Basics of non-Equilibrium Electrodynamics on the nano-Scale

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Heat Transfer and Conduction on the Nanoscale

WE Heraeus workshop 613

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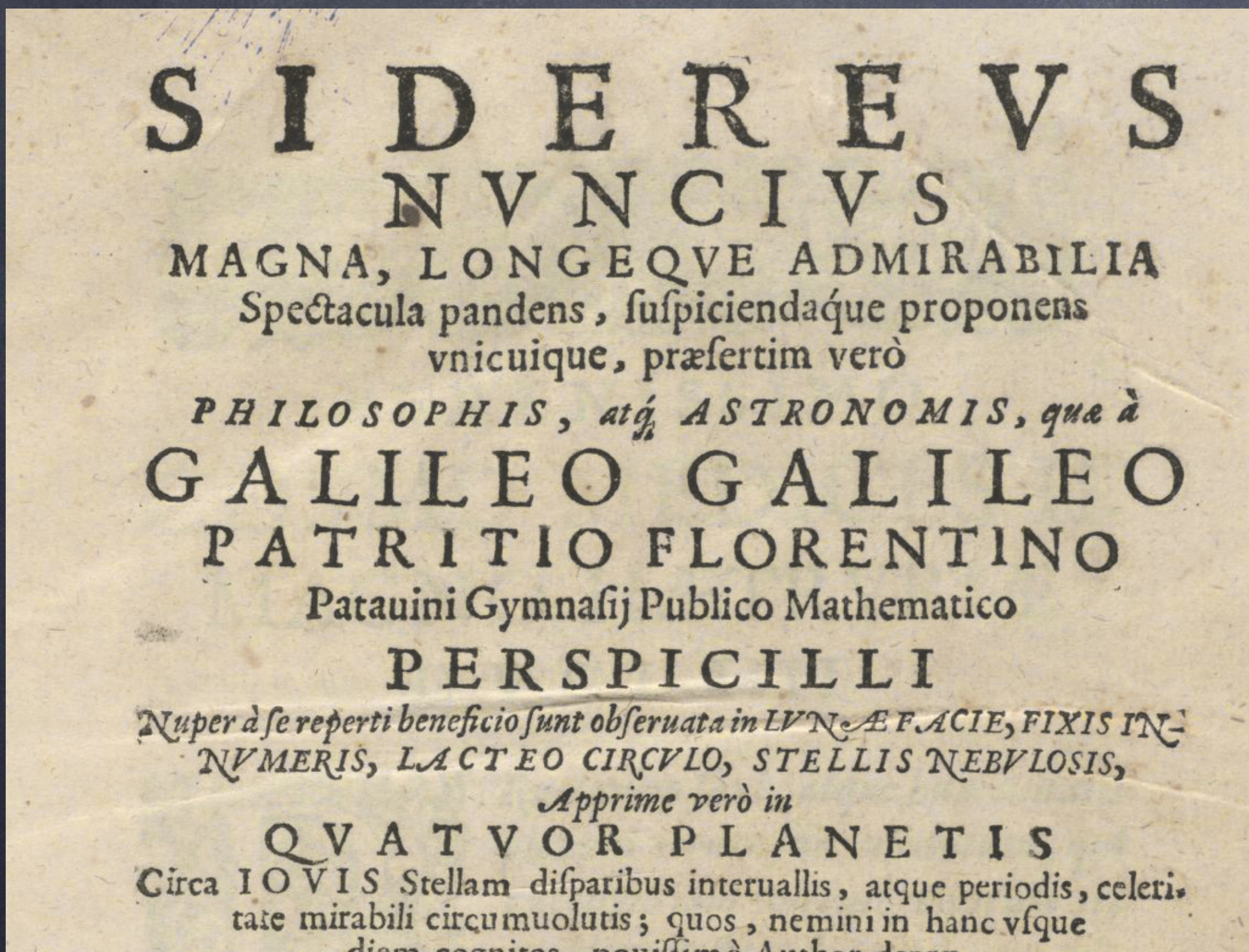
Non-equilibrium ... Light



SIDEREVS
NVNCIVS
MAGNA, LONGEQVE ADMIRABILIA
Spectacula pandens, suspiciendaque proponens
vnicuique, præsertim verò
PHILOSOPHIS, atq; ASTRONOMIS, quæ à
GALILEO GALILEO
PATRITIO FLORENTINO
Patauini Gymnasij Publico Mathematico
PERSPICILLI
Nuper à se reperti beneficio sunt obseruata in LVNÆ FACIE, FIXIS IN-
NVMERIS, LACTEO CIRCVLO, STELLIS NEBVLOSIS,
Apprime verò in
QVATVOR PLANETIS
Circa IOVIS Stellam disparibus interuallis, atque periodis, celeri-
tate mirabili circumuolutis; quos, nemini in hanc vsque
diem cognitos, nouissimè Author depræ-

Messenger of Stars (Venice 1610)

Hubble ultra deep field (NASA 2004)

Fundamental Interactions

- focus on condensed matter
- electric forces
- spin exchange "potential"
- electromagnetic ("collective") forces
- chemical bonds

Electrodynamics

$$-\partial_t \varepsilon_0 \mathbf{E} + \nabla \times \mathbf{H} = \mathbf{j}\,, \qquad \nabla \cdot \varepsilon_0 \mathbf{E} = \rho$$

$$\partial_t \mu_0 \mathbf{H} + \nabla \times \mathbf{E} = \mathbf{0}\,, \qquad \nabla \cdot \mu_0 \mathbf{H} = 0$$

- matter = sources
- matter = medium response

$$\mathbf{j} = \partial_t \mathbf{P} + \nabla \times \mathbf{M}$$

$$\rho = -\nabla \cdot \mathbf{P}$$

$$\mathbf{j} = \mathbf{j}_{\mathrm{ext}} - \mathrm{i}\omega(\varepsilon - \varepsilon_0)\mathbf{E} + \mathrm{mag}$$

$$\rho = \rho_{\mathrm{ext}} - \nabla \cdot (\varepsilon - \varepsilon_0)\mathbf{E}$$

- mesoscopic sources
- average response + fluctuations ("Rytov split")

Fluctuation Electrodynamics

[Rytov & al >1950s]

$$
\begin{aligned}
\mathrm{i}\omega\varepsilon\mathbf{E} + \nabla \times \mathbf{H} &= \mathbf{j}_{\mathrm{th}} + \mathbf{j}_{\mathrm{ext}}\,, \\
-\mathrm{i}\omega\mu\mathbf{H} + \nabla \times \mathbf{E} &= \mathbf{0}\,,
\end{aligned}
$$

random source
(Langevin force)

source: thermalised matter

$$\langle j(x) j(x') \rangle = \kappa T \,\mathrm{Re}\,\sigma\, \delta(x - x')$$

Johnson & Nyquist

$$\langle j^*_{\mathrm{th}k}(\mathbf{x}, \omega) j_{\mathrm{th}l}(\mathbf{x}', \omega') \rangle =$$

$$\frac{2\hbar\omega^2}{\mathrm{e}^{\hbar\omega/\kappa T} - 1} \mathrm{Im}\,\varepsilon_{kl}(\omega, \mathbf{x}, \mathbf{x}') 2\pi\delta(\omega - \omega')$$ + magn.

fluctuation–dissipation relation
[Callen & Welton, *Phys Rev* 1951]

whose Temperature?

