VI International Workshop on Nonequilibrium Thermodynamics

Thermodynamic analysis of irreversibilities in thin heat conducting films

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Outline

- Motivation
- Heat transport models for thin films
- The diffusive-ballistic transition.
  - Power spectrum of temperature fluctuations
  - Power spectrum of heat flux fluctuations
  - Thermodynamic susceptibility
  - Entropy production
  - Group and phase velocity
- Comments and conclusions

Motivation

- In small electronic structures heat is generated in a concentrated way which causes high temperatures operation
- This can affect their performance and reliability.
- Yet little has been done to analyze entropy generation in solids at length scales comparable with or smaller than the mean free path of heat carriers

- A fundamental knowledge of the entropy generation processes provides a thermodynamic understanding of heat transport in solid structures
- this is particularly important for the performance evaluation of thermal systems and microdevices

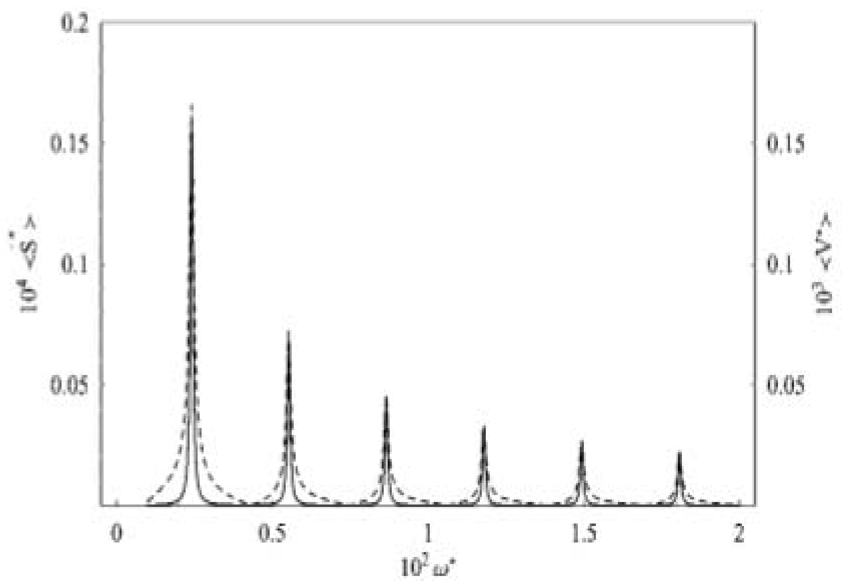
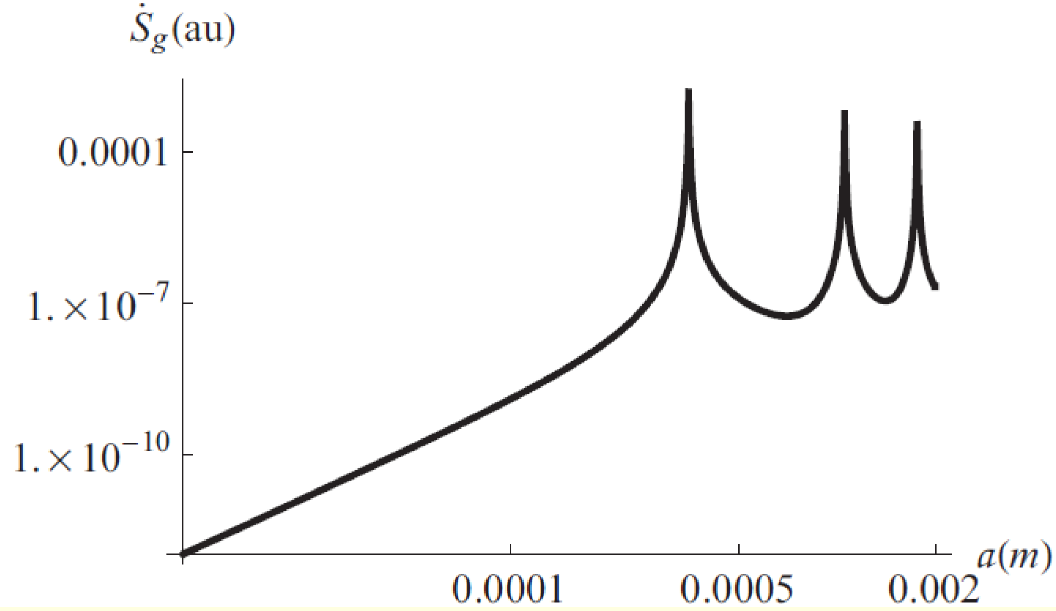


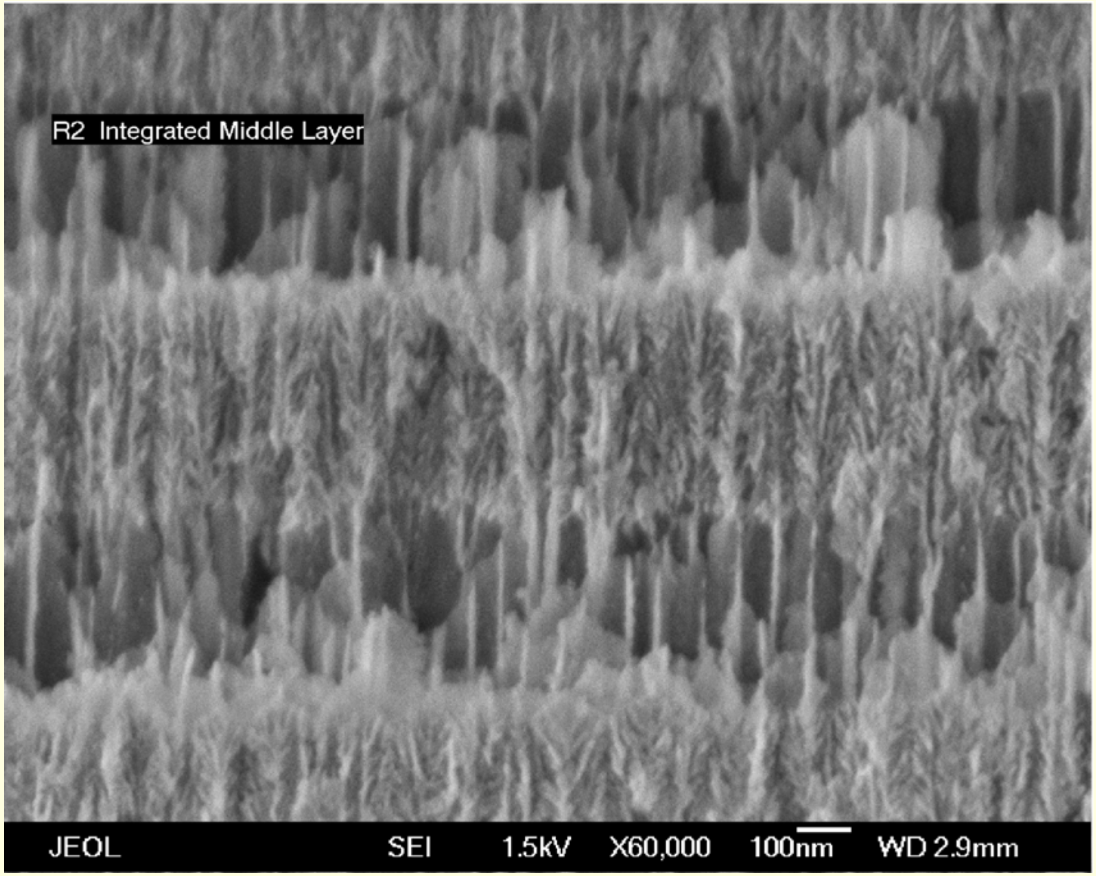
FIG. 1. Amplitude of the dimensionless velocity $\langle V^* \rangle$ (dashed line) and global entropy generation rate $\langle \dot{S}^* \rangle$ (solid line) as functions of the dimensionless frequency ω^* with $\alpha = 0.01$ and under isothermal conditions.

del Río et al., PRE 2004.

