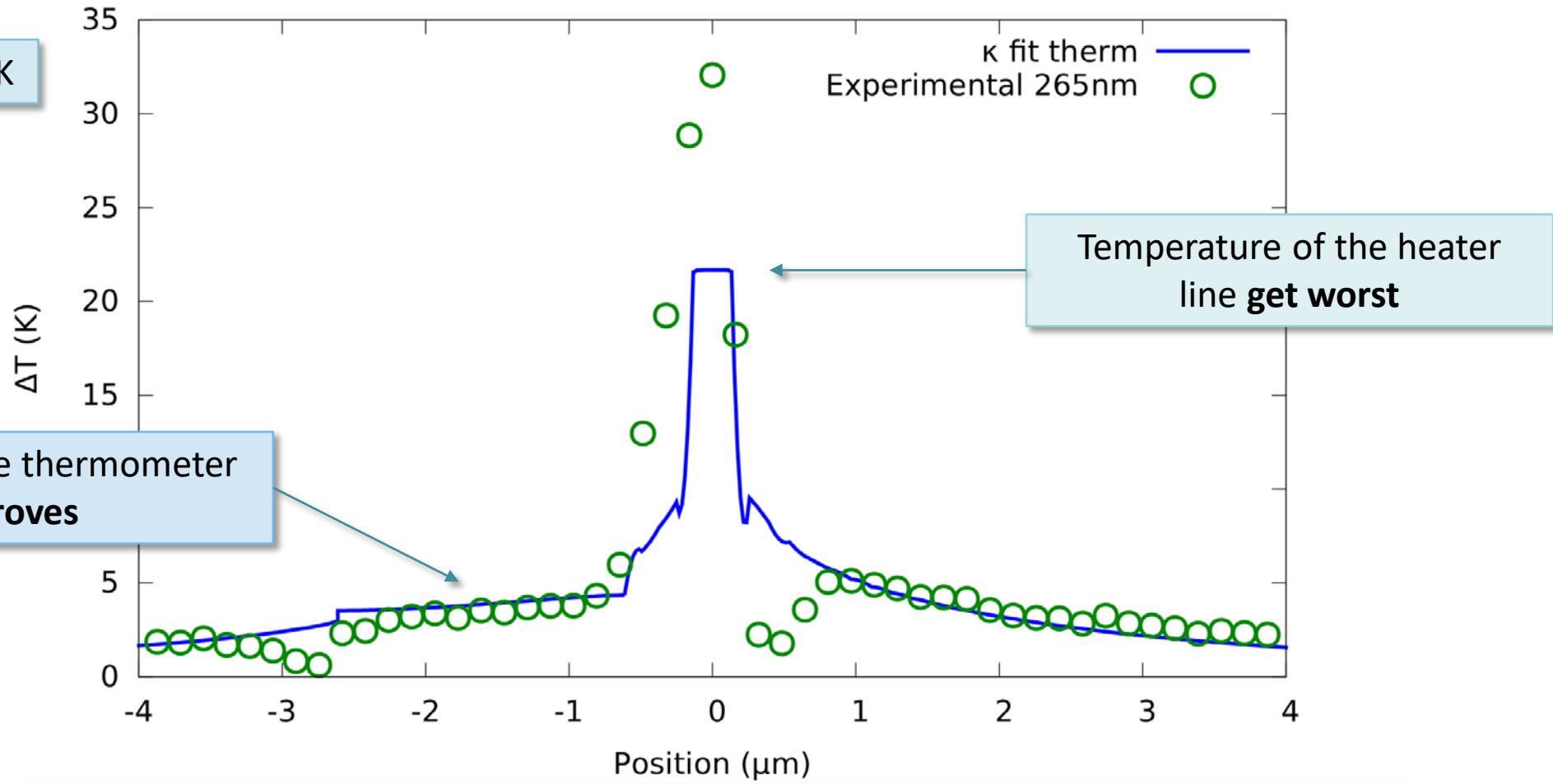
Temperature of the thermometer  
line **get worst**



Using a finite element software (COMSOL) we test the validity of the Fourier's law using a fitted value of the thermal conductivity of InGaAs to fit the heating line

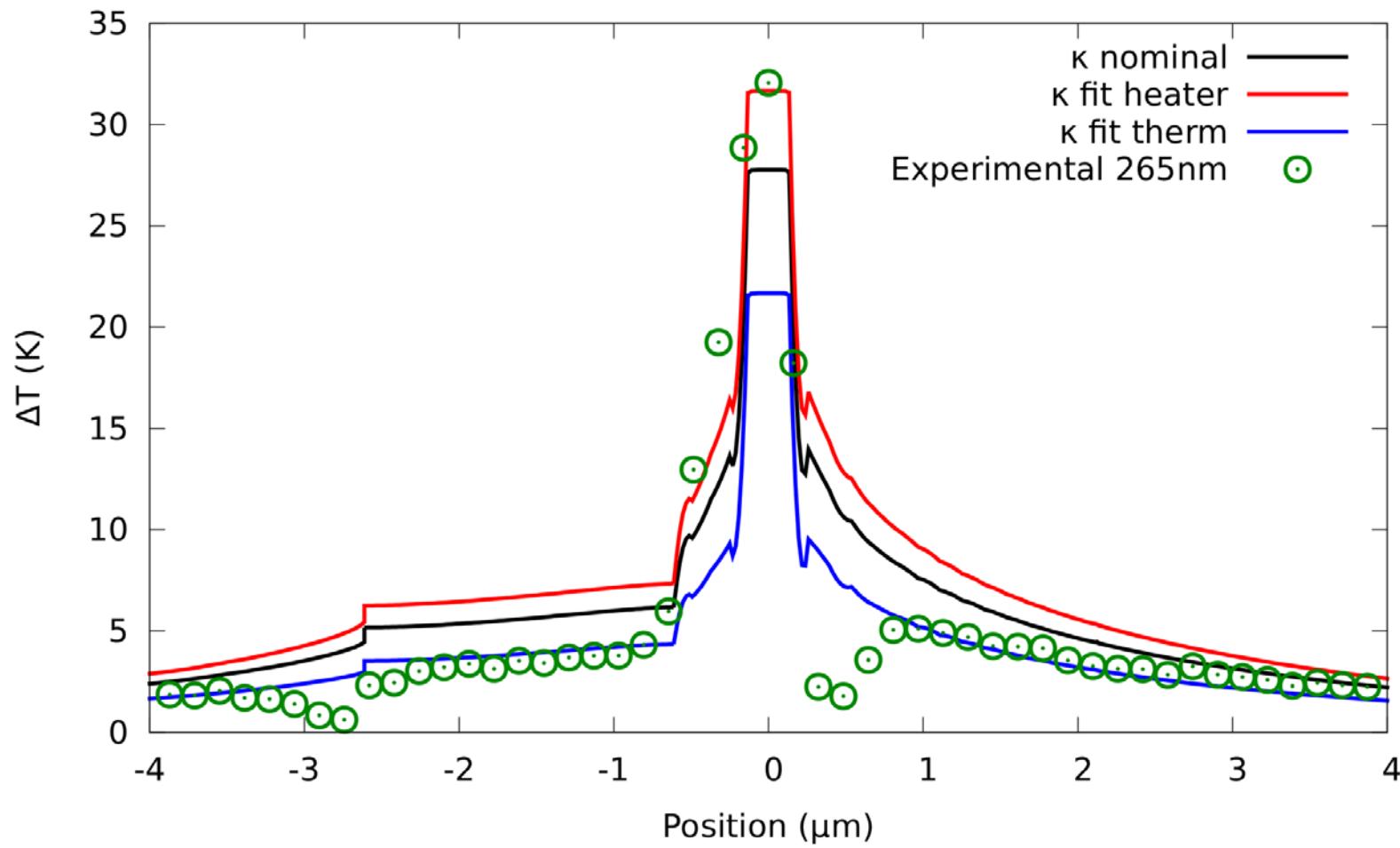
## Fourier's law test (III)

$$\kappa_{\text{InGaAs}} = 6.4 \text{ W/m}\cdot\text{K}$$



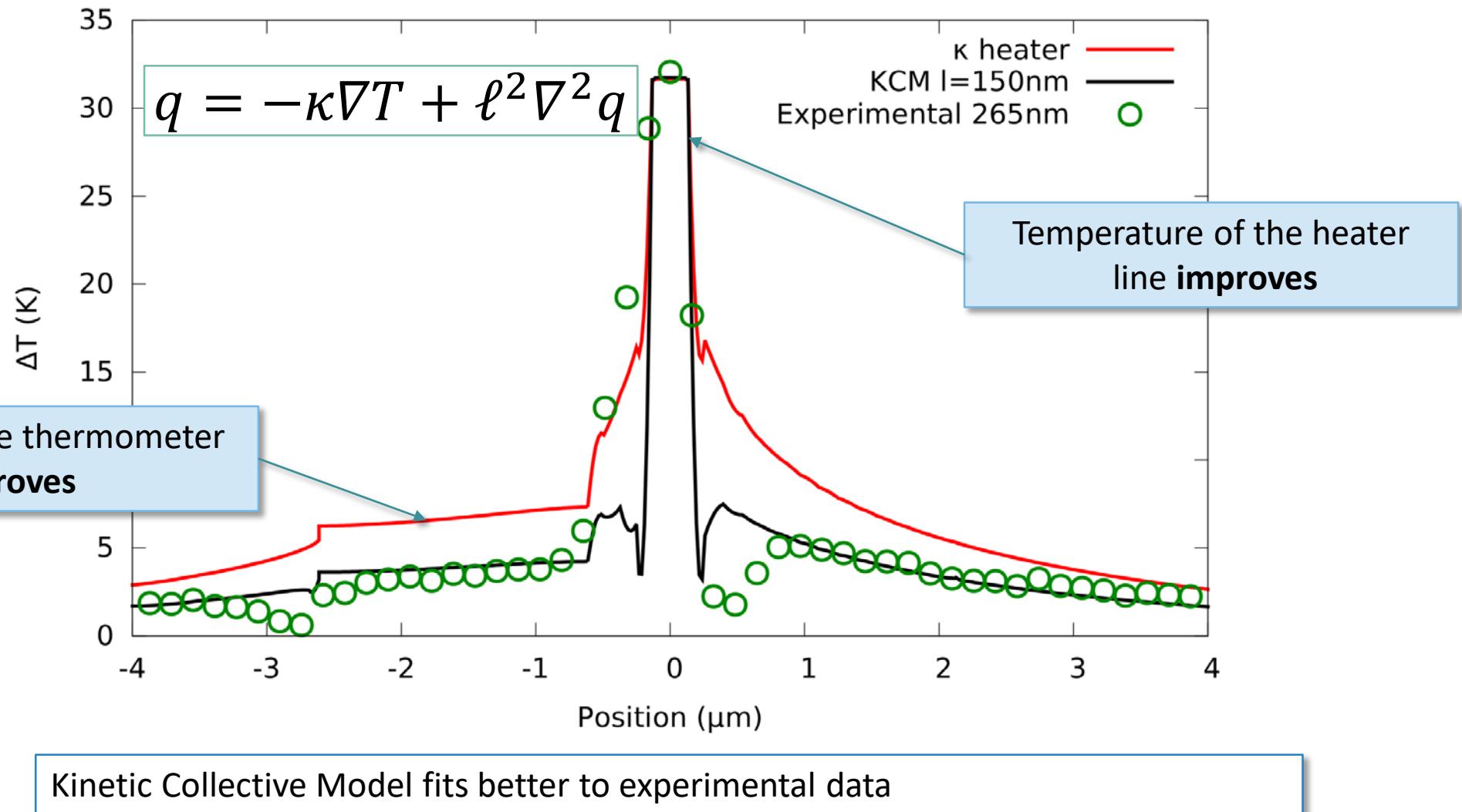
Using a finite element software (COMSOL) we test the validity of the Fourier's law using a fitted value of the thermal conductivity of InGaAs to fit the thermometer line

