Nanothermodynamics and near-field heat transfer

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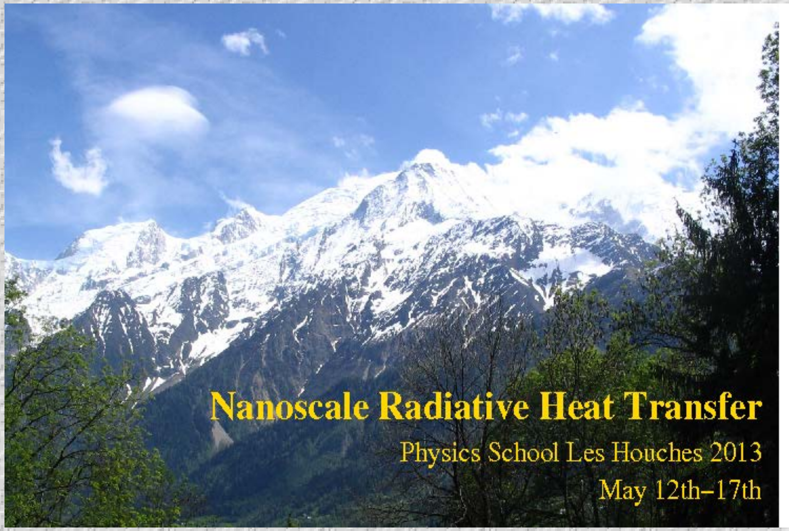