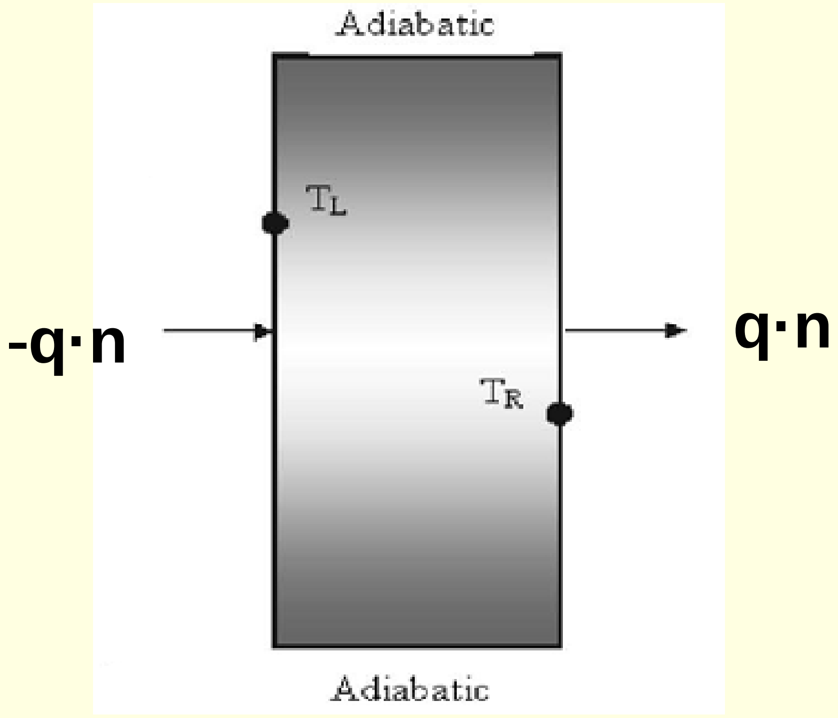
Figure 5. Global entropy production *vs.* plates separation. $\omega = 100$ Hz, $h_1 = 5000$ J/m^{2}K, $h_2 = 1000$ J/m^{2}K.



Vázquez et al., Entropy 2011.


R2 Integrated Middle Layer
JEOL
SEI
1.5kV
X60,000
100nm
WD 2.9mm

Heat conducting film



Effects of size reducing

A) Heat transport is no longer described by Fourier law (large space-time scales)

Other models (Cimmelli, JNET 2009):

Cattaneo

Guyer and Krumhansl

…

B) K depends on size

A) Heat transport model

Limiting cases

$$q = \lambda \frac{\Delta T}{L} \qquad \text{(diffusive transport)} \qquad \ell / L \ll 1$$

$$q = \Lambda \Delta T \qquad \text{(ballistic transport)} \qquad \ell / L \gg 1$$

Crossover from diffusive to ballistic heat transport

Generalized heat conductivity

(Jou et al. AML 2005)

$$q = \lambda(T, \ell/L)\frac{\Delta T}{L}$$

Properties

$$\lambda(T, \ell/L) \to \lambda(T) \qquad \text{for } \ell/L \to 0,$$

$$\lambda(T, \ell/L) \to \frac{\lambda(T)}{a}\frac{L}{\ell} \equiv \Lambda(T)L \qquad \text{for } \ell/L \to \infty$$

$\lambda(T, \ell/L)$ a generalized heat conductivity

Or

(Chen, J. Heat Transfer 2002).

$$\boldsymbol{q} = \boldsymbol{q}_d + \boldsymbol{q}_b$$

Heat transport models linking diffusive and ballistic regimes

Ballistic-diffusive equations (Chen, J. Heat Transfer 2002).

$$\boldsymbol{q} = \boldsymbol{q}_d + \boldsymbol{q}_b$$

$$C\left(\tau \frac{\partial^2 T_m}{\partial t^2} + \frac{\partial T_m}{\partial t}\right) = \nabla(k\nabla T_m) - \nabla \cdot \mathbf{q}_b$$

$\mathbf{q}_b$ given by solutions of Boltzmann´s equation

Lebon et al. model (Lebon et al., Proc. R. Soc. A 2011).

$$\boldsymbol{q} = \boldsymbol{q}_d + \boldsymbol{q}_b$$

$$\tau_d \frac{\partial \boldsymbol{q}_d}{\partial t} + \boldsymbol{q}_d = -\lambda_d \nabla T$$

Cattaneo

$$\tau_b \frac{\partial \boldsymbol{q}_b}{\partial t} + \boldsymbol{q}_b = -\lambda_b \nabla T + l_b^2 (\nabla^2 \boldsymbol{q}_b + 2\nabla\nabla . \boldsymbol{q}_b)$$

Guyer and Krumhansl

The C-F- model (Anderson and Tamma, PRL 2006).

$$q = q_C + q_F,$$

$$q_C + \tau \frac{dq_C}{dt} = -(1 - F_T)K\frac{dT}{dx},$$

$$q_F = -F_T K\frac{dT}{dx}.$$

$$F_T := K_F/(K_F + K_C)$$

GENERIC (Öttinger and Grmela, PRE 1997)

- Mesoscopic view

Gas of phonons

State variable: one-phonon distribution function

- Two level description for small systems

State variables: energy density, heat flux and one-phonon distribution function

GENERIC $\longrightarrow$ Chen's equations plus non linear terms and terms involving gradients

Grmela et al., APL 2005.

B) K dependent on size

Extended Irreversible Thermodynamics

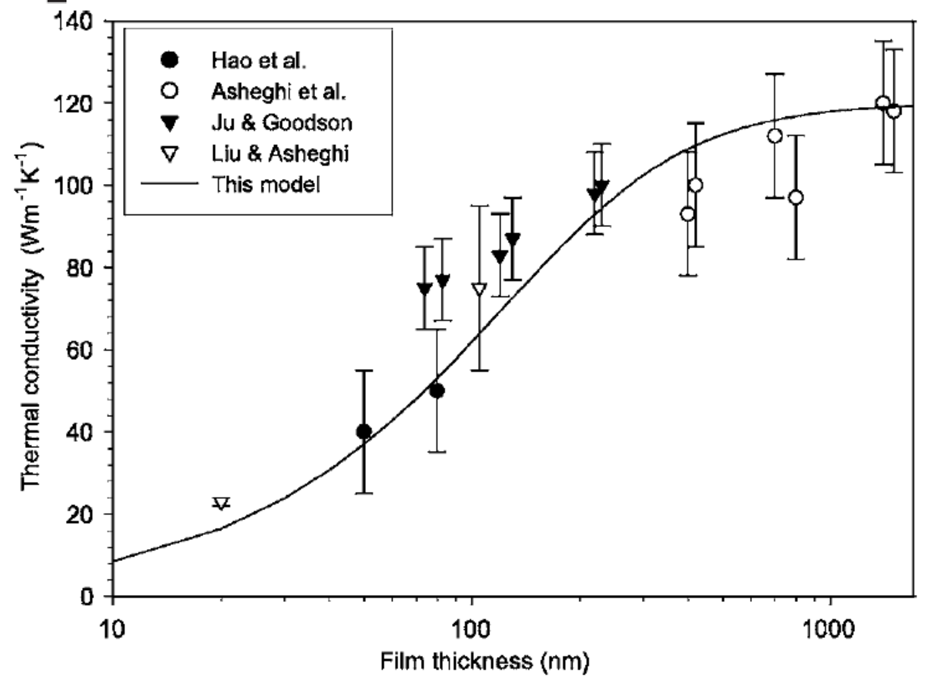
Dynamics of higher order fluxes

$$\lambda(\omega,k) = \frac{\lambda_0(T)}{1 + i\omega\tau_1 + k^2 l_1^2/\{1 + i\omega\tau_2 + k^2 l_2^2/[1 + i\omega\tau_3 + k^2 l_3^2/(1 + i\omega\tau_4 + \ \dots)]\}}$$