# Fourier's law summary



**Conclusion:** Fourier's law cannot describe thermal transport in this setup.  
New equation is needed.

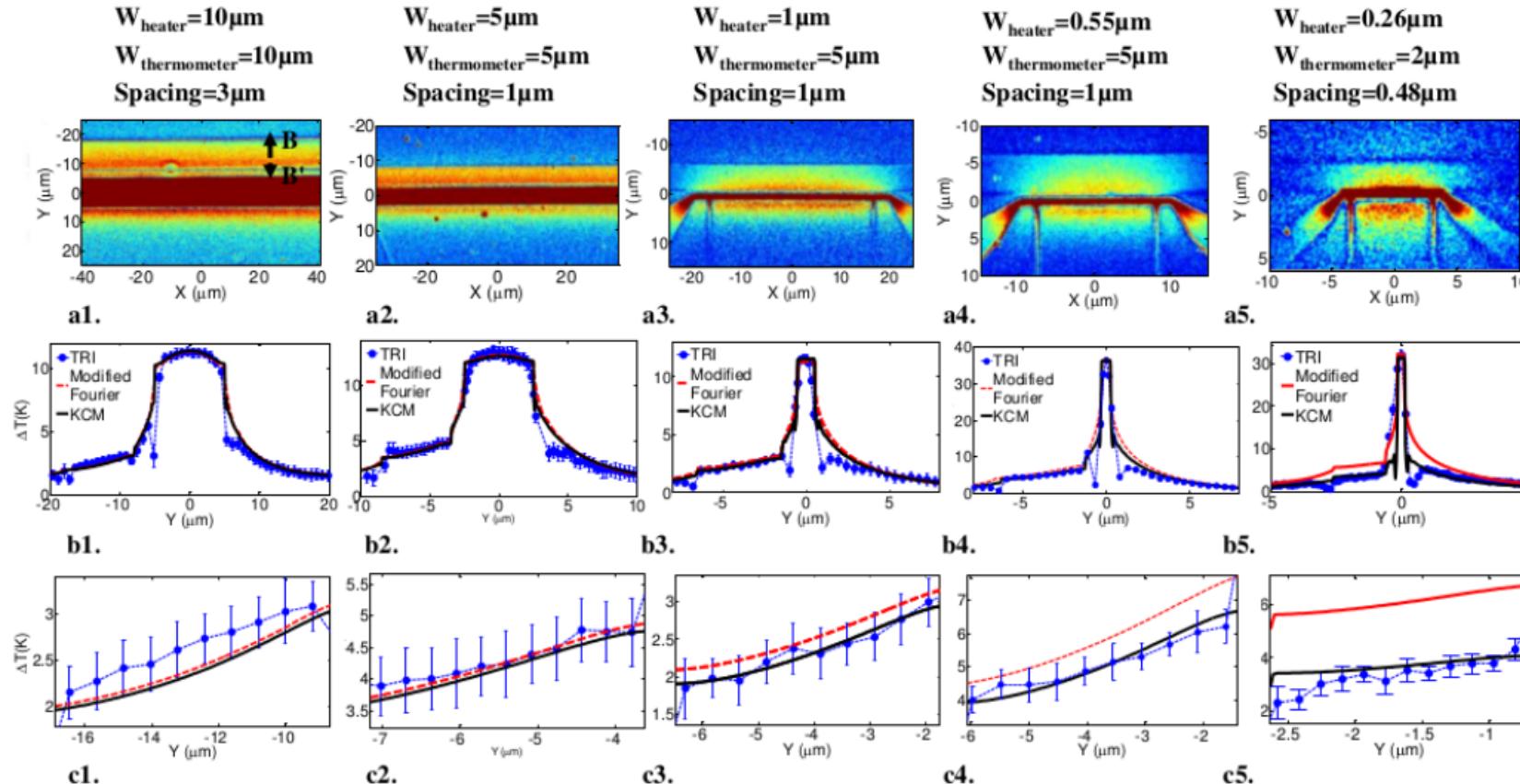
# GK equation



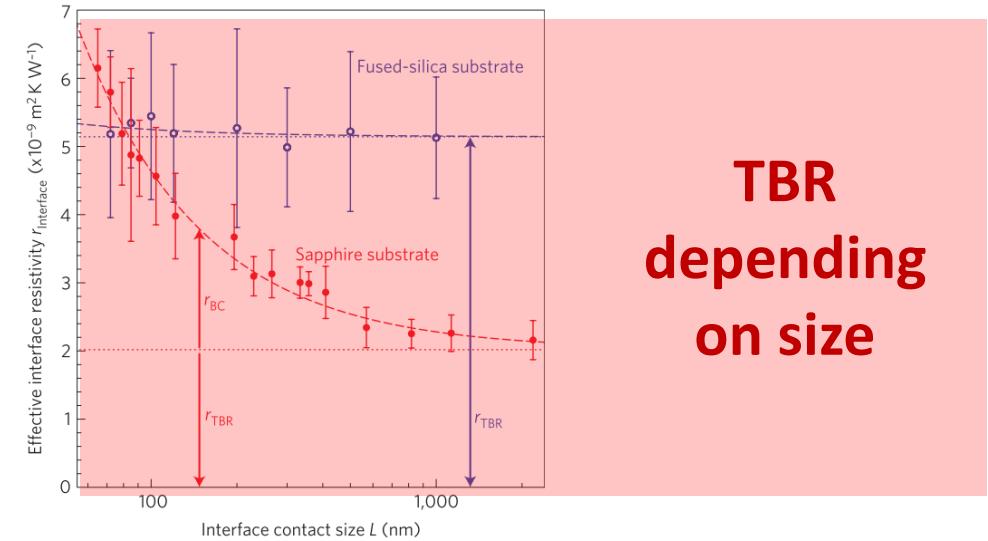
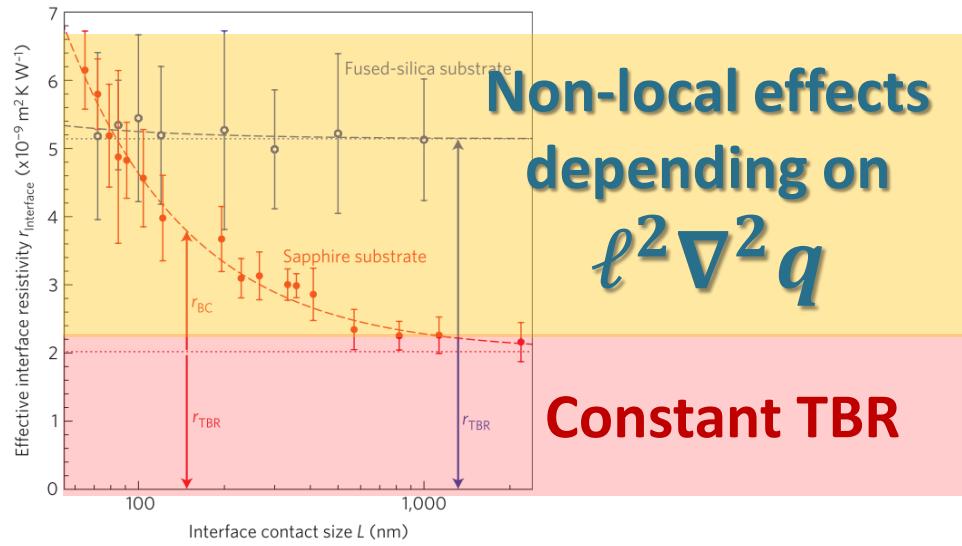
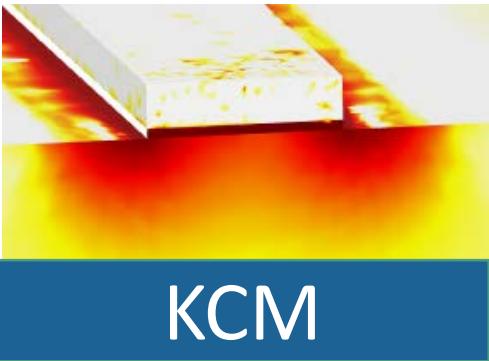
# Kinetic Collective Model + Guyer and Krumhansl

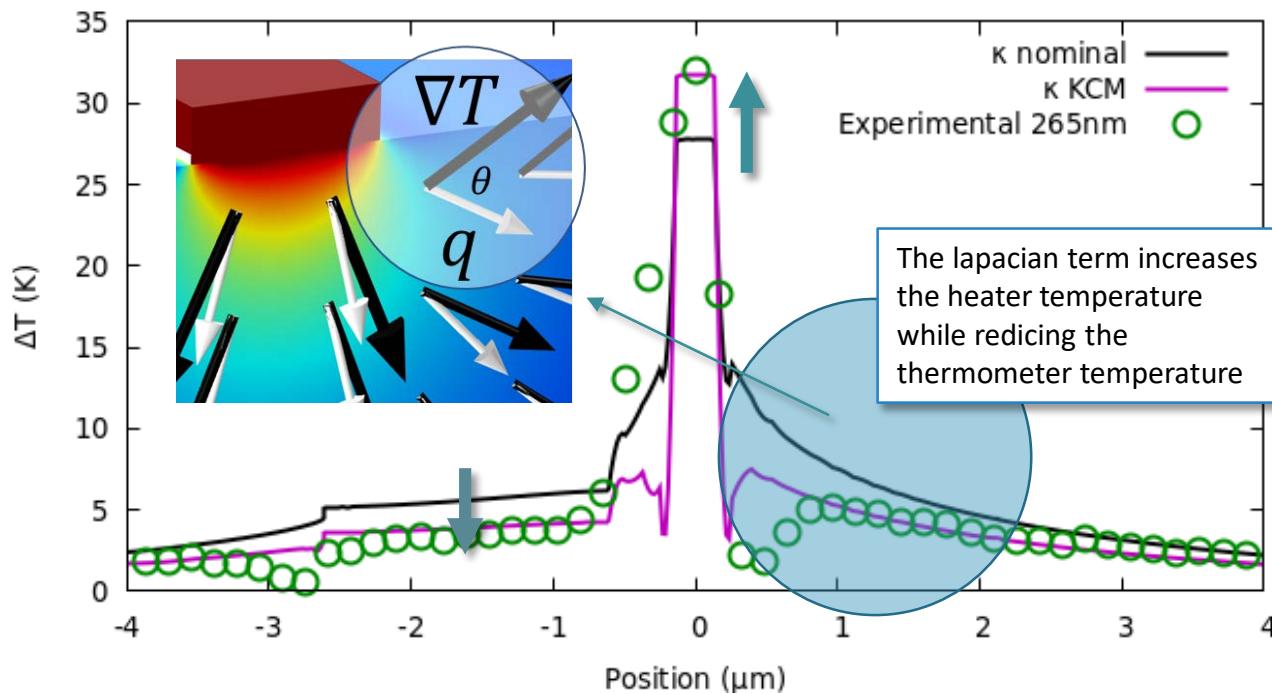
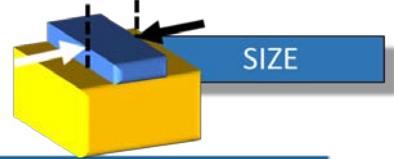
At large sizes we recover Fourier model

The smaller the size, the larger the effect

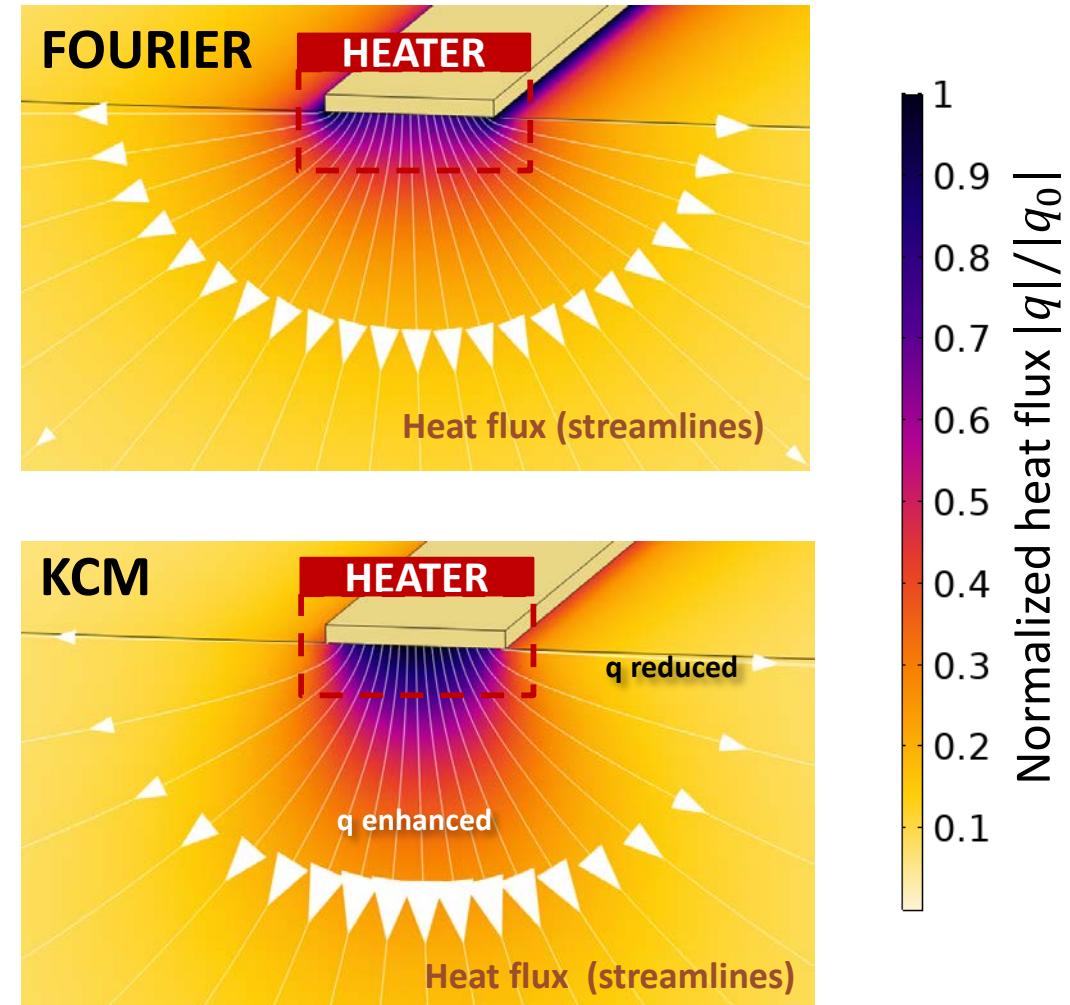


# TBR vs hydrodynamics





$$q = -\kappa \nabla T + \ell^2 \nabla^2 q$$



# OTHER HYDRODYNAMIC SIGNATURES IN SILICON



# OBSERVATION OF HYDRODYNAMIC TIME SCALES

# Temperature decay of metallic lines



Beardo, Knobloch et al.  
ACS Nano 15, 13019 (2021)