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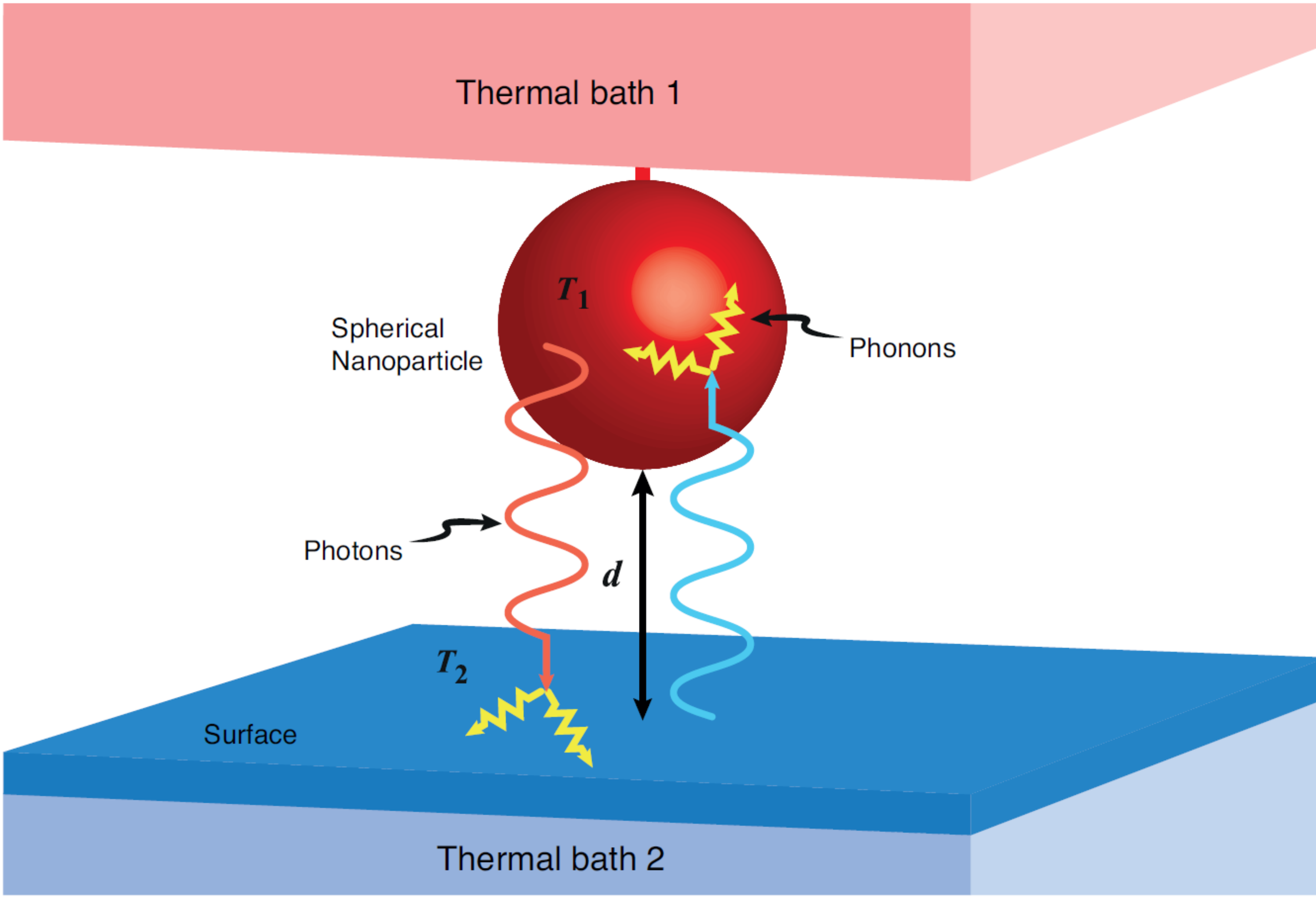
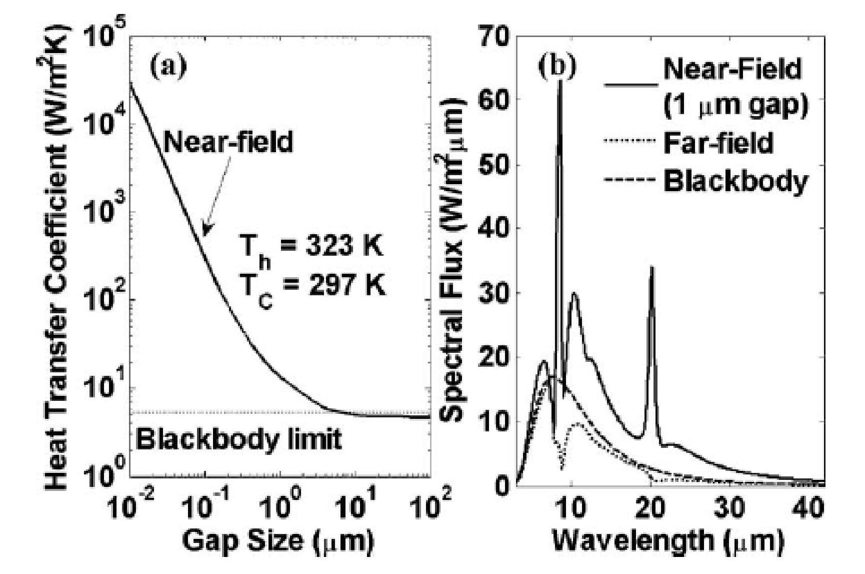
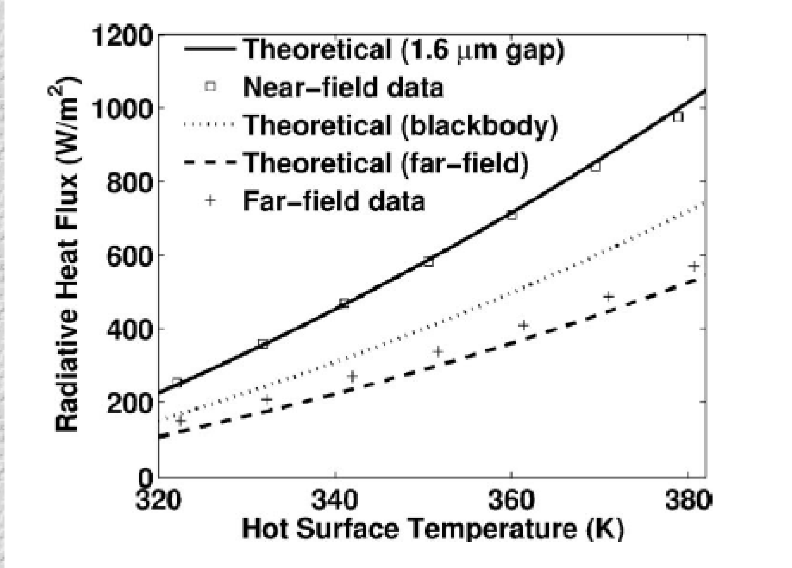