Size dependent heat conductivity

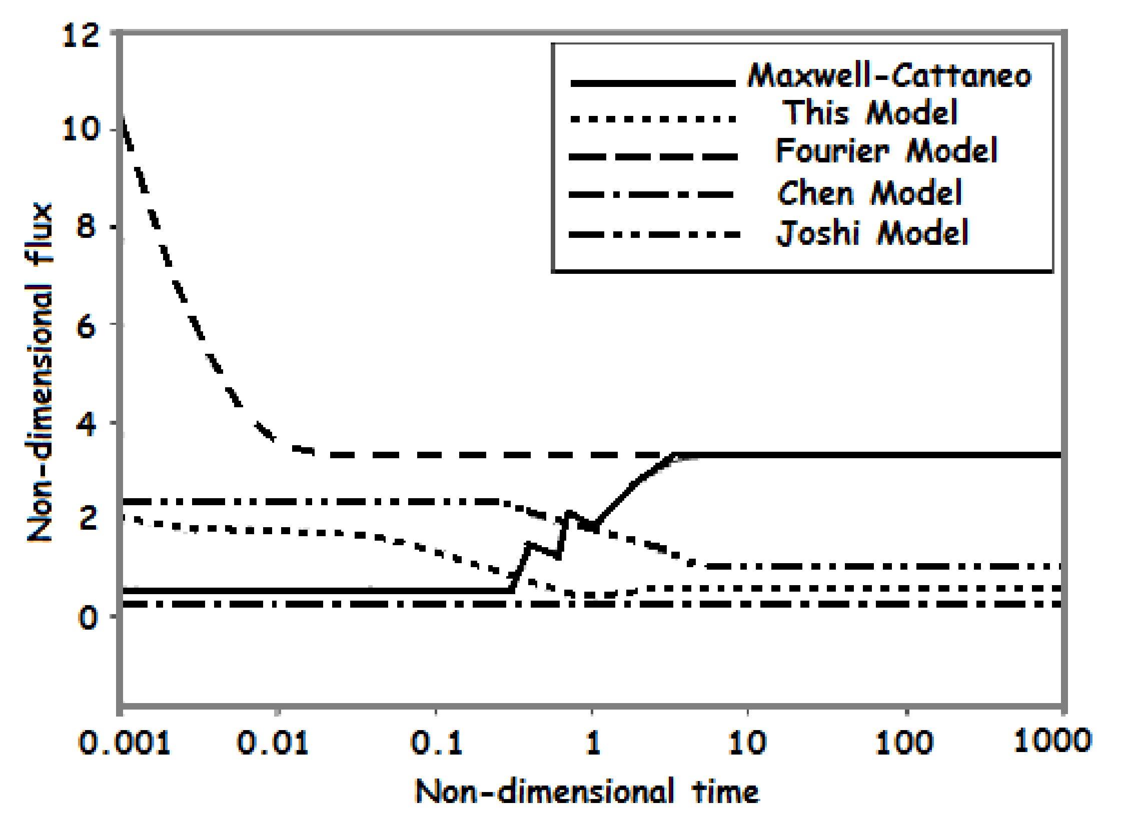
Stationary state, k=2π/L

$$\lambda(L) = \frac{\lambda_0 L^2}{2\pi^2 l^2}\left[\sqrt{1+4\left(\frac{\pi l}{L}\right)^2} - 1\right]$$



Jou et al., APL 2007

In favor of the use of K(Kn) in the transport equations:



Jou et al., APL 2007

FIG. 2. Evolution of the heat flux through the *x*=0 wall in a device with Knudsen number of 10. The dashed line represents the Fourier law, the solid line is the Maxwell-Cattaneo equation, the dotted line is the EIT equation, and the dash-dotted lines are Chen model Ref. 19 and model by Joshi and Majumdar Ref. 4.

We use C-F model

$$\boldsymbol{q} = \boldsymbol{q}_d + \boldsymbol{q}_b$$

Fourier

Cattaneo

+

$$K = \frac{\lambda_0 L^2}{2\pi^2 l^2}\left[\sqrt{1 + 4\left(\frac{\pi l}{L}\right)^2} - 1\right]$$

and

Model parameter F_T

Jeffrey like model

C-F model $\longrightarrow$

$$q + \tau \frac{dq}{dt} = -K \left[\frac{\partial T}{\partial x} + \tau F_T \frac{\partial}{\partial t} \left(\frac{\partial T}{\partial x} \right) \right] + \widehat{f}$$

$\widehat{f}$ is a δ-correlated function with zero mean.

with $$\mathrm{K} = \frac{\lambda_0 L^2}{2\pi^2 l^2} \left[\sqrt{1 + 4\left(\frac{\pi l}{L}\right)^2} - 1 \right]$$

Jeffrey's equation has been obtained from different theoretical schemes

- Double-lag method (Tzou, 1997),
- Extended Irreversible Thermodynamics (Jou et al. 2011),
- Internal variables formalism (Mauguin, 1990),
- Kernel (Joseph and Preziosi, 1989)

$$Q(s) = k_1 \delta(s) + \frac{k_2}{\tau} e^{-s/\tau}$$

Jeffrey’s model and the ballistic-diffusive transition

Temperature equilibrium fluctuations

FD Theorem

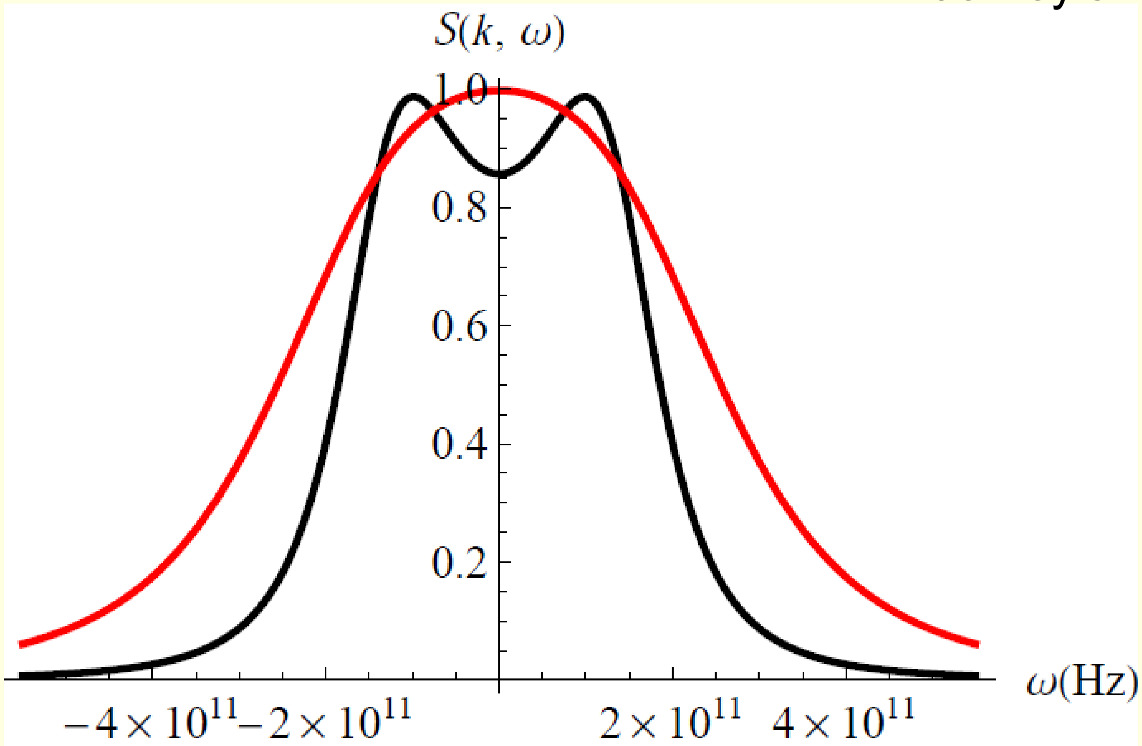
$$< \widehat{f}(k,\omega)\widehat{f}^*(k',\omega') > = (2k_B T_0^2/\tau^2)\lambda_0 \delta(k-k')\delta(\omega-\omega')$$