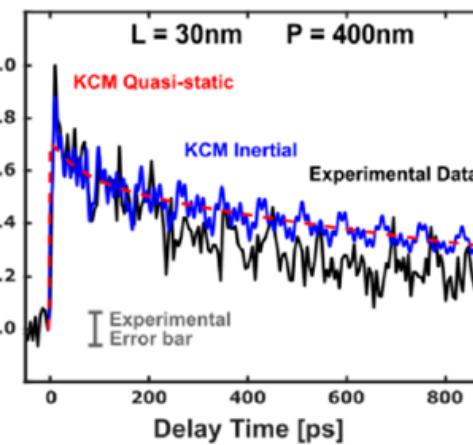
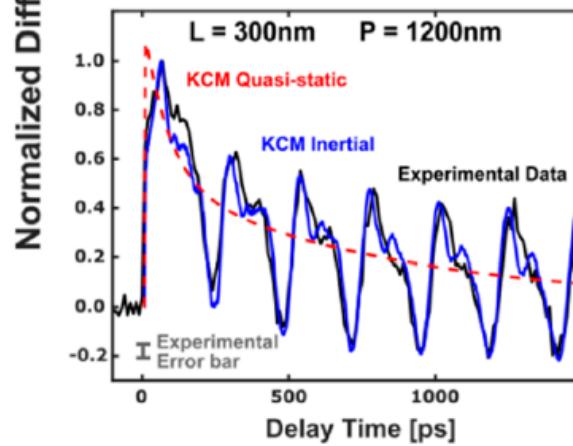
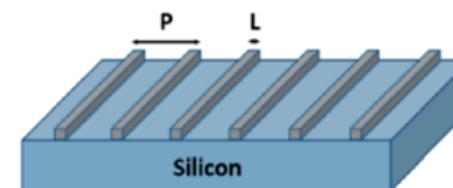
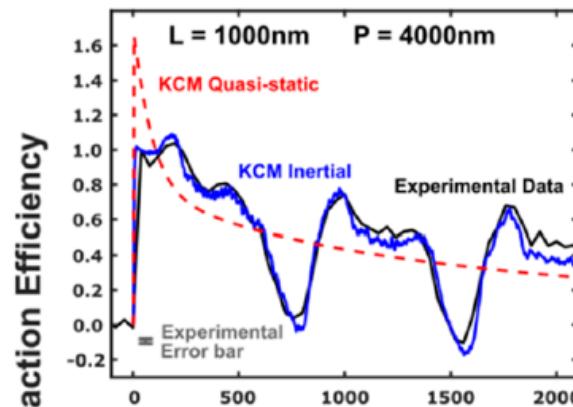
Margaret  
Murnane



University of Colorado  
Boulder

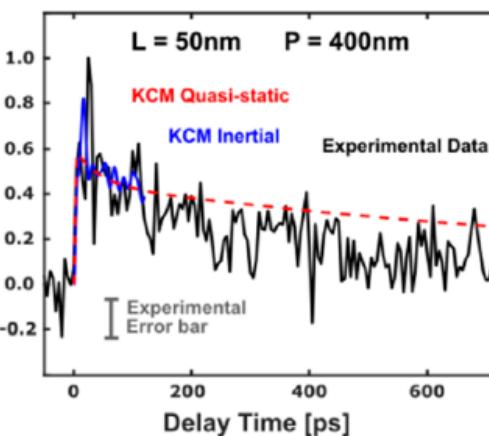
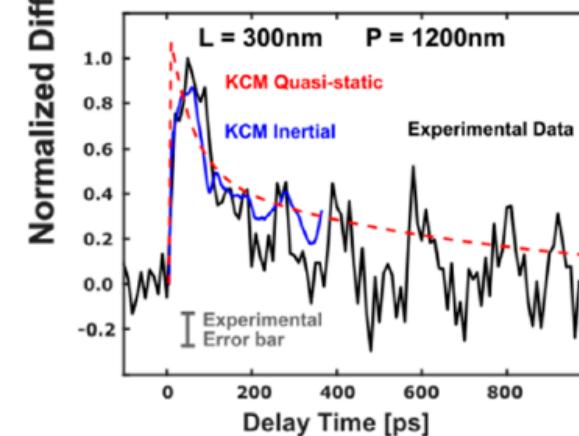
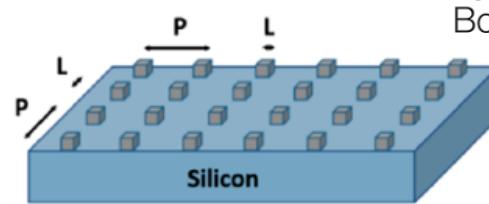
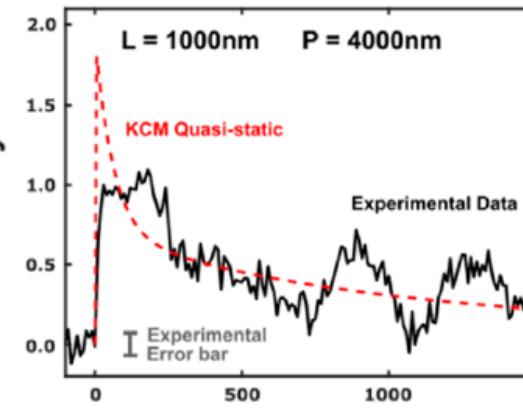
a

## Effectively isolated nanolines



b

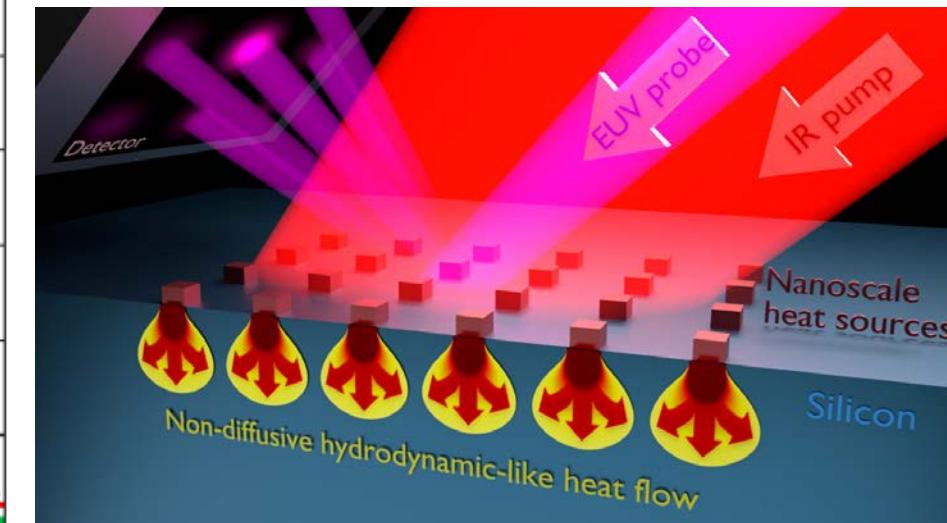
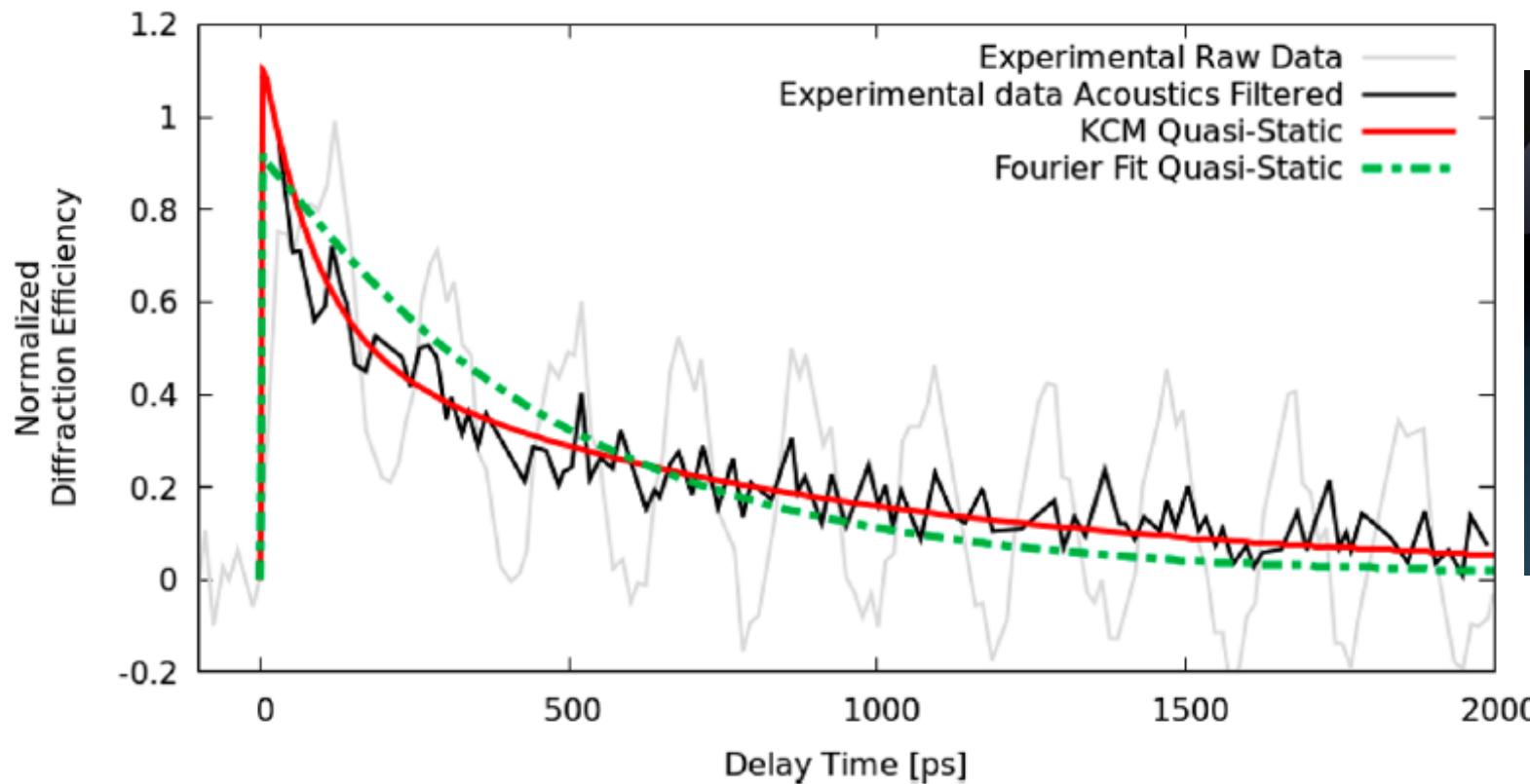
## Effectively isolated nanodots



# Non-Fourier decay / Double exponential



Beardo, Knobloch et al.  
ACS Nano 15, 13019 (2021)