- em field does *not* equilibrate
- matter thermalises (local eq = LTE)
- conservation laws and entropy production

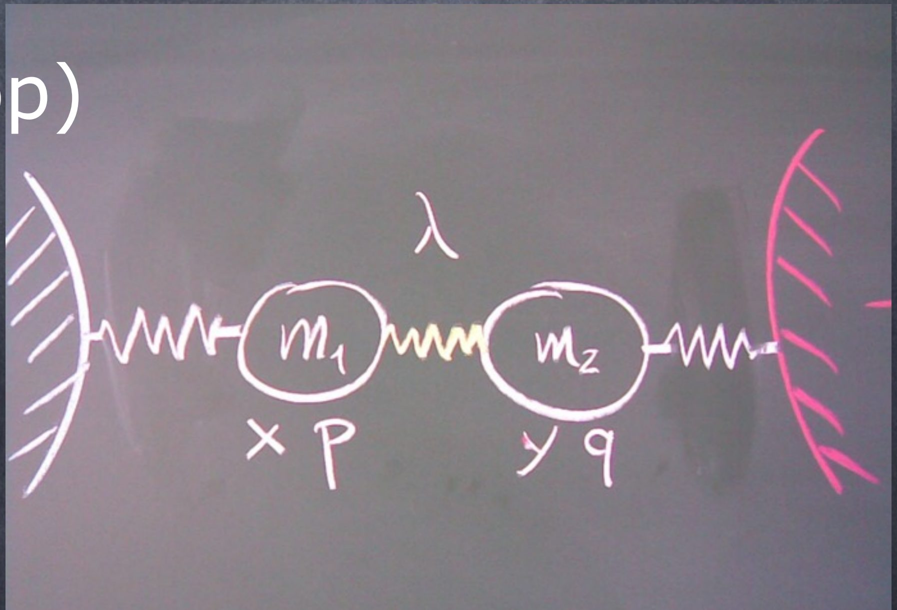
$$
\begin{aligned}
\frac{\partial}{\partial t}(\text{em energy } u) &= -\,\text{absorption} - \text{radiation} \\
c_V \frac{\partial}{\partial t}(\text{matter } T) &= +\,\text{absorbed heat}
\end{aligned}
$$

non-Equilibrium … non-LTE?

- **fast physics**
  excitation with short laser pulse
  – (few fs) plasmon dephases
  – hot electrons $T_{\rm el} > T_{\rm ph}$
  – (10 ps) equilibrate with lattice phonons

- concept: weak (thermal) contact

- **slow physics** (= this workshop)
  local thermal equilibrium (LTE)
  (steady) heat flux
  heat diffusion



toy model [... Barton *JPCM* 2015]

nano-Scale

$$a_0 \ll 1\,\mathrm{nm} \sim \lambda_{\mathrm{ph}} \ll \lambda_T(10\,\mu\mathrm{m})$$

- "local temperature", coarse grain $\mathrm{d}V = \text{many atoms}$
- mesoscopic electrodynamics ("Rytov split")

$$\mathbf{j} = \sigma(\mathbf{x})\mathbf{E} + \mathbf{j}_{\mathrm{th}}$$

"collective"

averaged field ("local"?)

thermal fluctuations

local Ohm: dx ≫ mfp (few nm)

non-local: "anomalous skin effect" $\sigma(\mathbf{q}, \omega)$

[Lindhard] [Singwi & Sjölander 1968]

nano-Scale

$$a_0 \ll 1\,\mathrm{nm} \sim \lambda_{\mathrm{ph}} \ll \lambda_T (10\,\mu\mathrm{m})$$

- spirit of 2nd FDT: local sources $\quad \mathrm{d}V = \text{many atoms}$

$$\langle j(x) j(x') \rangle = \kappa T \; \mathrm{Re}\, \sigma \, \delta(x - x')$$

local approx

$$\langle j^*_{\mathrm{th}k}(\mathbf{x}, \omega) j_{\mathrm{th}l}(\mathbf{x}', \omega') \rangle =$$

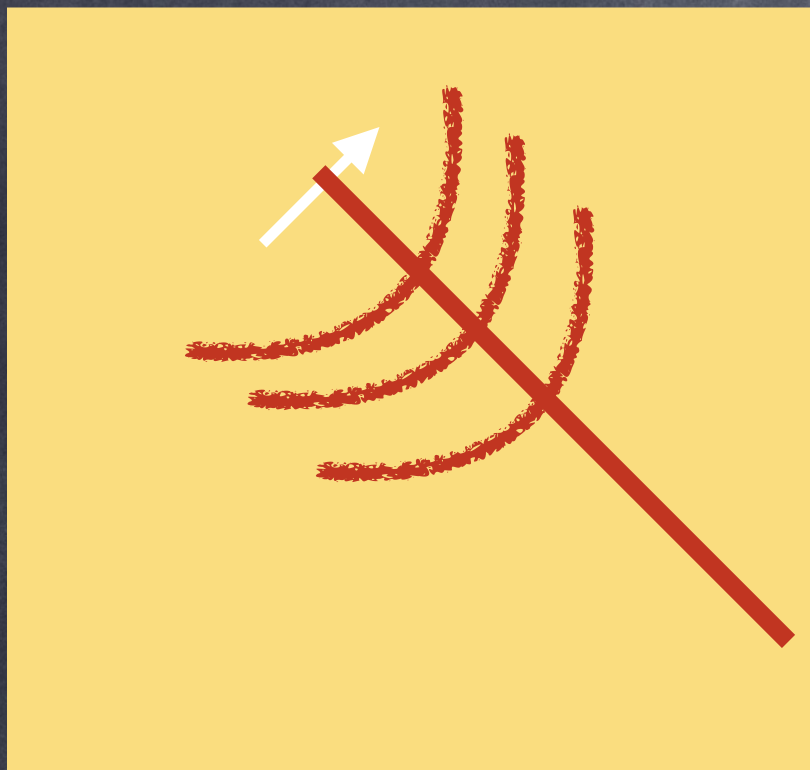
fluctuation–dissipation relation
[Callen & Welton, Phys Rev 1951]

$$\frac{2\hbar\omega^2}{\mathrm{e}^{\hbar\omega/\kappa T} - 1} \mathrm{Im}\, \varepsilon_{kl}(\omega, \mathbf{x}, \mathbf{x}') 2\pi\delta(\omega - \omega')$$

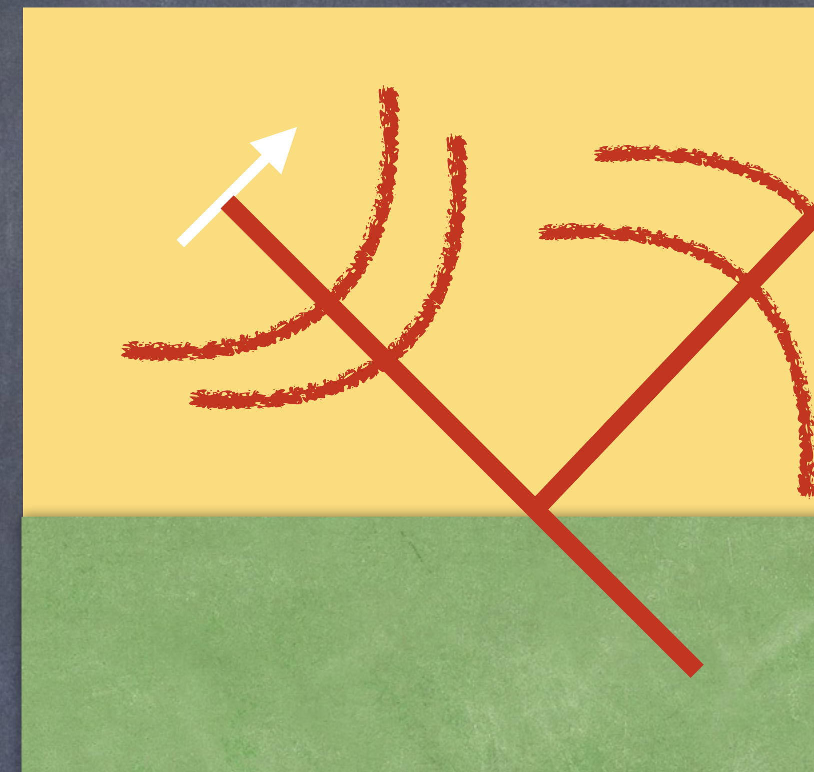
- Rytov-Maxwell → thermal radiation (Poynting v. etc)