Power spectrum

$$S(K_n,k,\omega) = \frac{(2k_B T_0^2/\tau^2)\lambda_0 k^2}{(K(K_n)\tau F_T k^2 - (1+\tau^2\omega^2)\rho c_v)^2\omega^2 + (K(K_n)k^2 - \rho c_v \tau\omega^2)^2}$$

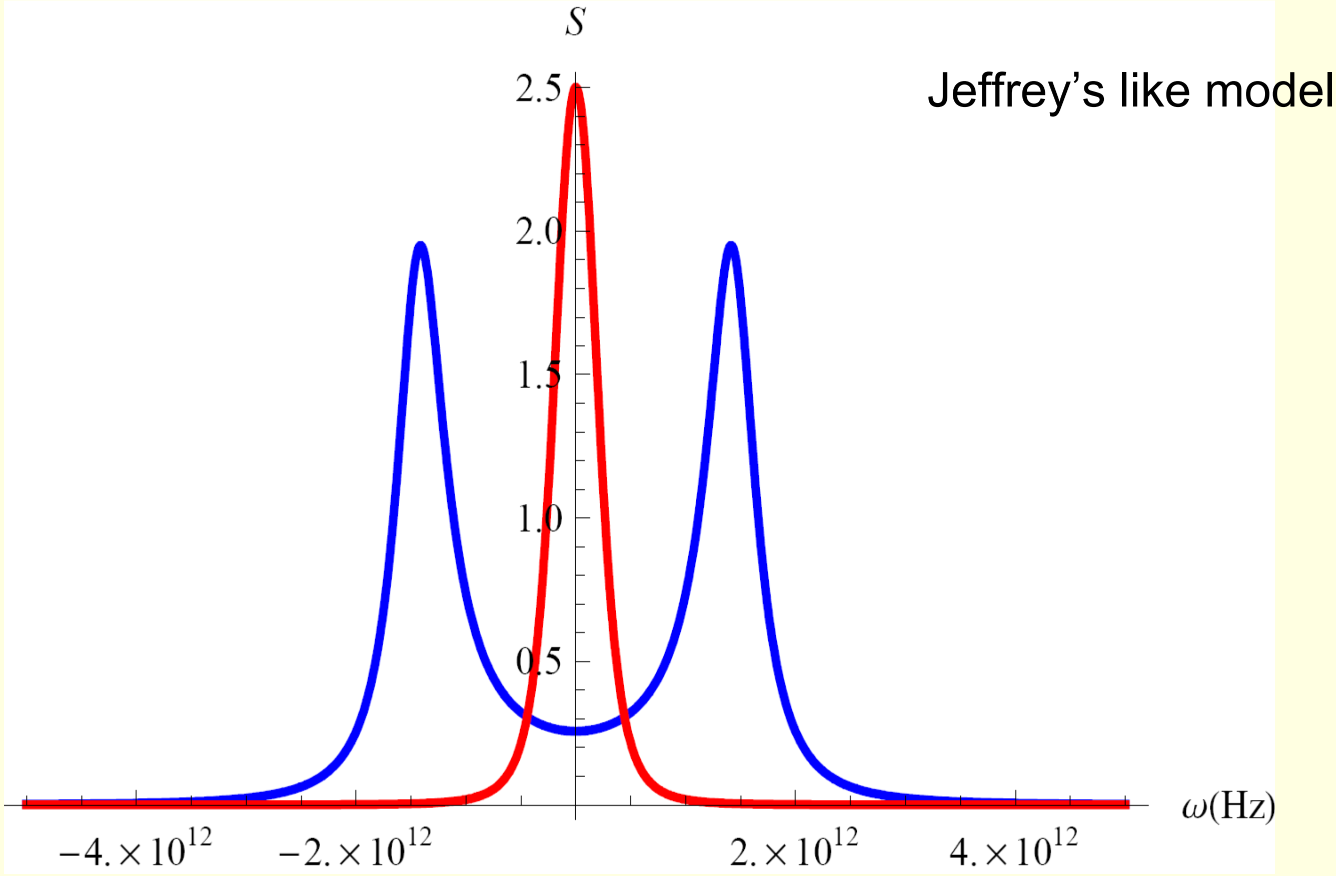
Power spectrum of temperature fluctuations

Jeffrey's like model



As a function of Kn (Knudsen number) and frequency. Red line corresponds to Kn = 0.2 (diffusive transport) and the black one to Kn = 2.5 (wave propagation). The WP −DT transition occurs at Kn = 2.3 and FT = 0.1. The material is Silicon.

Power spectrum of temperature fluctuations



Blue kn=1>knt (ballistic), red kn=0.38<knt (diffusive), knt=0.43.

Diffusive transport and wave propagation

Physical meaning of the maxima:

They appear at $\pm\omega_{max}$

If $\omega_{max} = 0$ one maximum exists.

Other case:

There exists propagation of thermal waves with velocity

$$\omega_{max}/k$$

Transition Knudsen number:

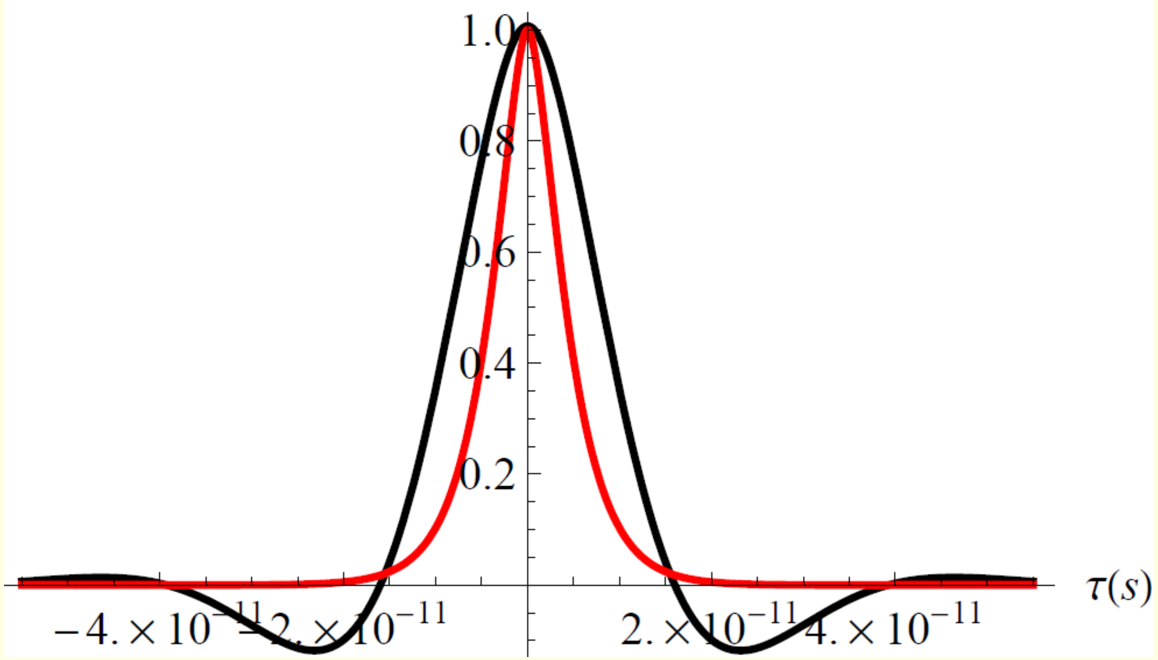
$$dS(K_n, \omega)/d\omega = 0$$

For $K_n < K_{nt}$ the transport of thermal signals is diffusive and ballistic otherwise.