EUV SCATTEROMETRY SETUP

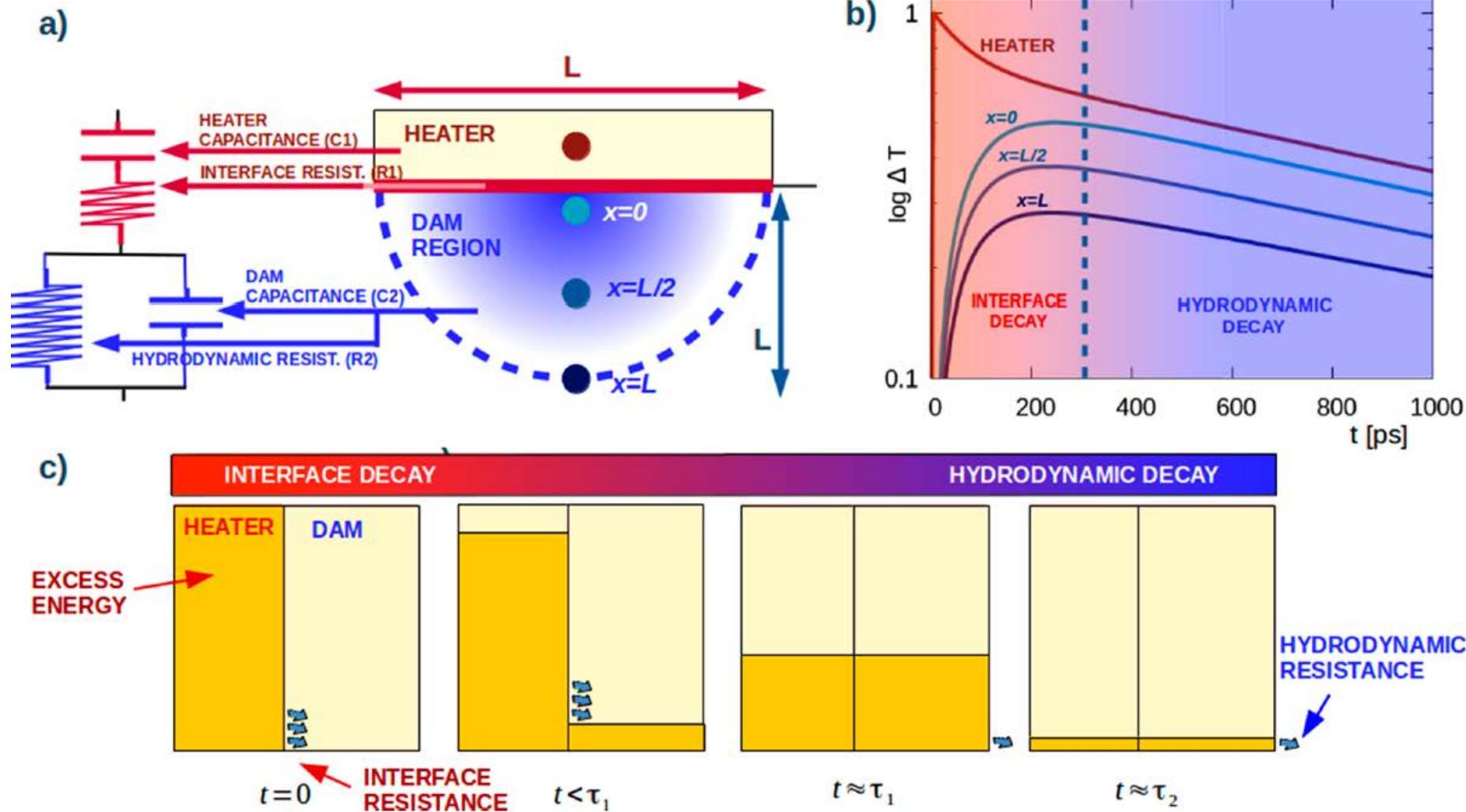


University of Colorado  
Boulder

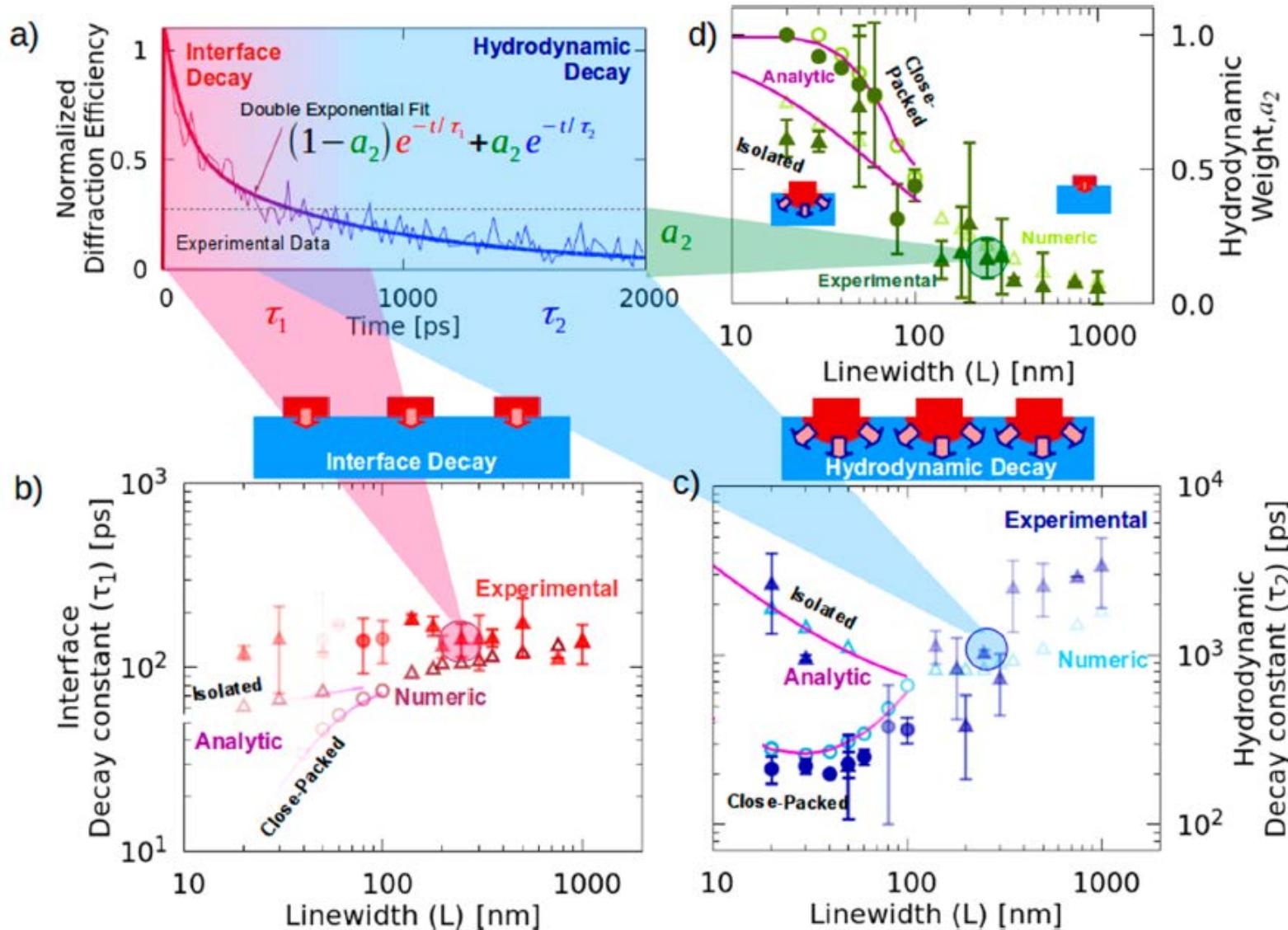
# Two Box model – The Dam region



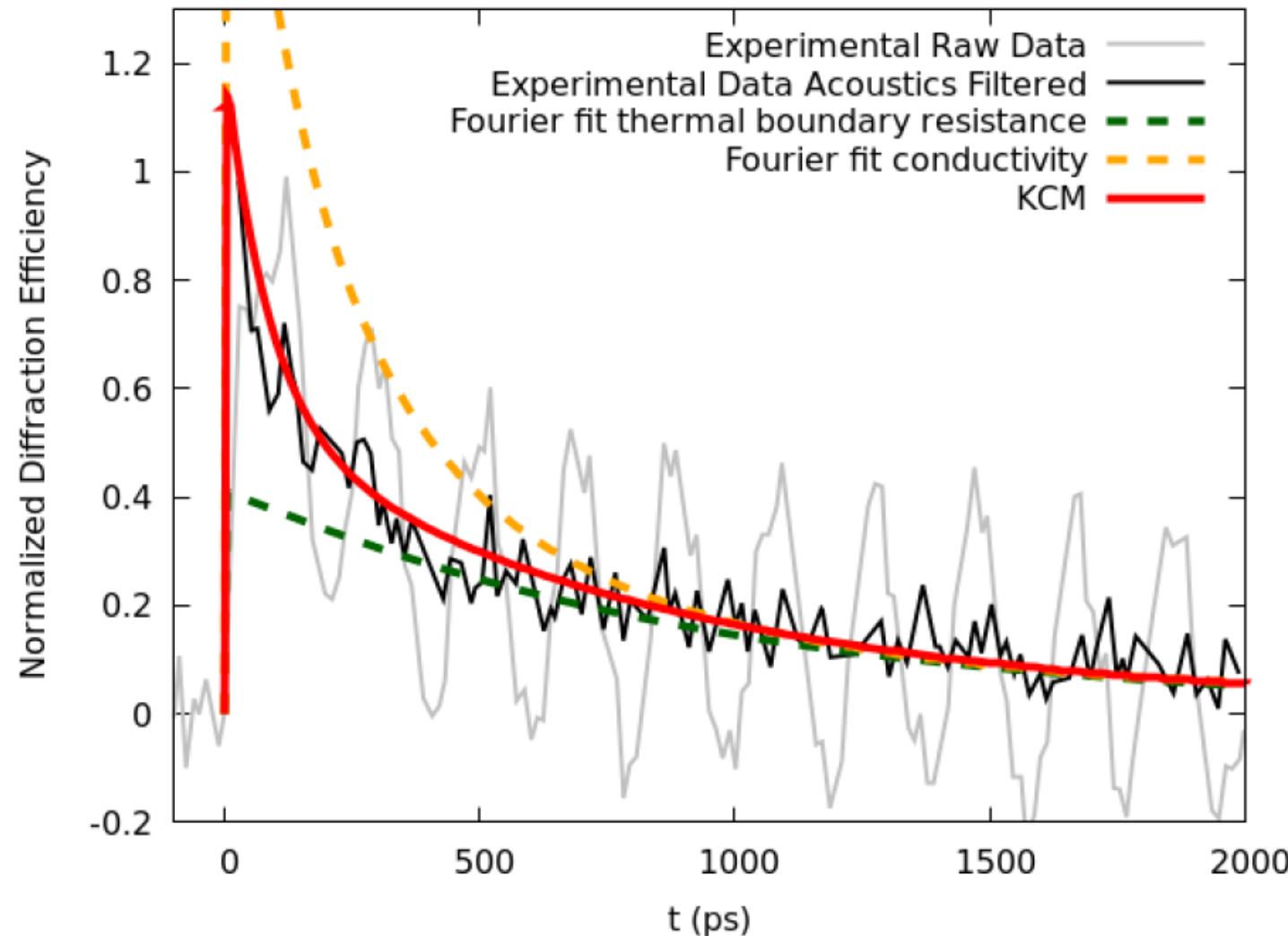
Beardo, Knobloch et al.  
ACS Nano 15, 13019 (2021)