Thermal bath 1
T_1
Spherical Nanoparticle
Phonons
Photons
d
T_2
Surface
Thermal bath 2

Heat Transfer coefficient

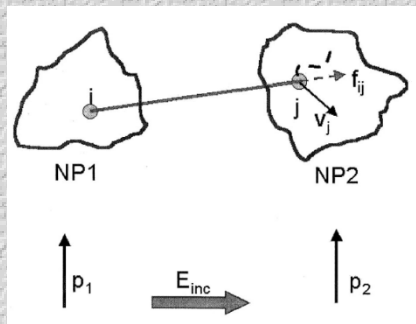


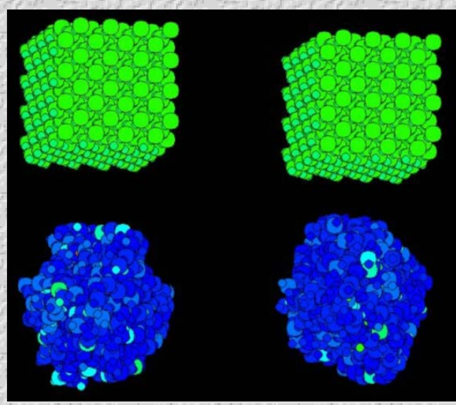


Enhancement of the heat flux in the near-field

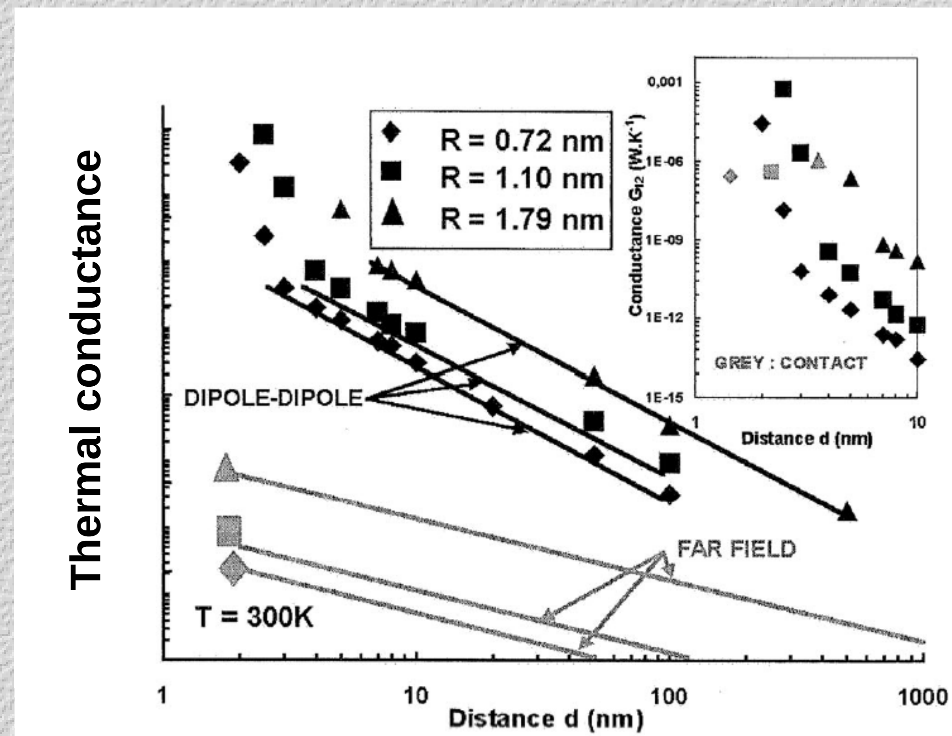
Hu et al., Appl. Phys. Lett. 92, 133106 (2008)