Autocorrelation function of temperature fluctuations

$$C(K_n, k, \tau) = 2k_B T_0 \lambda_0 \int_{-\infty}^{\infty} S(K_n, k, \omega) e^{i\omega\tau} d\omega$$

Jeffrey's like model



As a function of Kn (Knudsen number) and delay time. Red line corresponds to Kn = 0.2 (diffusive transport) and the black one to Kn = 2.5 (wave propagation). The WP − DT transition occurs at Kn = 2.3 and FT = 0.1. The material is Silicon.

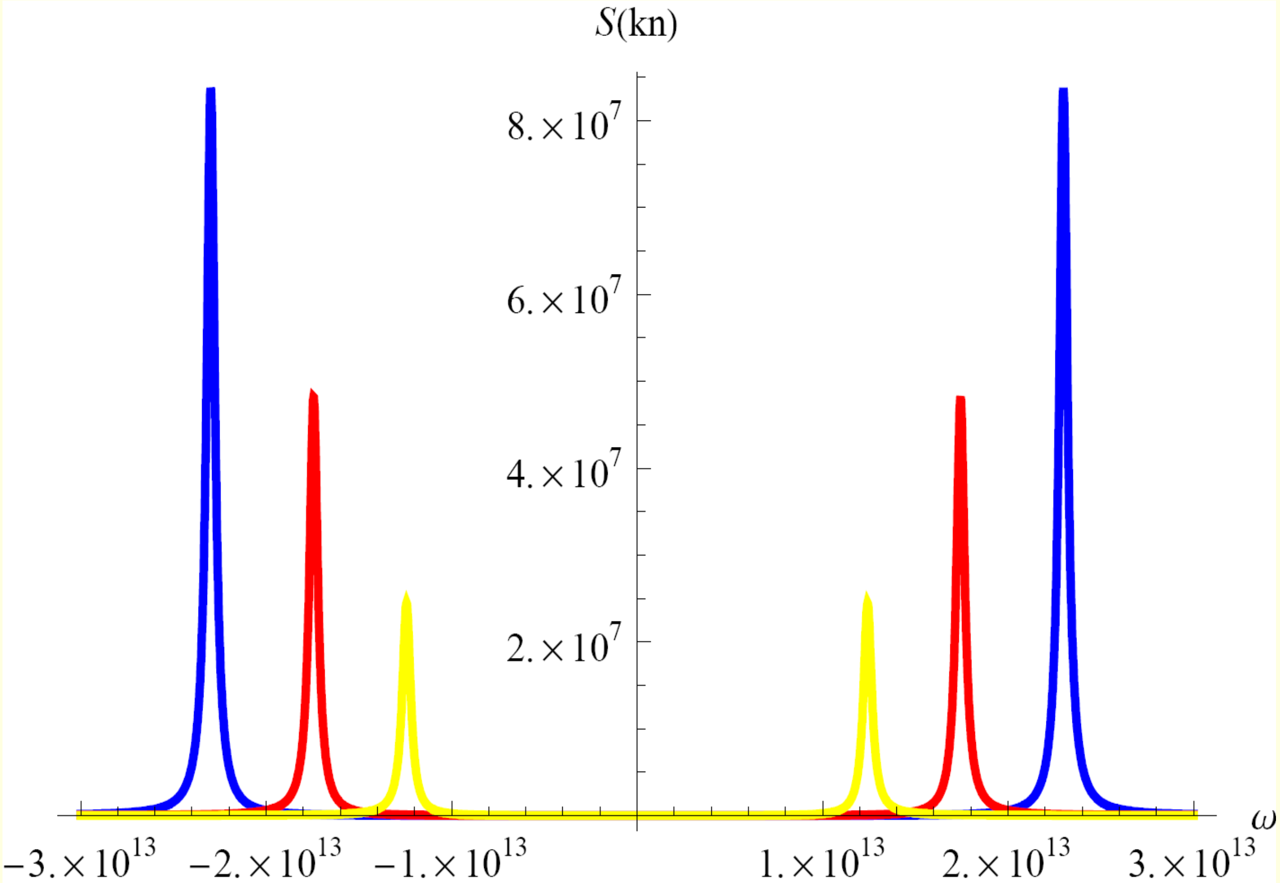
Summary

	F_T	Transition
Fourier	1	NO
Cattaneo	0	YES
Jeffrey	---	YES
Guyer-Krumhansl	---	NO

Power spectrum of heat flux equilibrium fluctuations

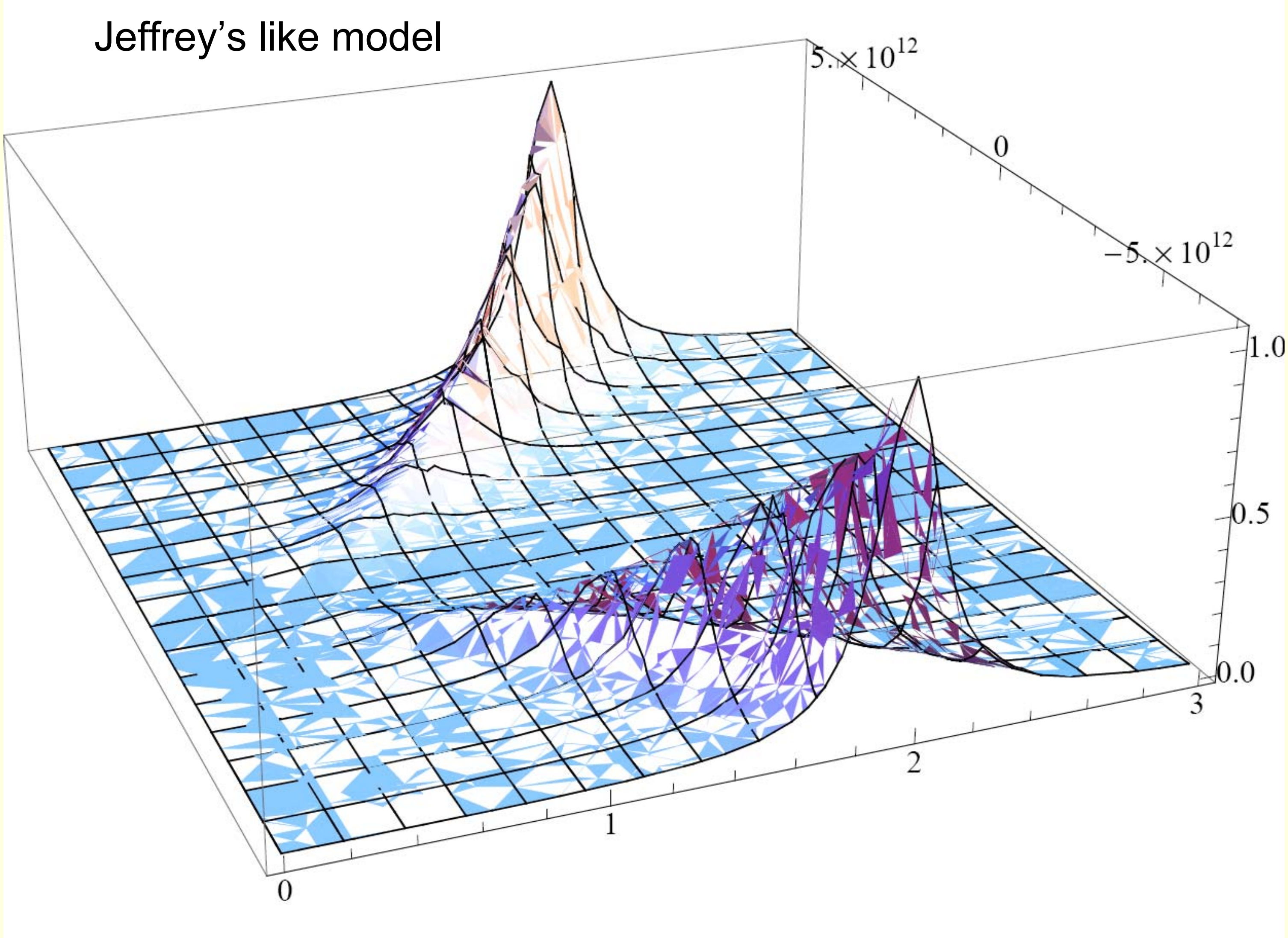
Transition can not be seen.