## Two Box model / TBR and hydrodynamic relaxation times



## Two Box model / TBR and hydrodynamic relaxation times



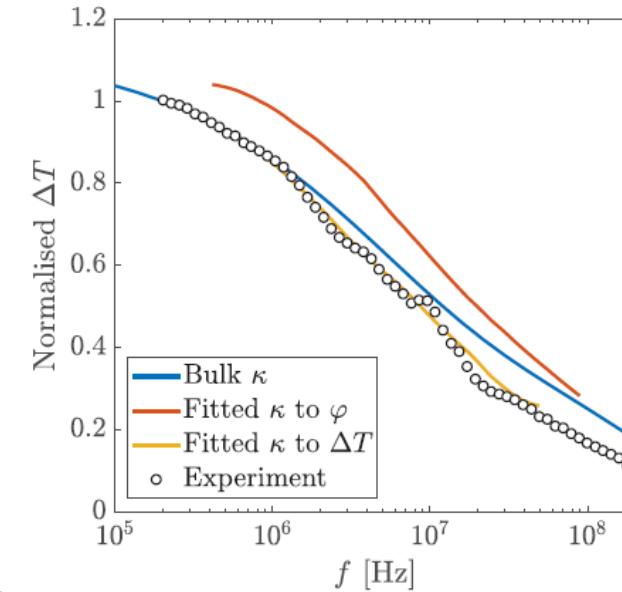
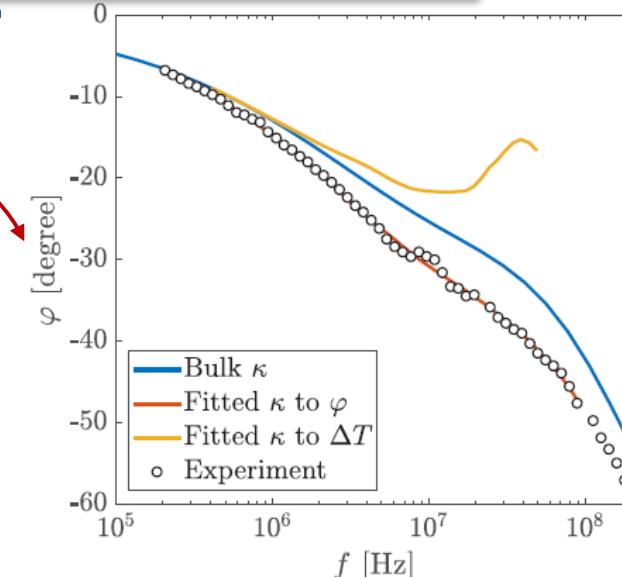
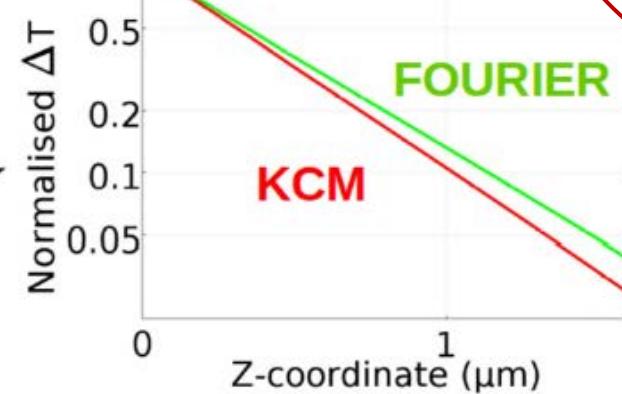
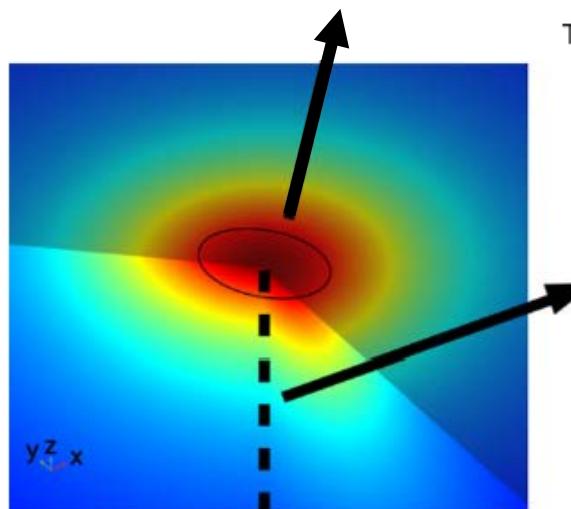
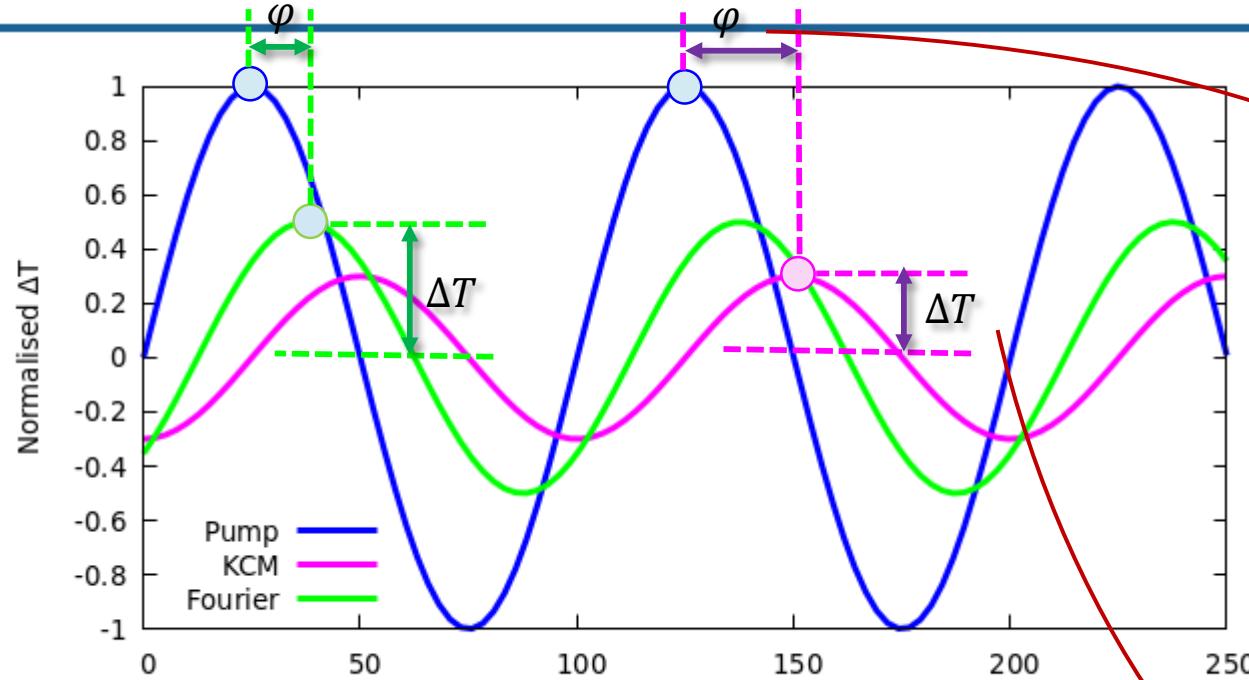
# **SECOND SOUND**

# Frequency Domain Thermoreflectance (FDTR)



Regner et al.  
Nat. Commun. 4, 1640 (2013)

FREQUENCY

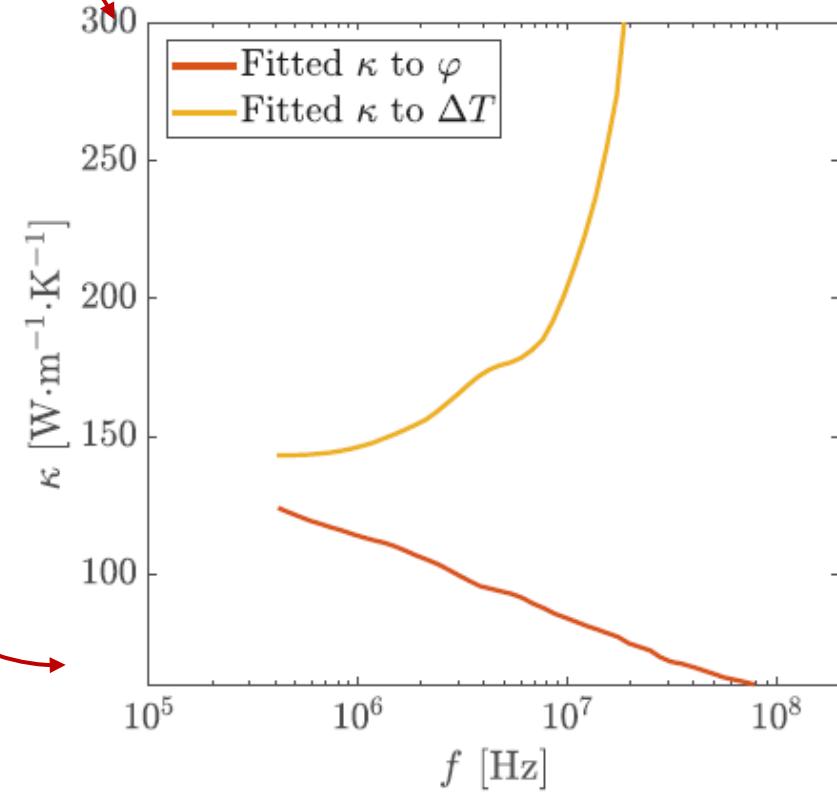
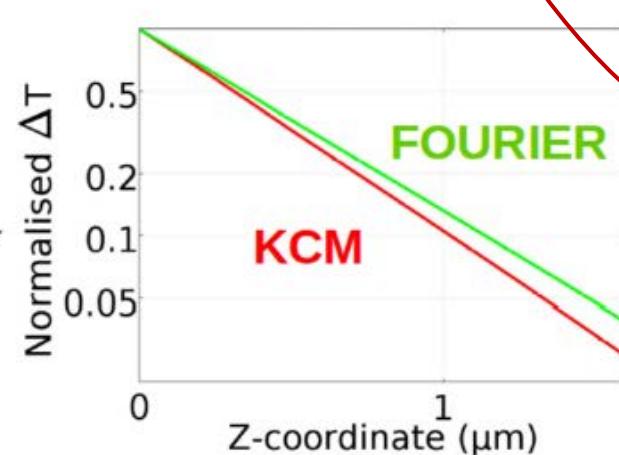
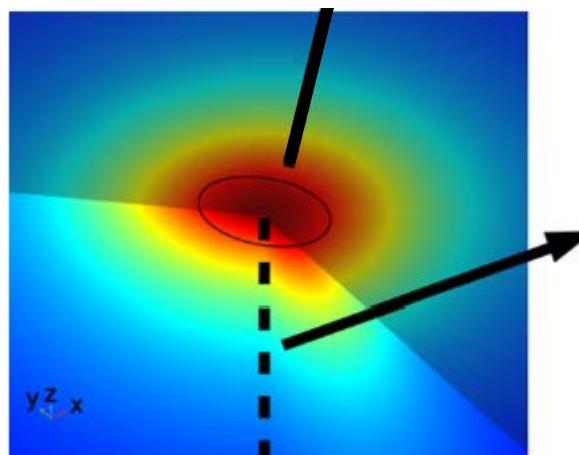
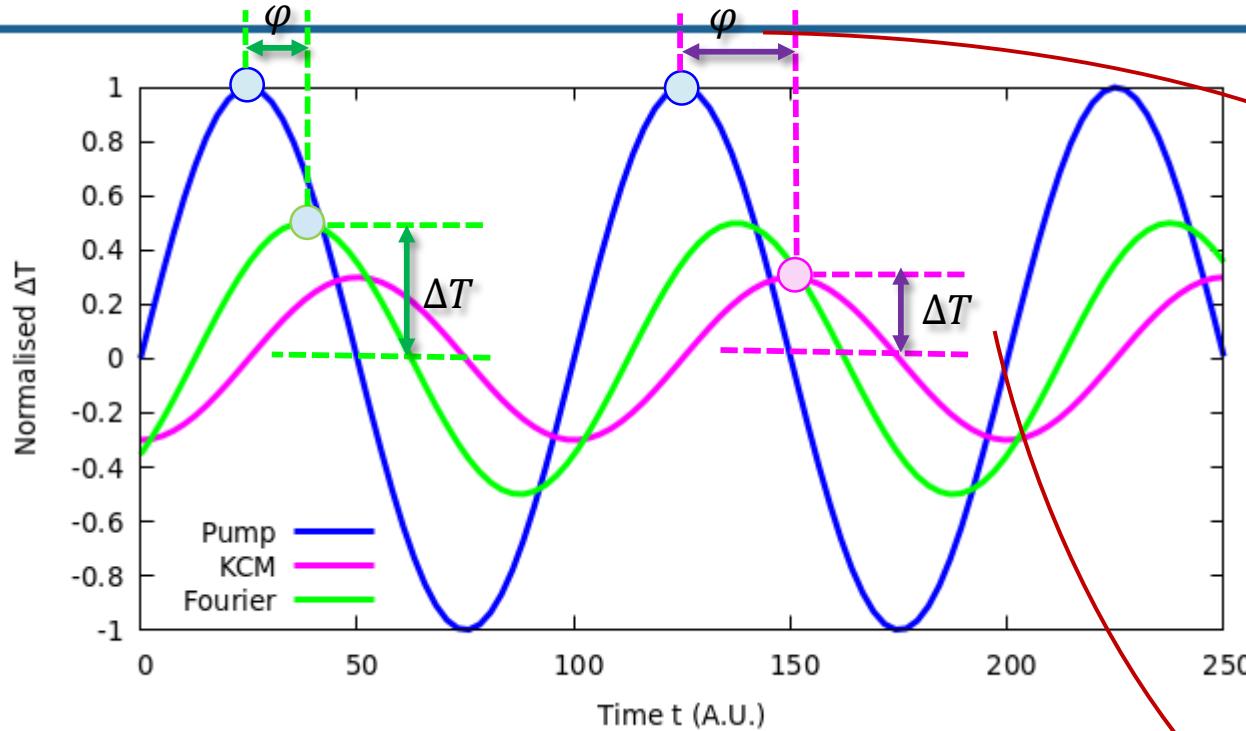