- how to work with this (numerical schemes)

painless Green



$$\mathbf{E}(\mathbf{x}) = \mathbf{G}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{d}(\mathbf{x}')$$



$$\mathbf{G}(\mathbf{R}, z, \mathbf{R}', z') = \mathbf{G}_0 + \mathbf{G}_{\mathrm{ref}}$$

- solve radiation by point source (Green tensor)
- homogeneous medium

$$\mathbf{G}(\mathbf{r}, \mathbf{r}'; \omega) = \left(\frac{\omega^2}{c^2} + \nabla \otimes \nabla \right) \frac{e^{i\omega|\mathbf{r}-\mathbf{r}'|/c}}{4\pi\varepsilon|\mathbf{r} - \mathbf{r}'|}$$

Mode Densities "LDOS"

$$\langle \mathbf{E}(x)\mathbf{E}(x')\rangle_\omega = \frac{\hbar\omega^3}{\cdots\varepsilon_0(\mathrm{e}^{\hbar\omega/\kappa T}-1)}\sum_\mu \int \mathrm{d}\Omega\, \mathbf{f}^*_\mu(\mathbf{r})\mathbf{f}_\mu(\mathbf{r}')$$

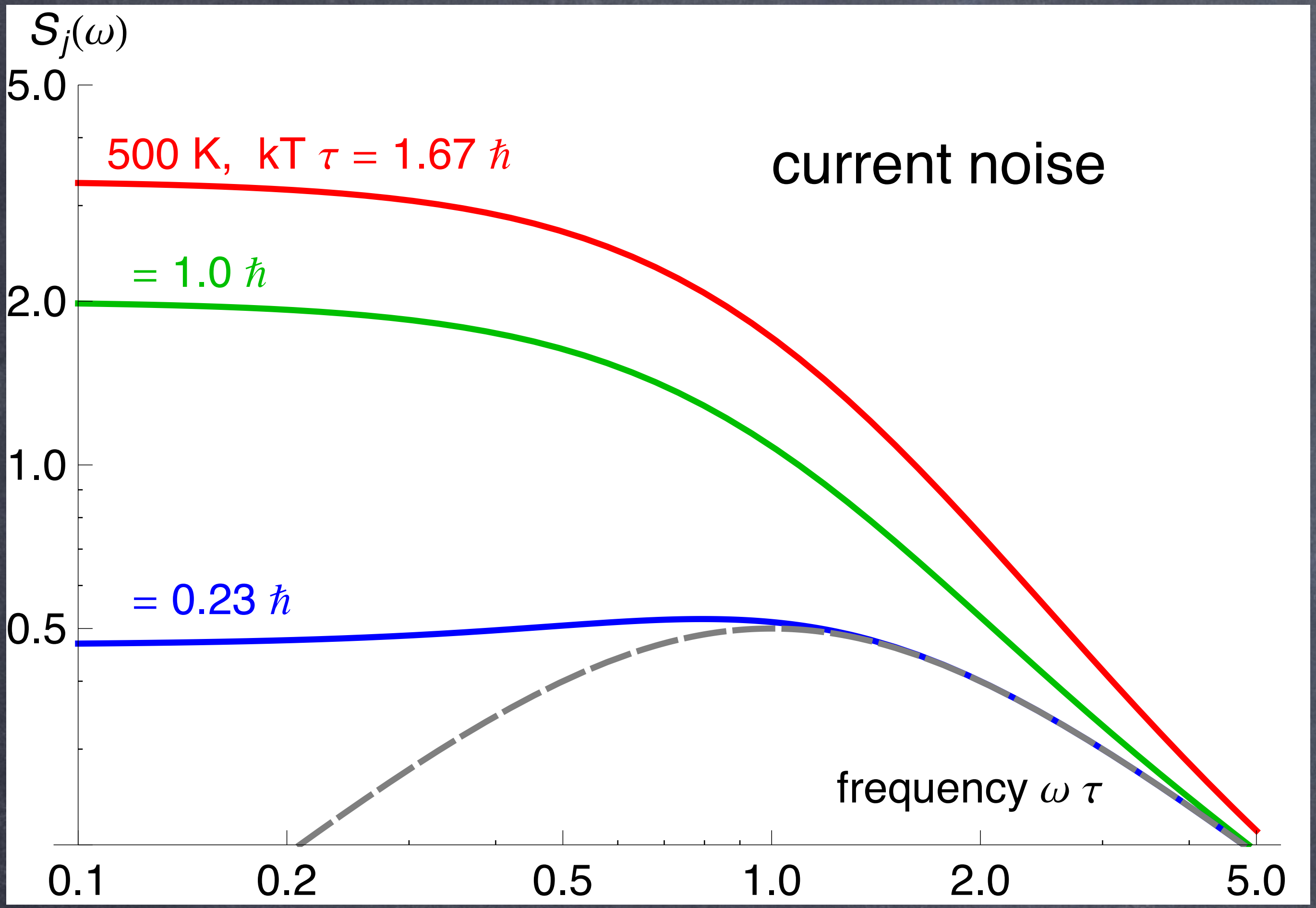
$$= \frac{2\hbar}{\mathrm{e}^{\hbar\omega/\kappa T}-1}\,\mathrm{Im}\,\mathbf{G}(\mathbf{r},\mathbf{r}';\omega)$$

occupation / mode

mode density

- blackbody radiation [Planck 1900]
- FD relation "1st kind"
  [Callen & Welton 1951] [Eckhardt *Opt Commun* 1984]
- local mode density LDOS = Im G, **r**-dependent
- global vs local temperature(s)

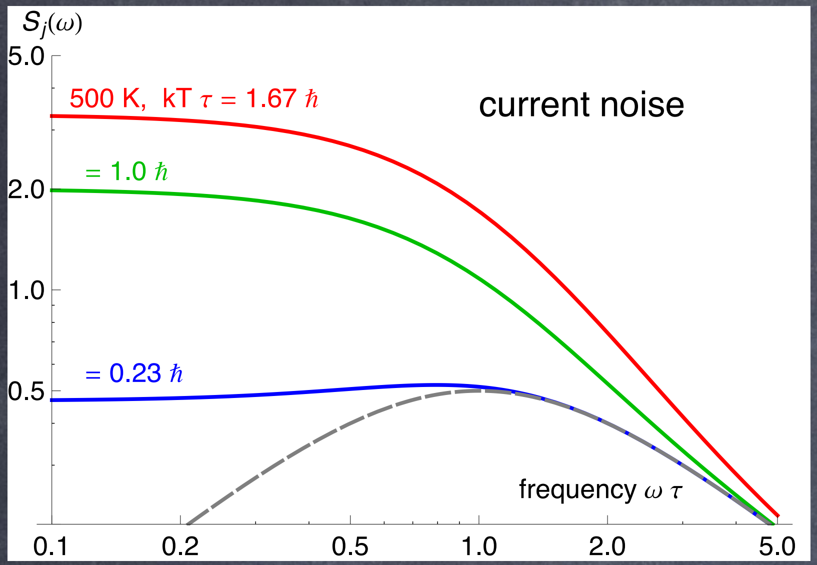
"thermal Photons" in Metal



spectrum in bulk
(Drude)