Jeffrey's like model

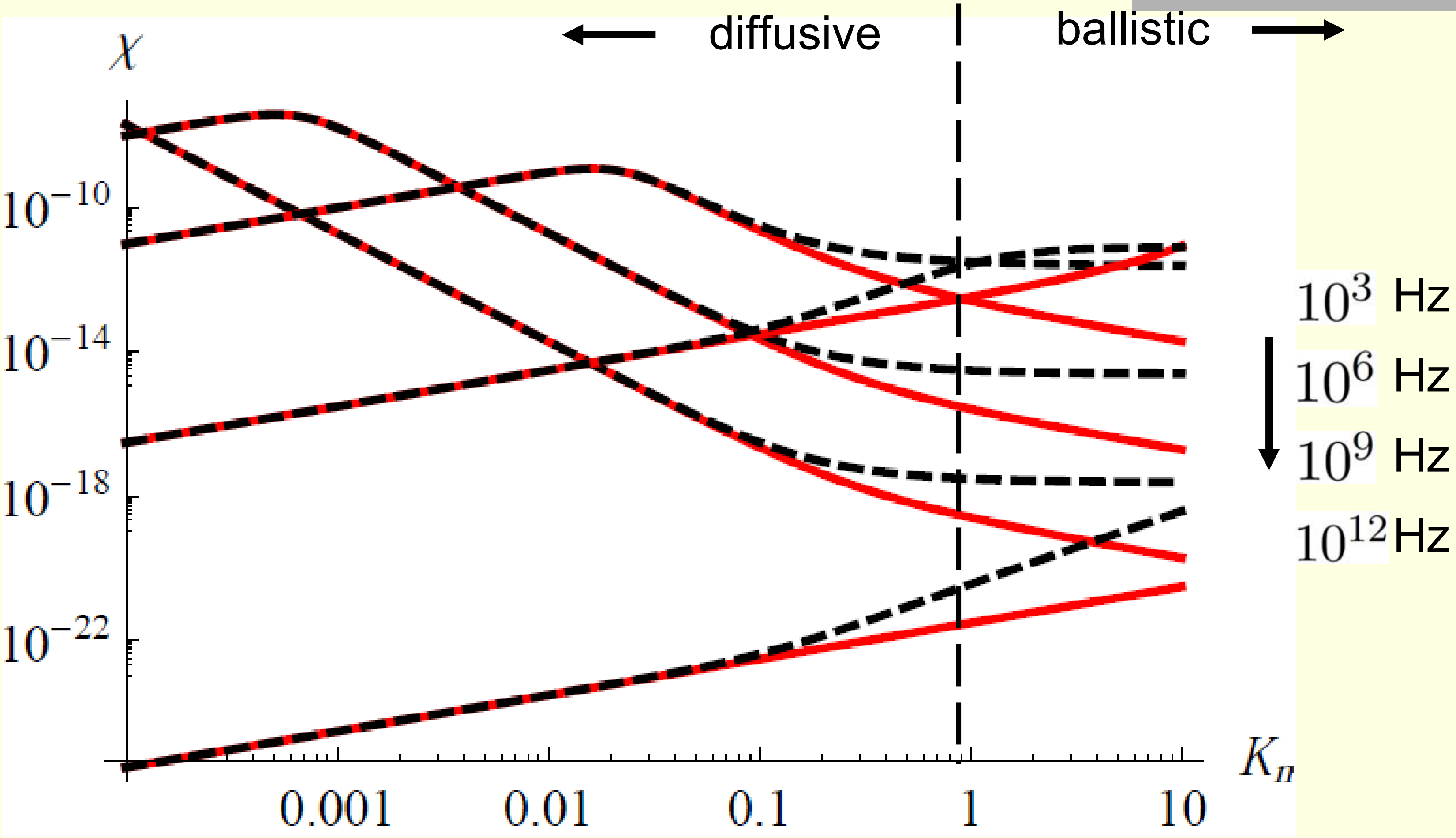


Blue kn=l/L, red kn=l/(1.2L), yellow kn=l/(1.5L)

Power spectrum of heat flux fluctuations vs. Knudsen number



Spectral thermodynamic susceptibility vs. Knudsen number



Transition can not be seen.

Jeffrey's like model F_T=0.27

Entropy production

$$s(u,q) = s_{eq}(u) + \frac{\tau}{2K(K_n)T^2} q^2$$

Compatibilidad termodinámica

$$\sigma(q) = \frac{1}{K(K_n)T^2} q^2$$

Álvarez et al., PRE 2008

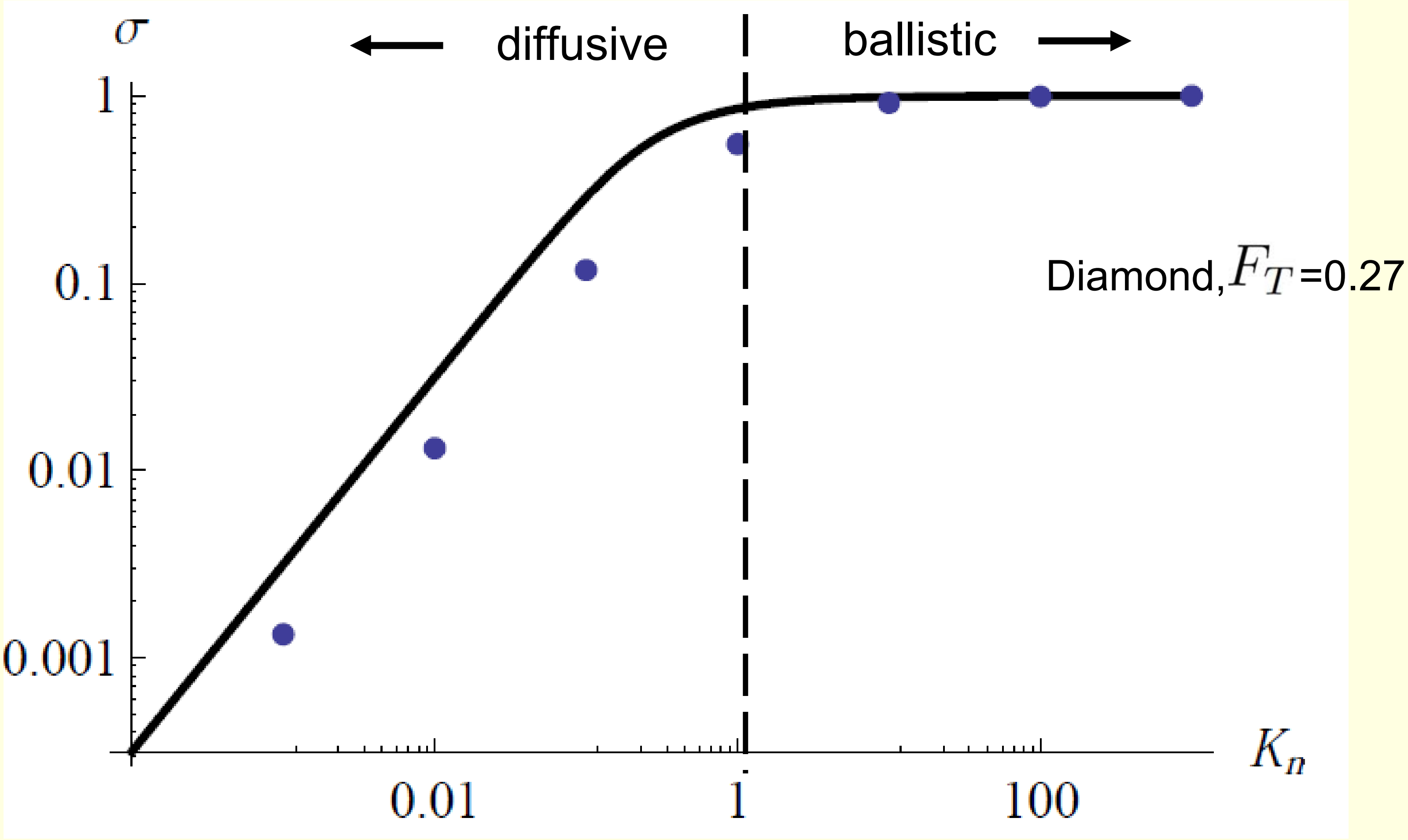
In the stationary state:

$$\sigma(q) = \frac{K(K_n)}{T_0^2 L^2} (\Delta T)^2$$

Entropy production in the volume:

$$\dot{s}(K_n) = \frac{l K_0 \left[\sqrt{1 + 4\pi^2 K_n^2} - 1\right]}{T_0^2 K_n} \left(\frac{\Delta T}{L}\right)^2$$

Entropy production in stationary state vs. Knudsen number



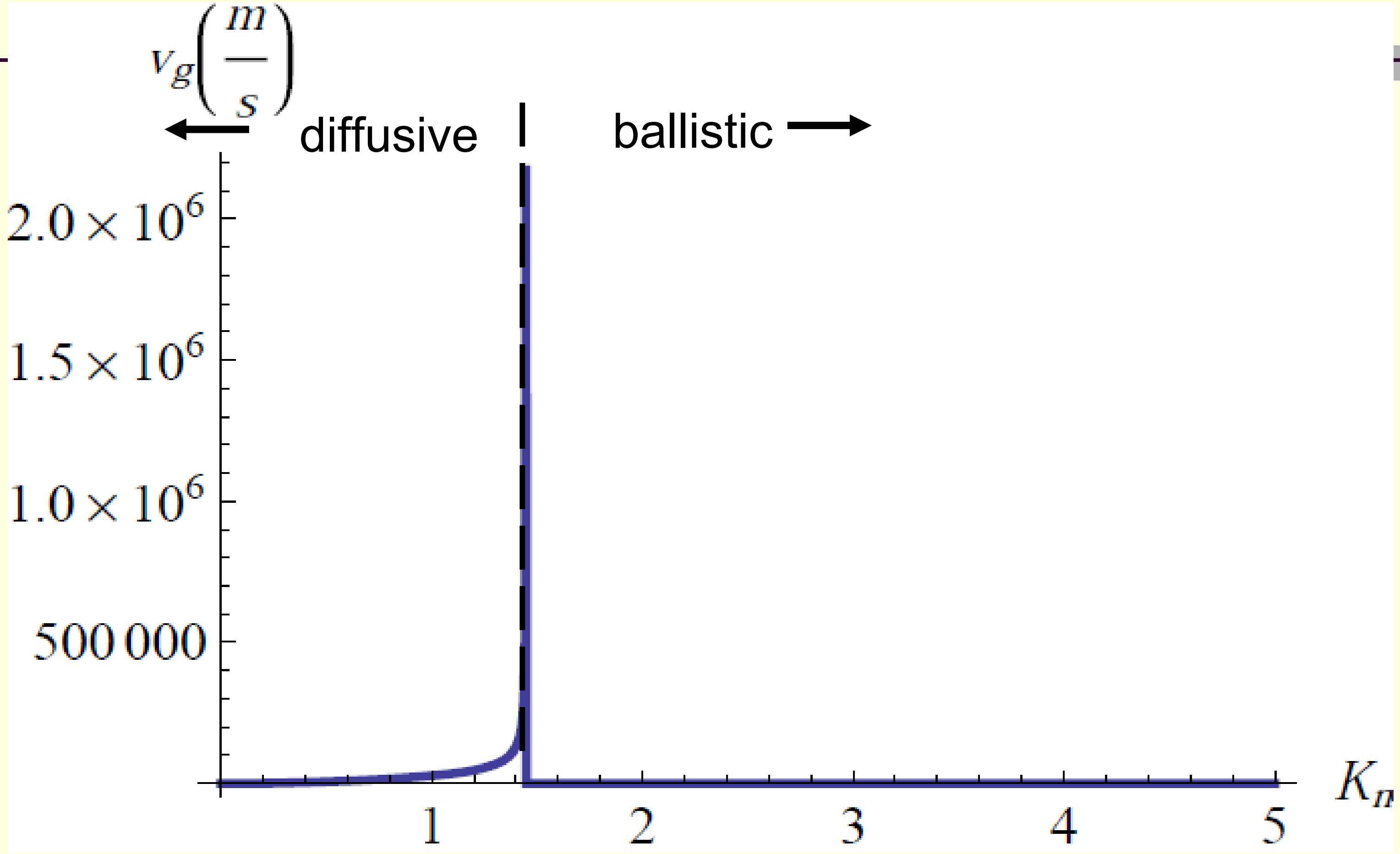
Jeffrey's like model

Equation of phonon radiative transfer results

- Bright, J. Heat Transfer 2010

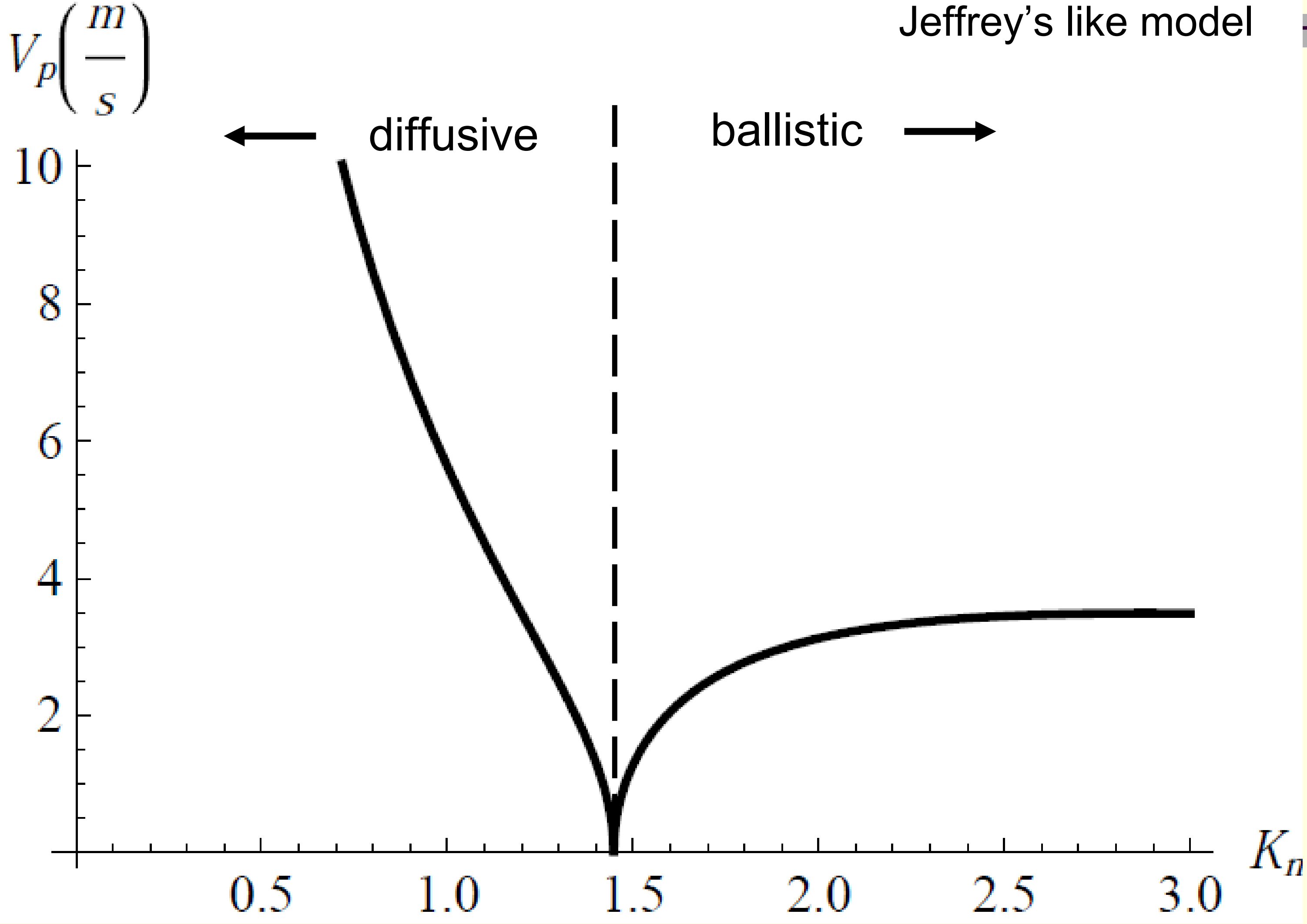
Kn	Medium (radiation)	Left wall	Right wall	Percentage of walls (%)	Total	Medium (diffusion)	Relative difference (%)
1000	1.612×10^{4}	2.320×10^{7}	2.036×10^{6}	99.98	2.524×10^{7}	6.754×10^{3}	58
100	1.177×10^{5}	2.297×10^{7}	1.934×10^{6}	99.50	2.503×10^{7}	6.496×10^{4}	45
10	6.285×10^{5}	2.109×10^{7}	1.415×10^{6}	97.26	2.314×10^{7}	4.695×10^{5}	25
1	1.491×10^{6}	1.211×10^{7}	3.511×10^{5}	89.33	1.395×10^{7}	1.230×10^{6}	17
0.1	8.723×10^{5}	2.080×10^{6}	1.188×10^{4}	70.58	2.964×10^{6}	7.447×10^{5}	15
0.01	2.037×10^{5}	1.272×10^{5}	1.416×10^{2}	38.46	3.311×10^{5}	1.933×10^{5}	5.1