# Frequency Domain Thermoreflectance (FDTR)



Regner et al.  
*Nat. Commun.* **4**, 1640 (2013)

FREQUENCY

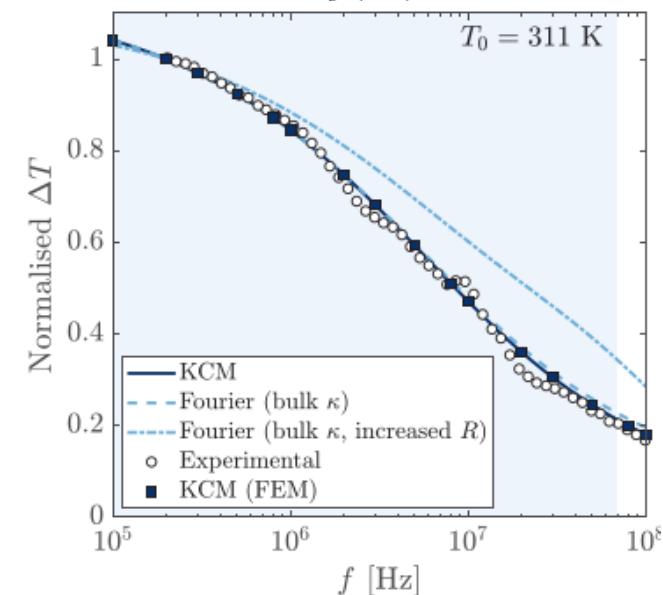
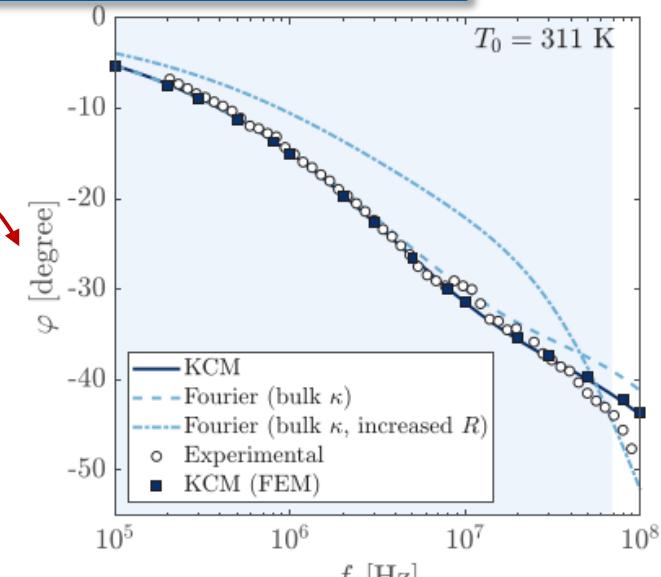
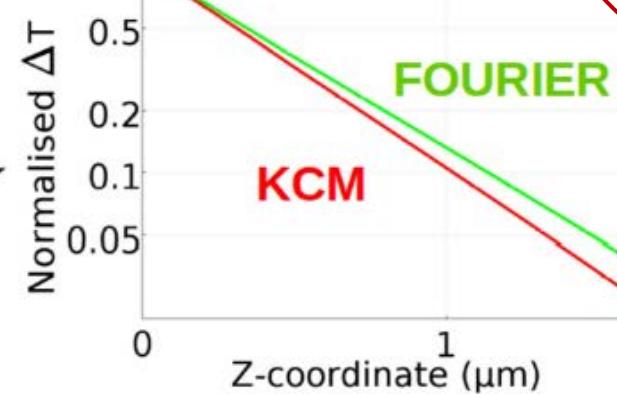
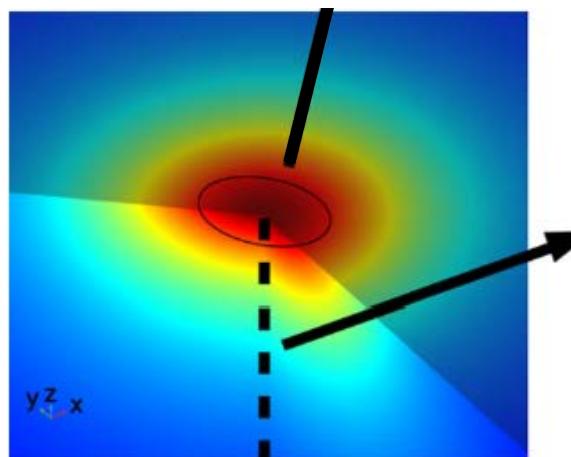
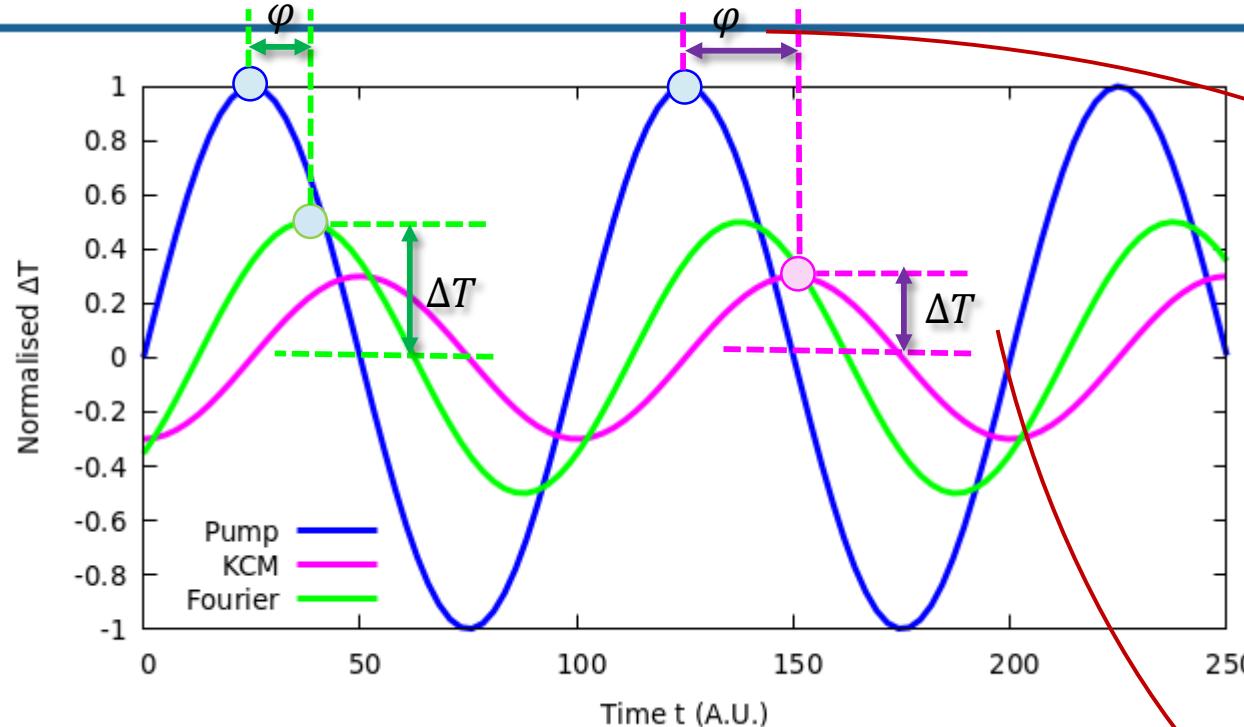


# Frequency Domain Thermoreflectance (FDTR)



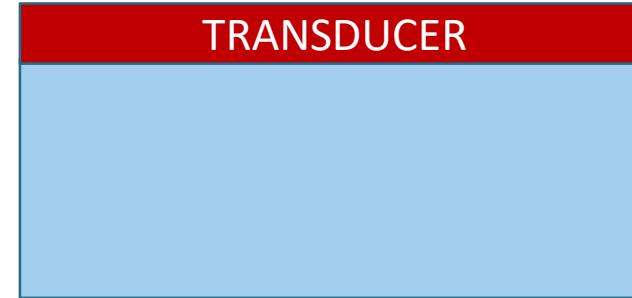
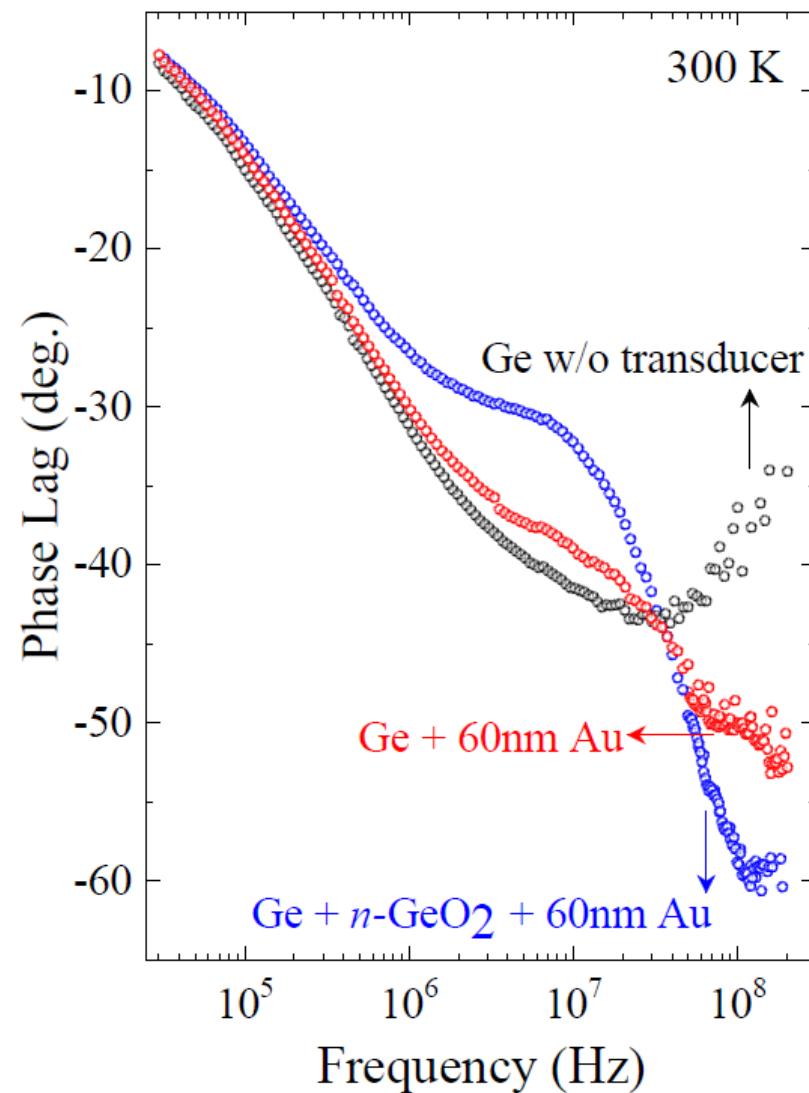
Regner et al.  
*Nat. Commun.* **4**, 1640 (2013)