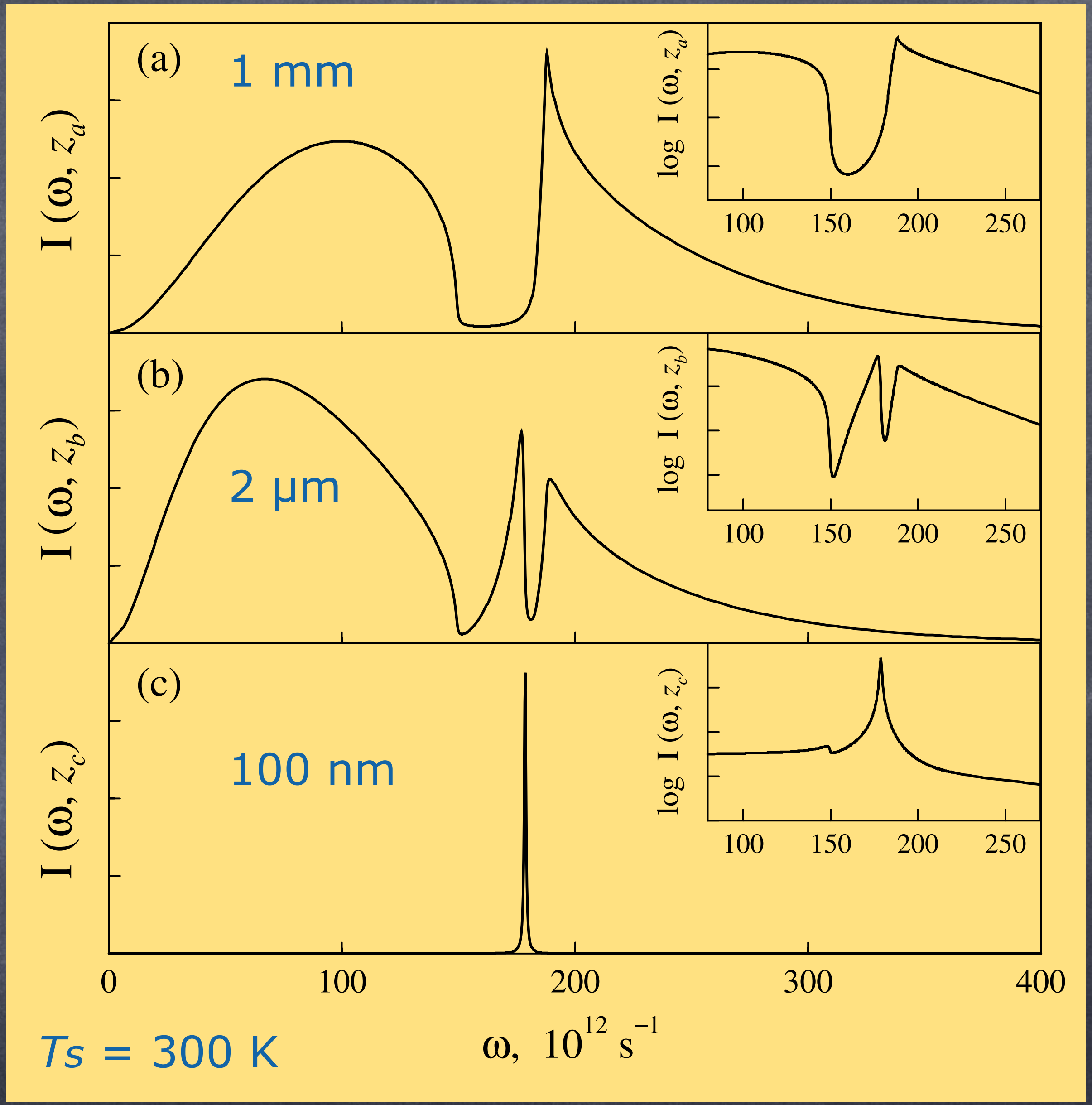
$$\sim \frac{\hbar\omega \; \mathrm{Re}\, \sigma(\omega)}{\mathrm{e}^{\hbar\omega/\kappa T} - 1}$$

"thermal Photons" near SiC



spectrum in bulk

$$\sim \frac{\hbar\omega \, \mathrm{Re}\, \sigma(\omega)}{e^{\hbar\omega/\kappa T} - 1}$$



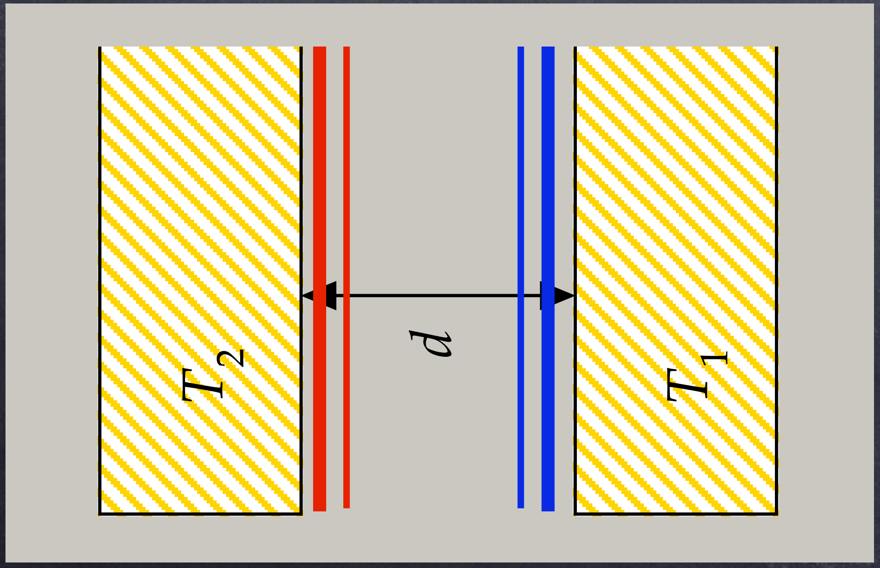
Shchegrov & al [Phys Rev Lett 2000]

near field spectrum
• surface plasmon

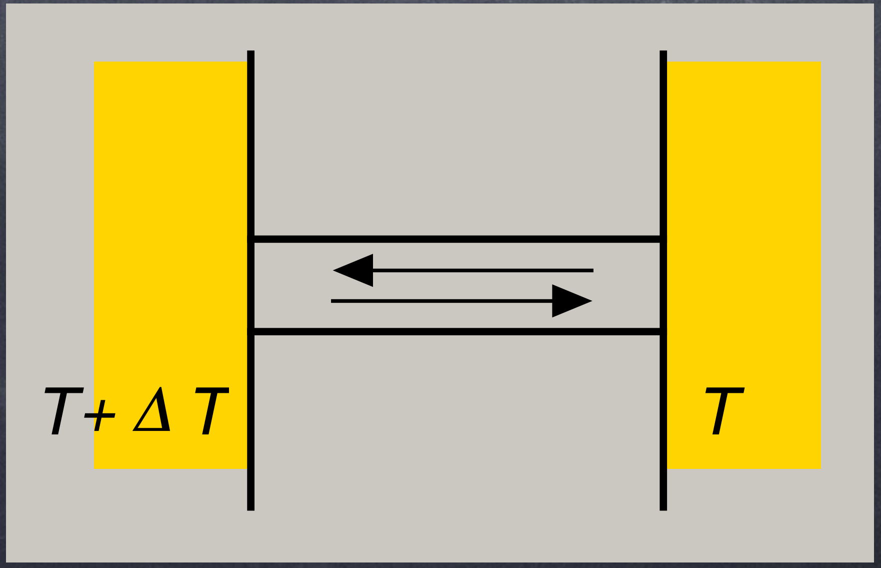
$$\sim \frac{\hbar}{e^{\hbar\omega/\kappa T} - 1} \, \mathrm{Im}\, \frac{\varepsilon(\omega) - \varepsilon_0}{\varepsilon(\omega) + \varepsilon_0}$$

Photons v Phonons

- T = 300K: wavelengths 2-10µm ≫ ~ 1nm
- elastic field theory, heat capacity, local temperature, defects, kinetic theory (Boltzmann)
- ballistic v diffusive: conduction
- "heat transfer across vacuum" = "ballistic wire"