0.001	3.015×10^{4}	3.389×10^{3}	1.443×10^{0}	10.11	3.354×10^{4}	3.013×10^{4}	0.07
0.0001	3.323×10^{3}	4.359×10^{1}	1.445×10^{-2}	1.30	3.367×10^{3}	3.315×10^{3}	0.26
0.00001	3.365×10^{2}	4.501×10^{-1}	1.444×10^{-4}	0.13	3.369×10^{2}	3.351×10^{2}	0.40

Group velocity of propagating Fourier modes

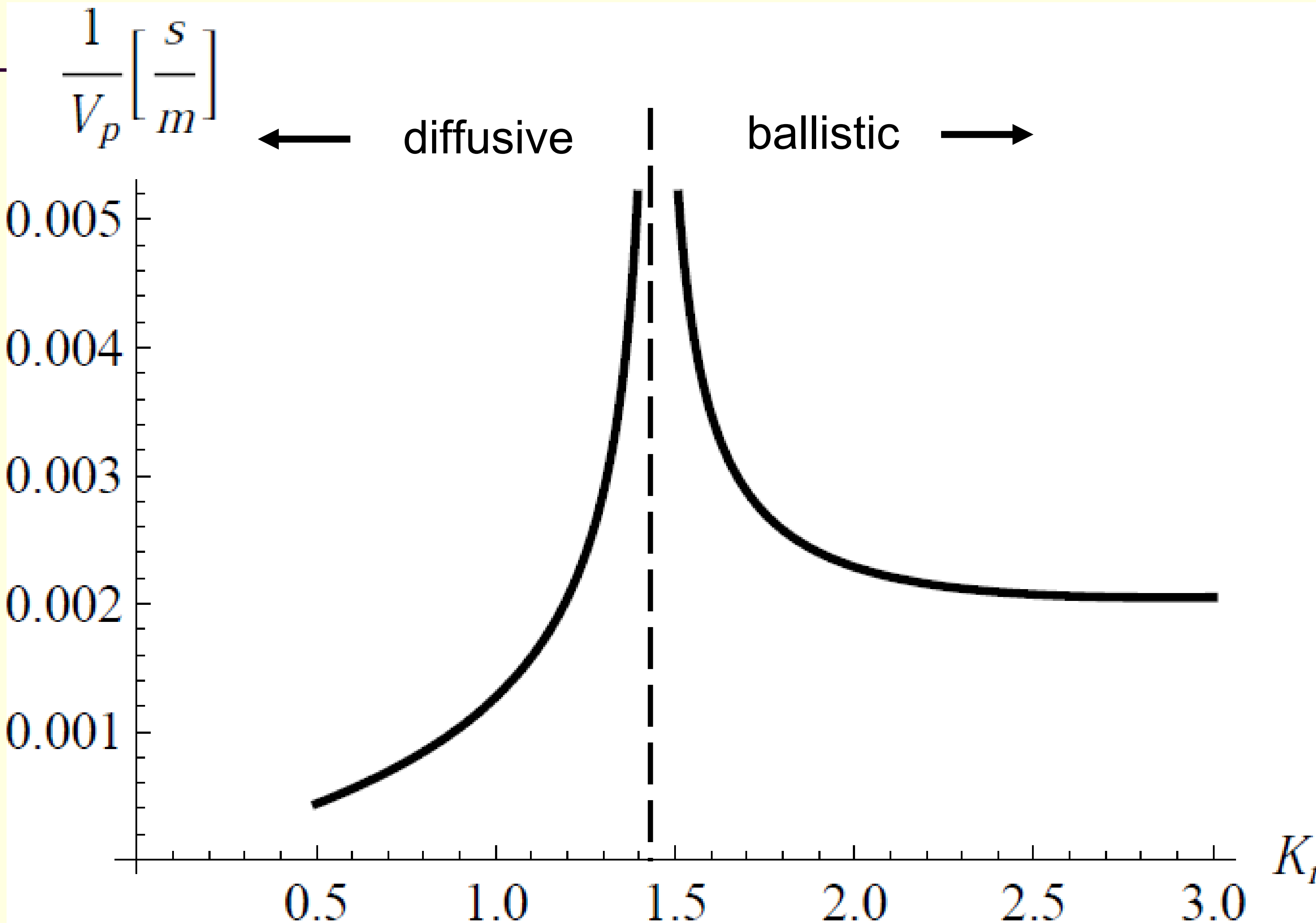


$$\omega = \frac{1}{2\rho C_v \tau}\left(-i\left(\rho C_v + \tau F_T K k^2\right) + \left(4\rho C_v \tau K k^2 - \sqrt{\rho C_v + \tau F_T K k^2}\right)^2\right)$$

Phase velocity of propagating Fourier modes



Inverse of phase velocity of propagating modes



Jeffrey's like model

Gámbar and Márkus, PLA 2007

Conclusions

When the size of the film is reduced, the Kn=1 crossover shows

1) A transition in the power spectrum of temperature fluctuations

2) A transition in the autocorrelation function of temperature fluctuations

3) A quick increasing of the entropy production when Kn $\longrightarrow$ 1

4) A regime of high entropy production when Kn > 1

5) The features of a dynamical phase transition

Thank you!

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