FREQUENCY





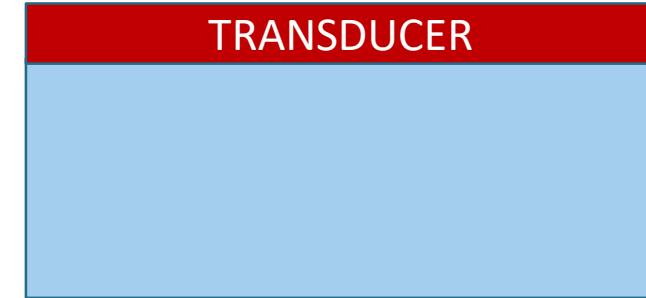
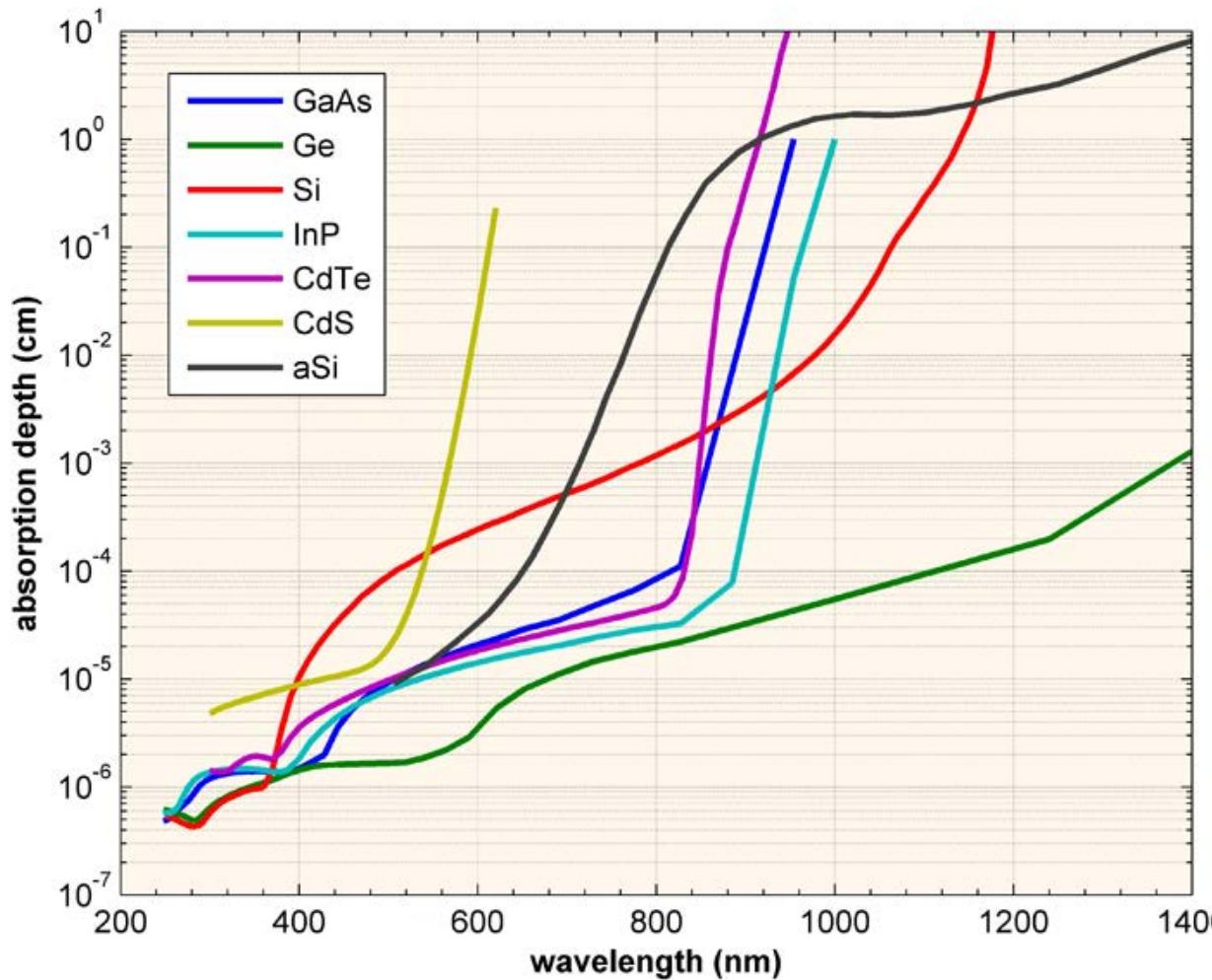
Sebastian  
Reparaz



# Memory effects / Second sound



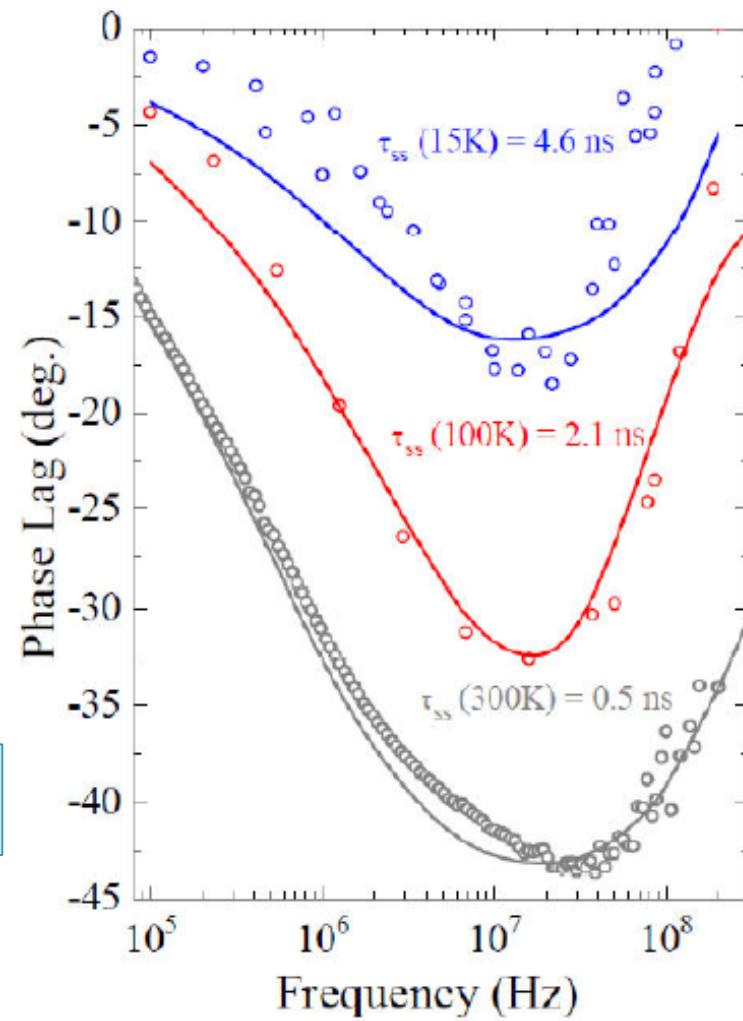
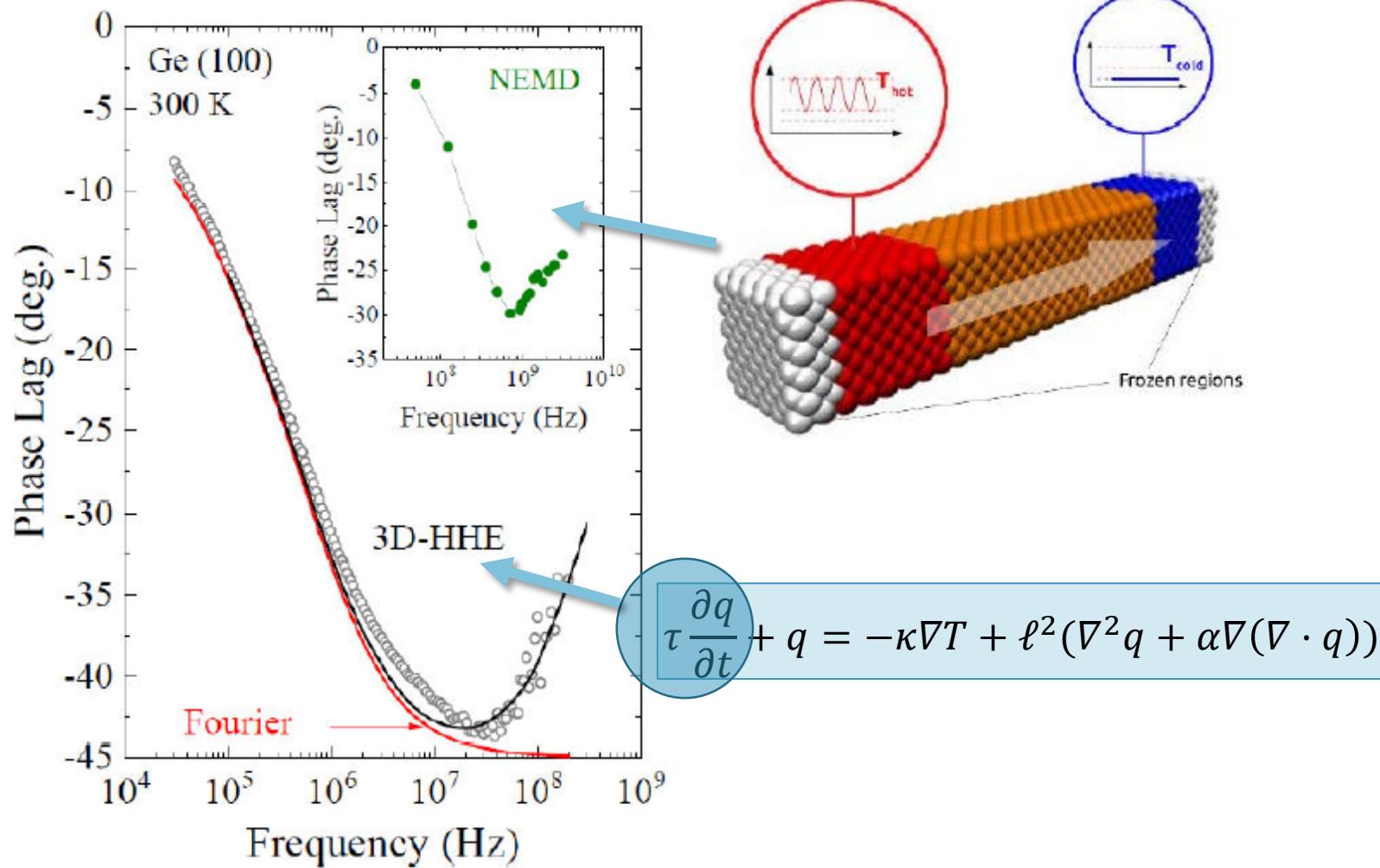
Beardo et al.  
*Sci. Adv.* 7, eabg4677 (2021)



# Memory effects / Second sound



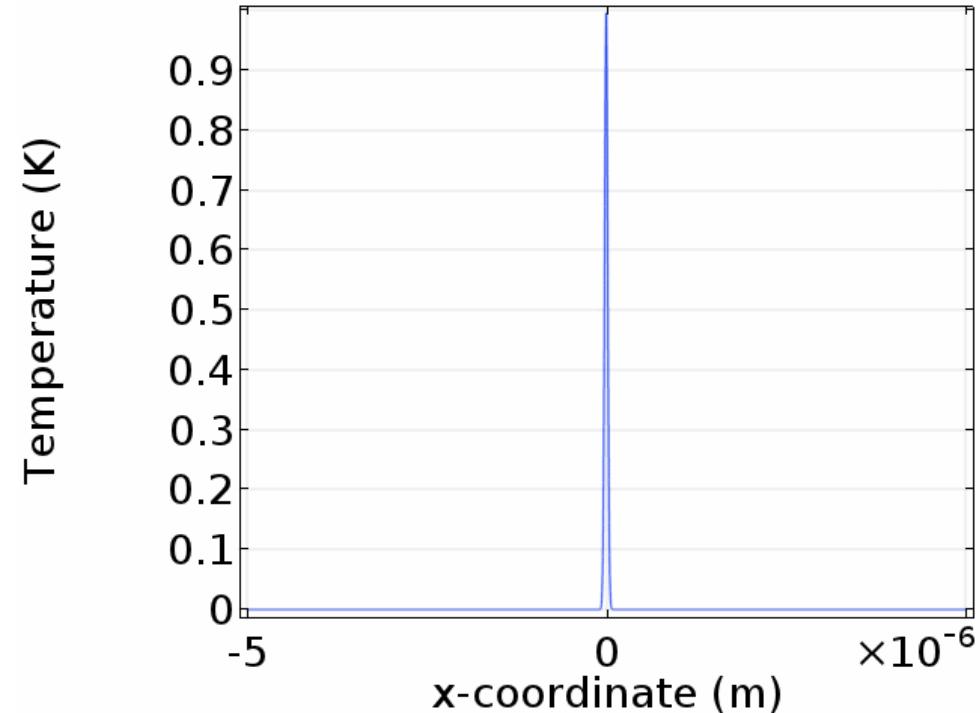
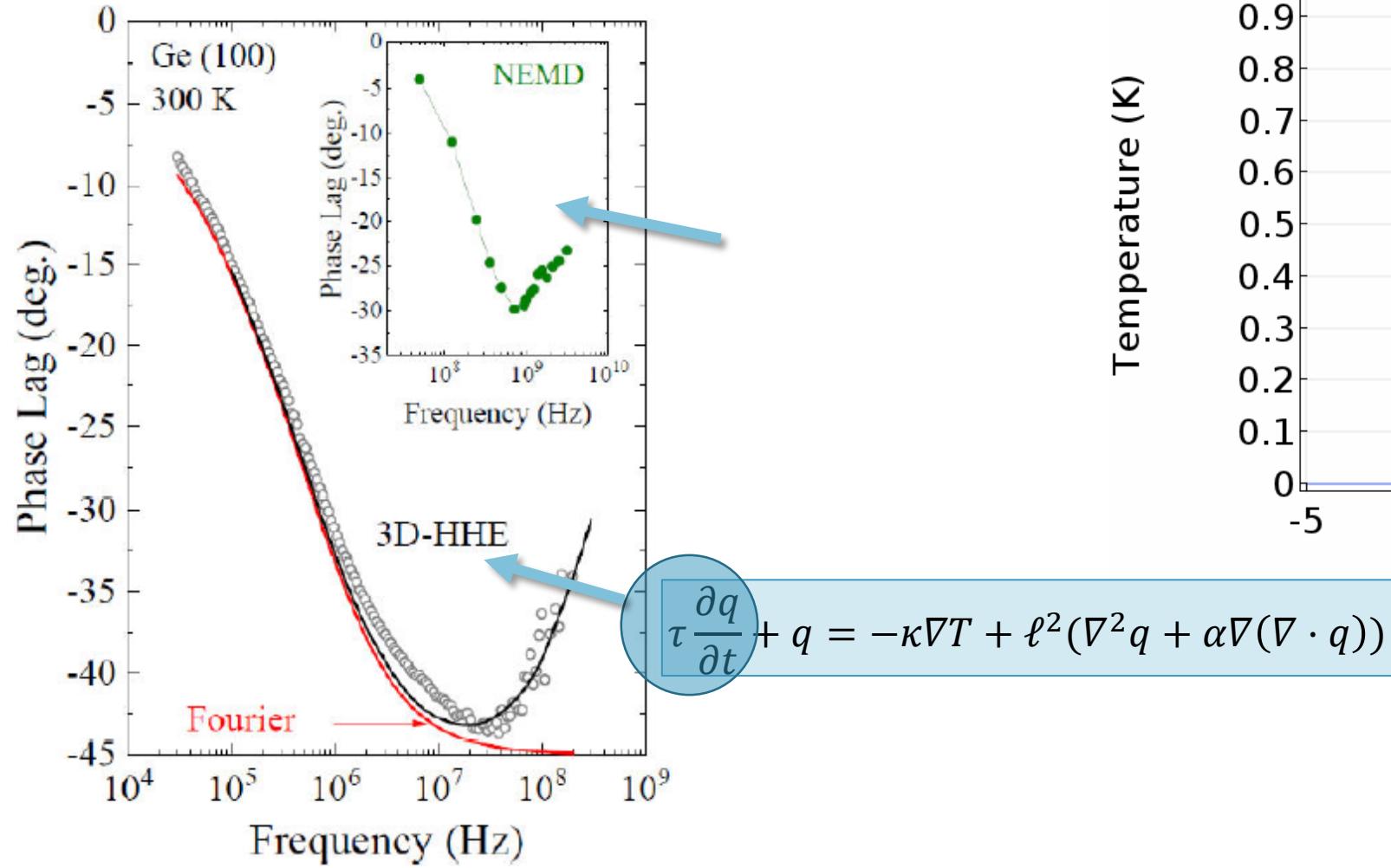
Beardo et al.  
Sci. Adv. 7, eabg4677 (2021)