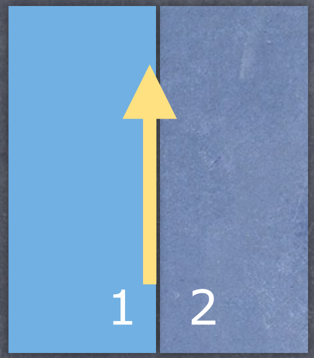


photon tunnelling



phonon shooting

Boundaries



- connection rules:
  Maxwell fields, surface charges/currents

$$\mathbf{n} \times \mathbf{H}_1 - \mathbf{n} \times \mathbf{H}_2 = \mathbf{J}_{\|}$$

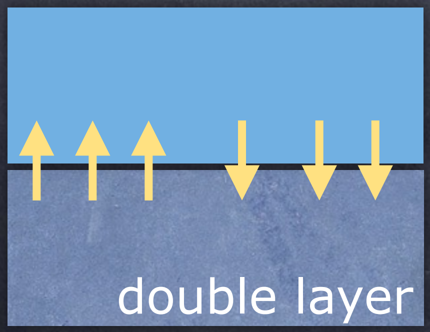
fluctuates, too

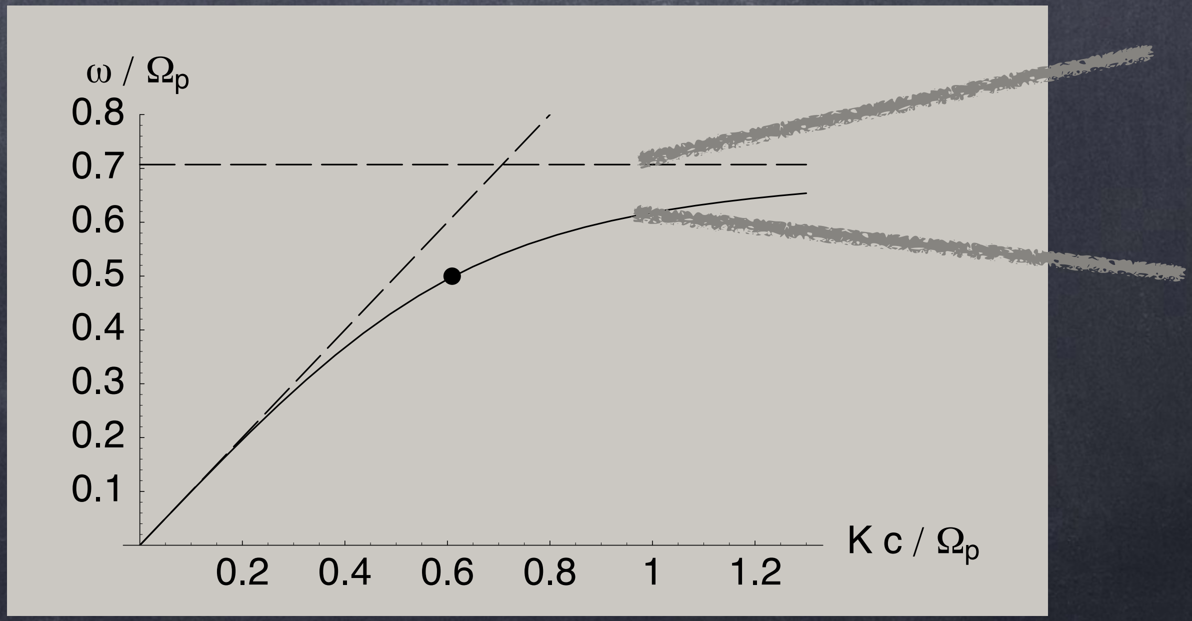
- matter currents (add'l boundary cond's "ABC")

- genuine surface response
  example: plasmon dispersion

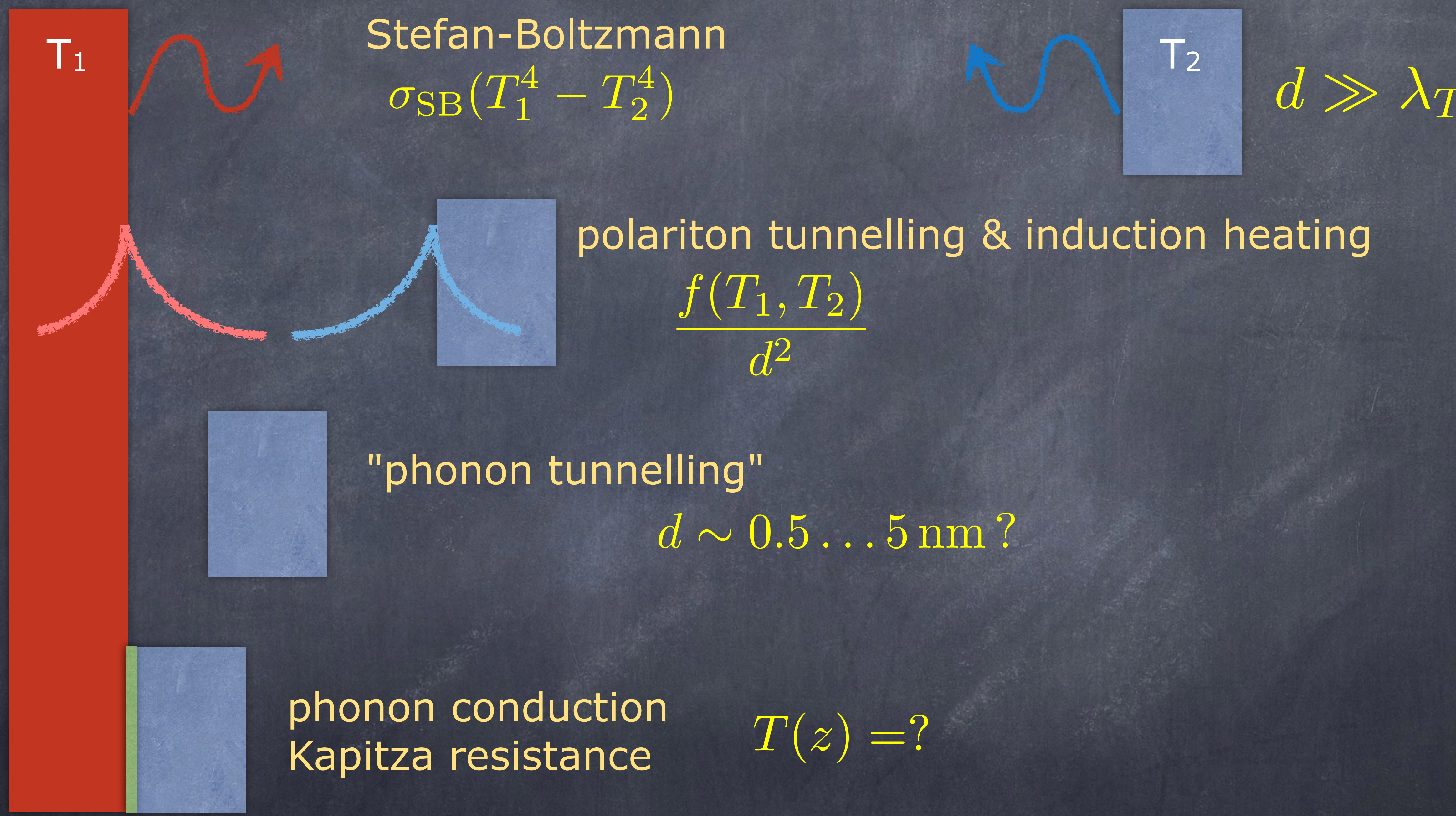
[Flores & al SSC 1972]
[Feibelman *PRB* 1989]
[Horovitz & H *EPL* 2012]

$$\mathbf{n} \cdot \mathbf{P} = \varepsilon_0 d_{\perp}(\omega)\, \mathbf{n} \cdot \mathbf{E}_2$$