# Memory effects / Second sound



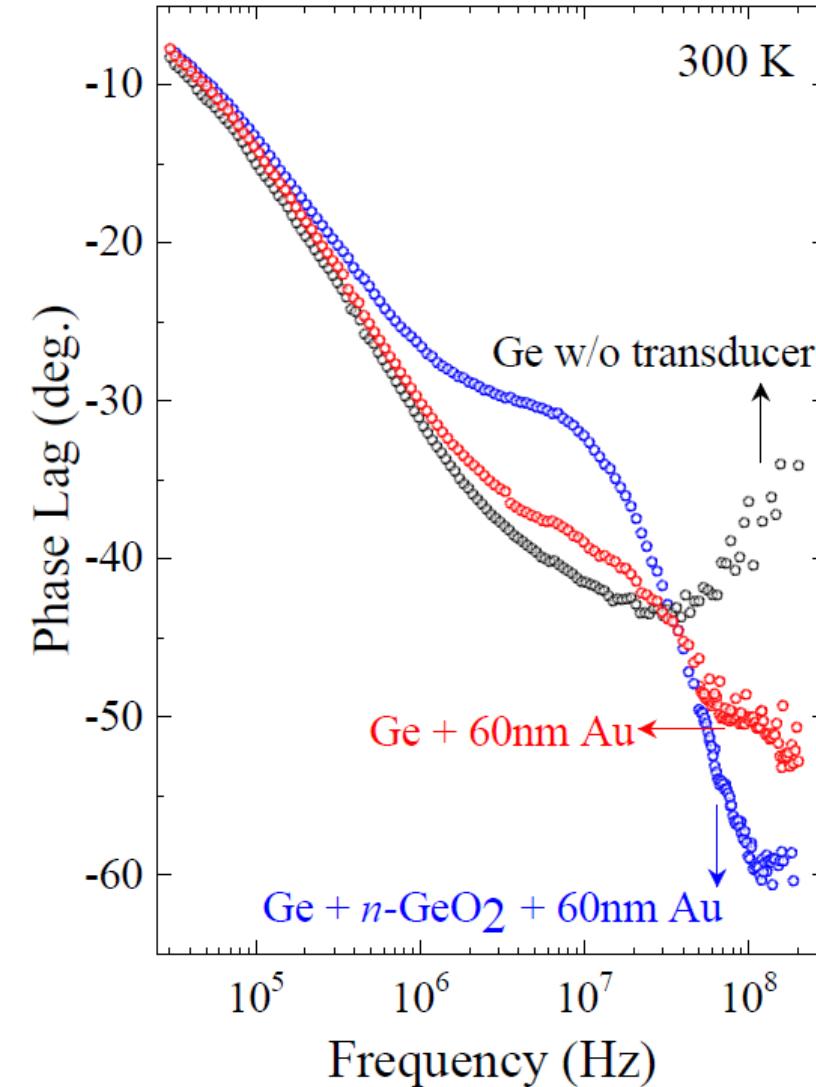
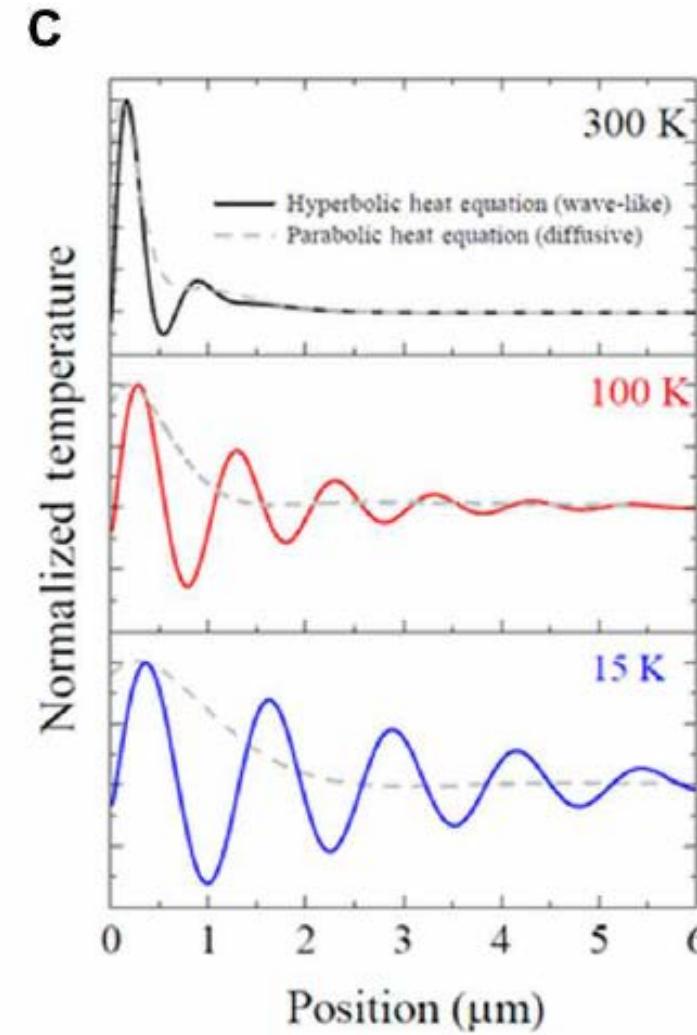
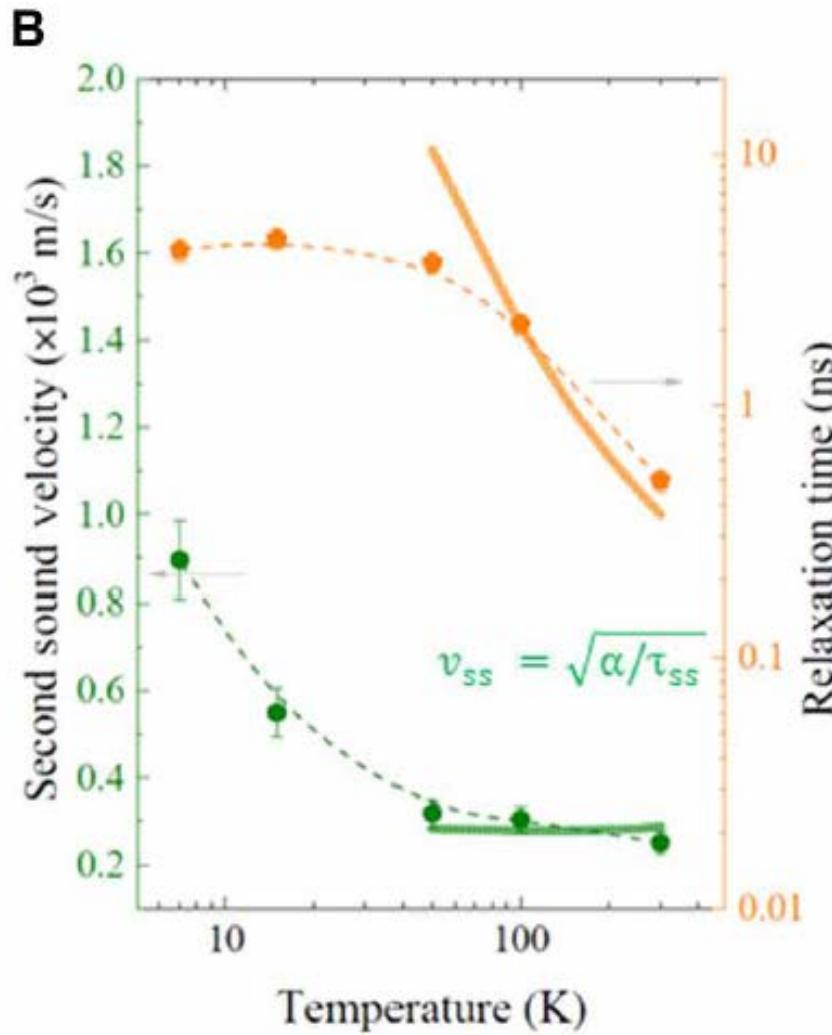
Beardo et al.  
Sci. Adv. 7, eabg4677 (2021)



# Memory effects / Second sound



Beardo et al.  
Sci. Adv. 7, eabg4677 (2021)



## Conclusions



My approach is fundamental

I'm pure



He's a phenomenological approach

He's a wrong approximation to the field

## Conclusions



H and S approaches are connected!

## Conclusions

---

- Combination of **Guyer and Krumhansl** equation with **ab-initio Kinetic Collective Model** for the transport properties allows the prediction of a large set of experiments
- The possibility to solve this model in a **Finite Element (COMSOL)** allows the direct comparison with any experimental setup despite its geometrical complexity
- The large set of experimental data on silicon explained by GK with a single abinitio set of parameters is an evidence in favor of a **hydrodynamic regime** in silicon

# Thank you

## THERMOREFLECTANCE IMAGING

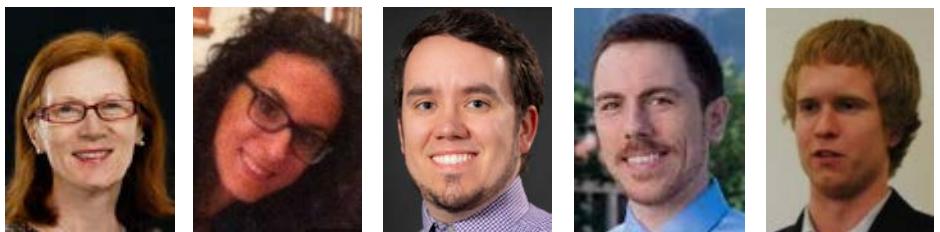


Sami Alajlouni   Amirkoushyar Ziabari   Ali Shakouri

## EUV SCATTEROMETRY SETUP

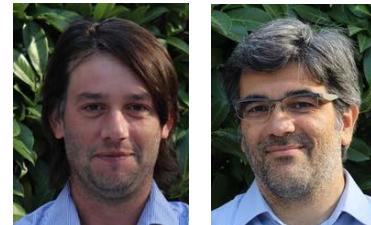


University of Colorado  
Boulder



Margaret Murnane   Begoña Abad   Joshua L. Knobloch   Travis Frazer   Brendan McBennett

## FDTR SETUP



Sebastian Reparaz   Riccardo Rurali

## GK-KCM MODEL



Lluc Sendra   Albert Beardo   Javier Bafaluy   Juan Camacho