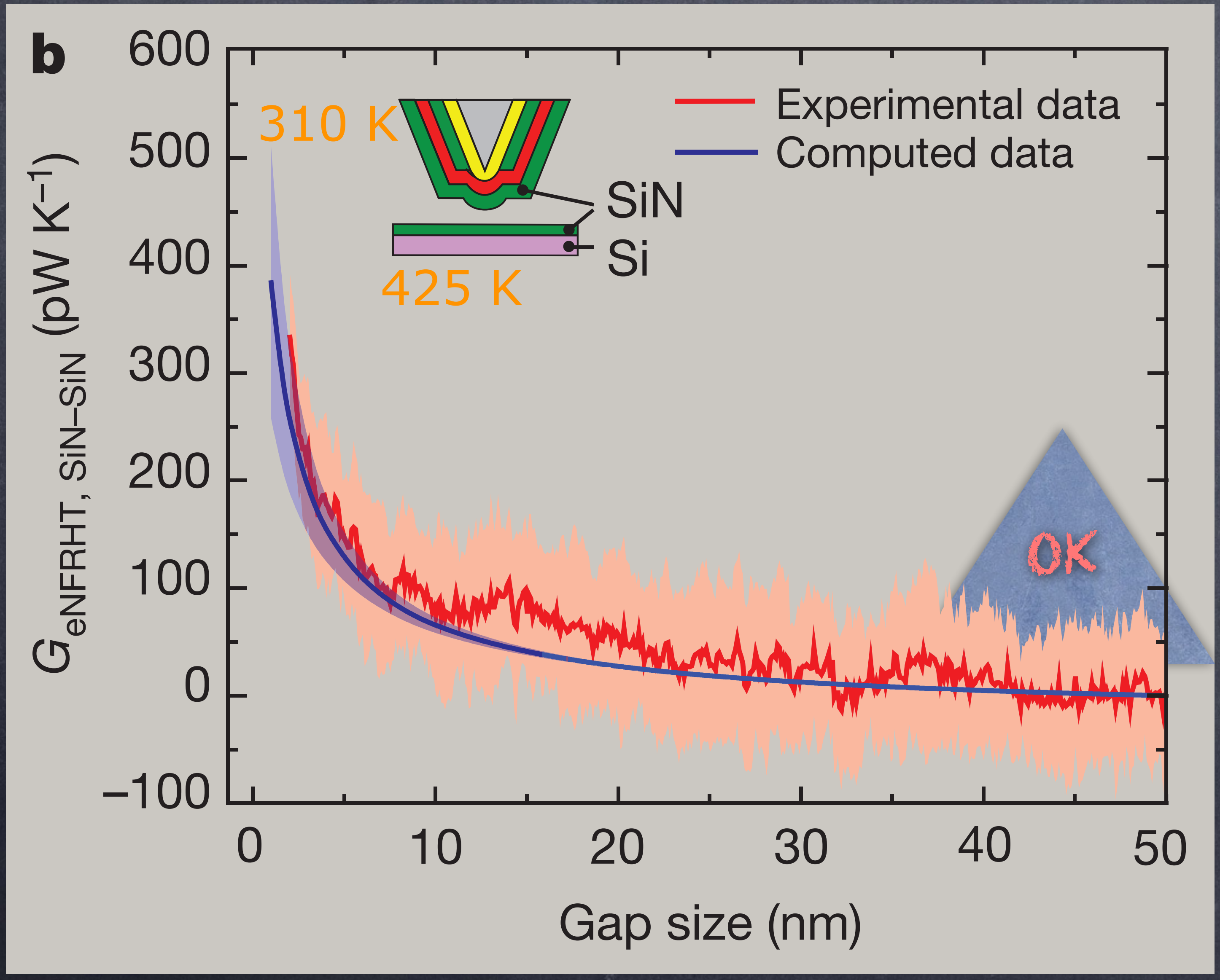
Regimes of Heat Transfer

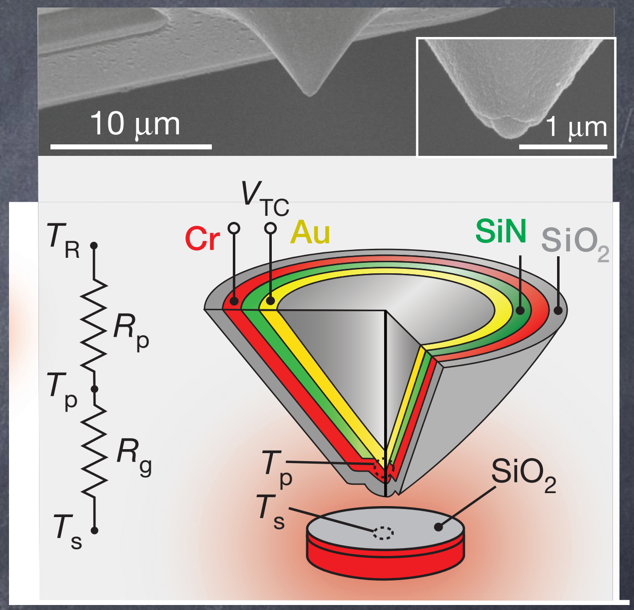


expts:
A. Kittel, T. Kralik, Pramod S. Reddy, Y. de Wilde ...
theory:
A. Rodriguez, K. Sasihithlu, S. Volz ...

Challenges

- heat transfer across 1–10nm gap ("xnf")
- expt P Reddy group & comp MT Homer Reid





tip ~ 400 nm diam

Kim & al [*Nature* 2015]

Challenges

- heat transfer across 1–10nm gap ("xnf")
- expt P Reddy group & comp MT Homer Reid

OK

- expt A Kittel group & comp AW Rodriguez

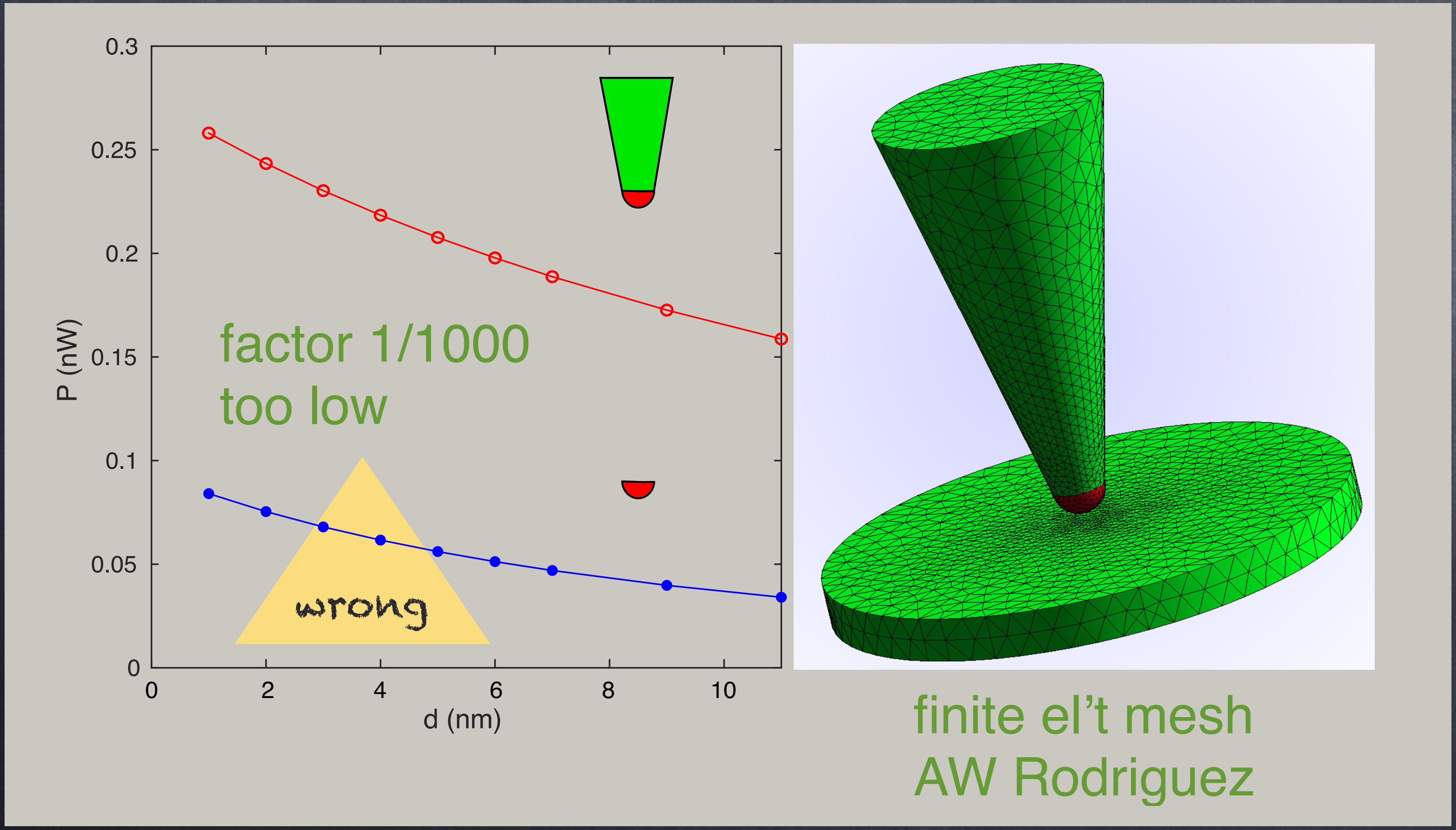
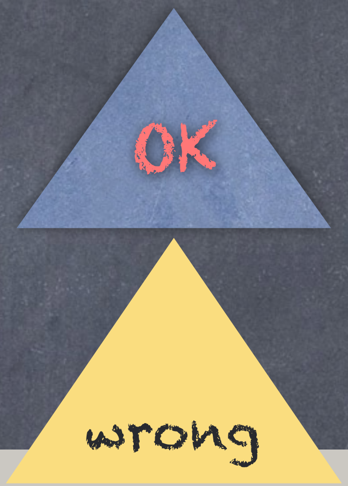


Figure 3: **Theoretical results of the transfered heat**

Kloppstech & al [arXiv:1510.06311]

Challenges

- heat transfer across 1–10nm gap ("xnf")
- expt P Reddy group & comp MT Homer Reid
- expt A Kittel group & comp AW Rodriguez



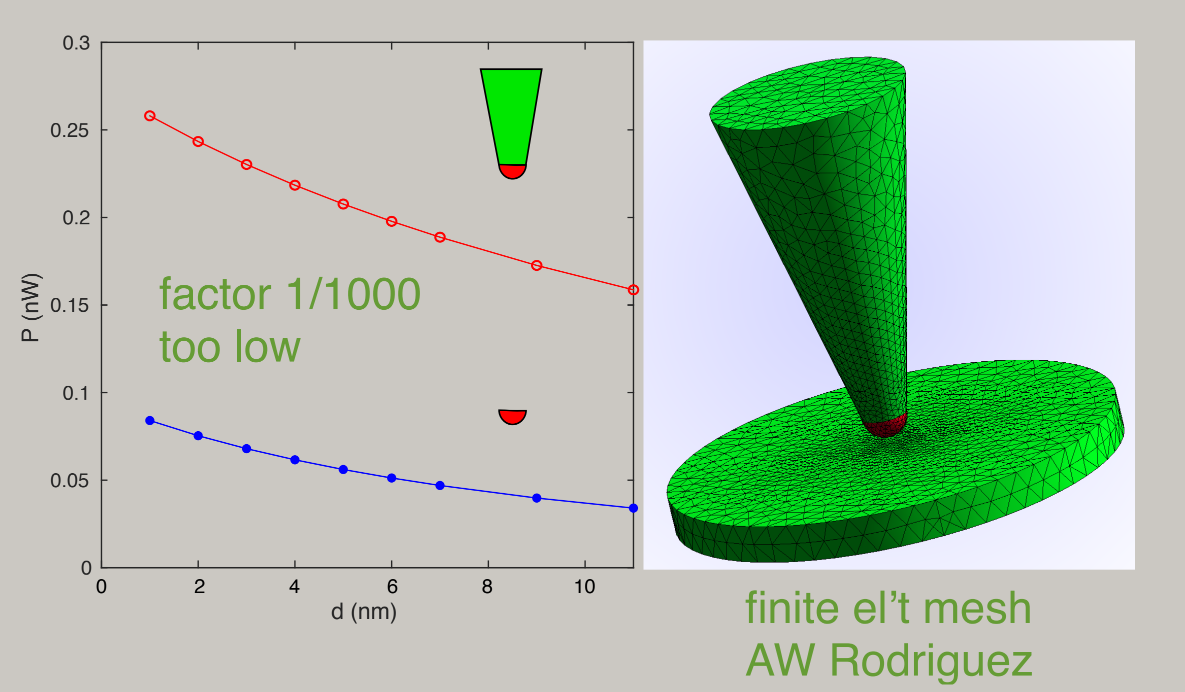
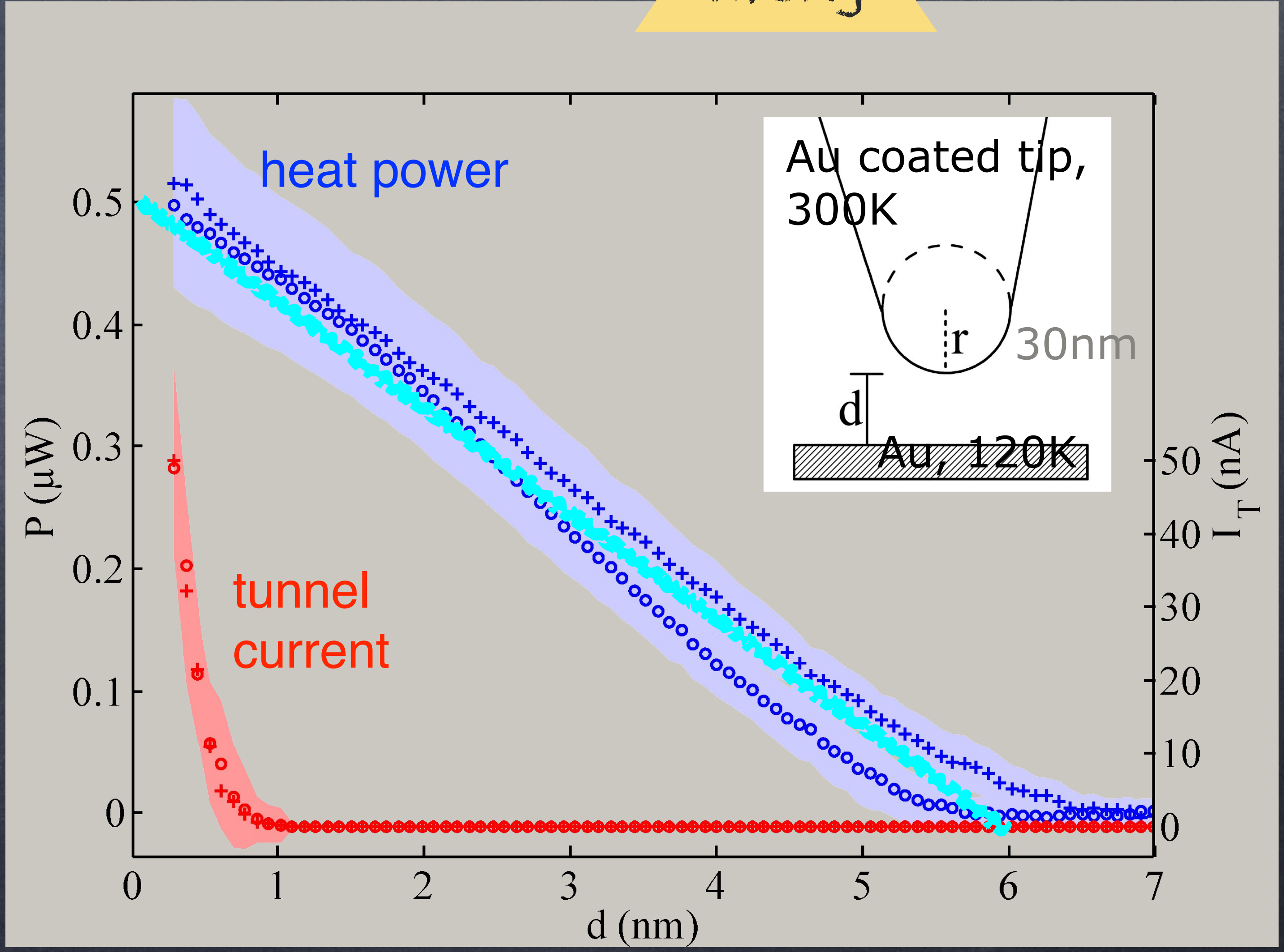


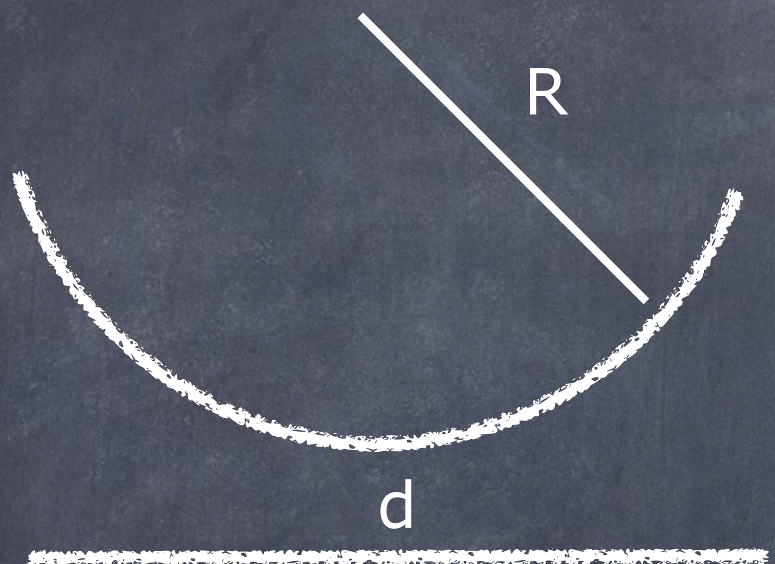
Figure 3: **Theoretical results of the transfered heat flux.** Sketch of the considered geometry (righthand side) and numerical results using exact numerical calculations for the spherical tip and the cone-like protruding part. We have dyed



Kloppstech & al [arXiv:1510.06311]

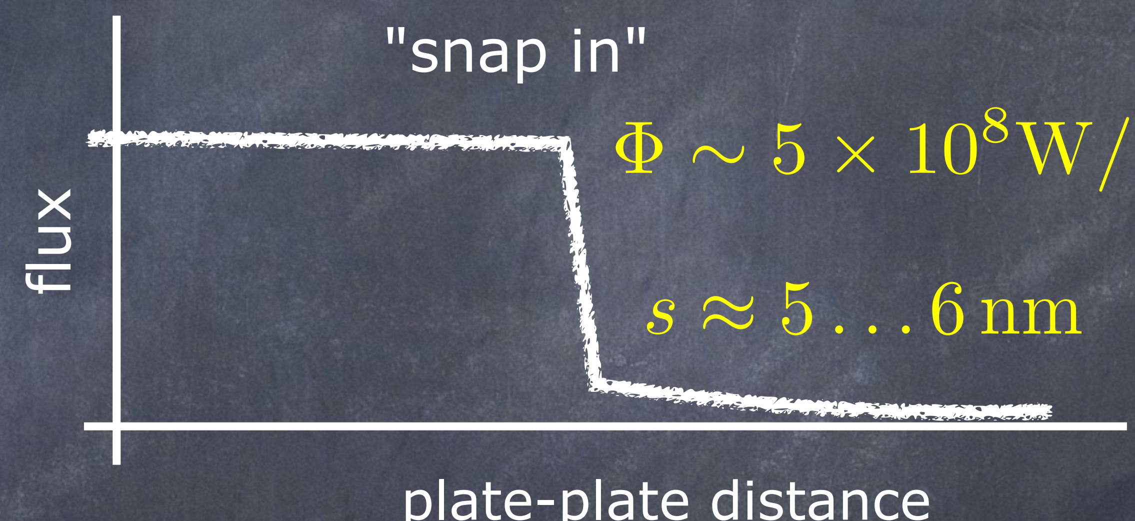
Sketch of a "theory"

Idea: proximity force (Deryagin) approximation



$$D(z) \approx d + x^2/2R$$

$$\mathrm{area}(D < s) \approx 2\pi R(s - d)$$



$$\Phi \sim 5 \times 10^8 \mathrm{W/m^2}$$

$$s \approx 5 \ldots 6\,\mathrm{nm}$$

$$\text{flux}\ \Phi \ll \text{ballistic phonons}$$

Teasers

- radiation near metals is mainly magnetic (LMDOS)
  [J. D. Jackson] [K. Joulain, *PRB* 2003]

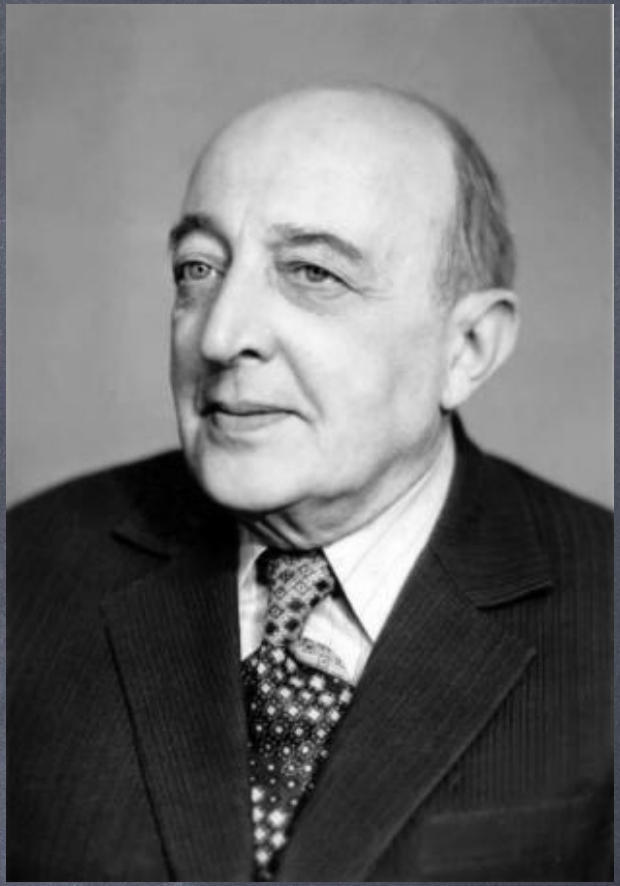
- electrodynamics & relativity:
  medium edyn & general relativity
  [U. Leonhardt & Th. Philbin, *Progr Opt* 2009]

- relative motion is a non-eq setting (4-vector field)
  similar to temperature gradients
  [G. Neugebauer] [Zh. Ch. Wu, *EPL* 2009]

- quantum aspects / multiple-scale simulations

friction (Cherenkov) forces:
I. Nefedov, A. Volokitin ...

Summary



Summary

- fluctuation EDyn (Rytov theory) = Maxwell + Langevin
- matter thermalises to $T(\mathbf{r})$,
  equilibrates the e.m. field via absorption / fluctuation
  (FD relations 1+2)
- super-Planck heat transfer:
  "activate" matter degrees of freedom (SPP, phonons)
- n-scale: non-sharp boundaries, non-local response