Thermal conductance





Molecular dynamics



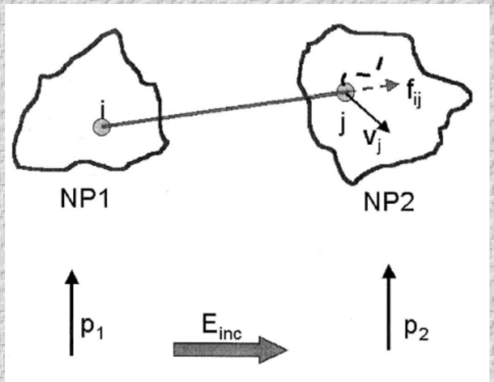
Domingues et al., Phys. Rev. Lett. 94, 085901 (2005)

Fluctuation-dissipation regime

Fluctuating electrodynamics

$$\mathbf{E}_{inc} = \mathbf{G} \cdot \mathbf{p}$$

$$Q_{1 \longrightarrow 2}(\omega) = \frac{\omega \varepsilon_0}{2} \alpha_2'' \left| \mathbf{E}_{inc}(\mathbf{r}_2) \right|^2$$



$$\left| \mathbf{E}_{inc}(\mathbf{r}_2) \right|^2 \sim \langle p_k p_l \rangle$$

FDT

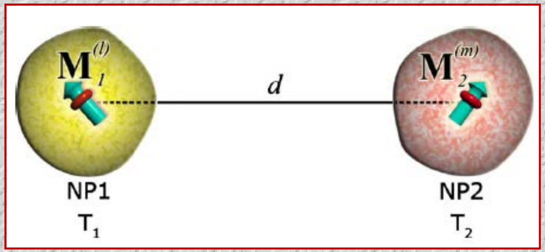
$$\langle p_k p_l \rangle = \frac{\varepsilon_0 \alpha_1''(\omega)}{\pi \omega} \Theta(\omega, T_1) \delta(\omega - \omega') \delta_{kl}$$

$$Q_{12}^{NF}(\omega) = \frac{3}{4\pi^3} \frac{\alpha_1''(\omega) \alpha_2''(\omega)}{d^6} \left[\Theta(\omega, T_1) - \Theta(\omega, T_2) \right]$$

Domingues et al., PRL, 94, 085901 (2005)

Valid when thermalization is very fast

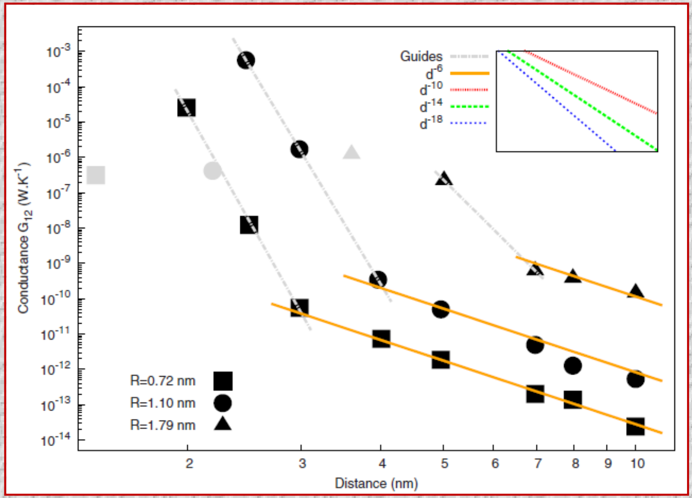
Beyond the dipolar approximation…

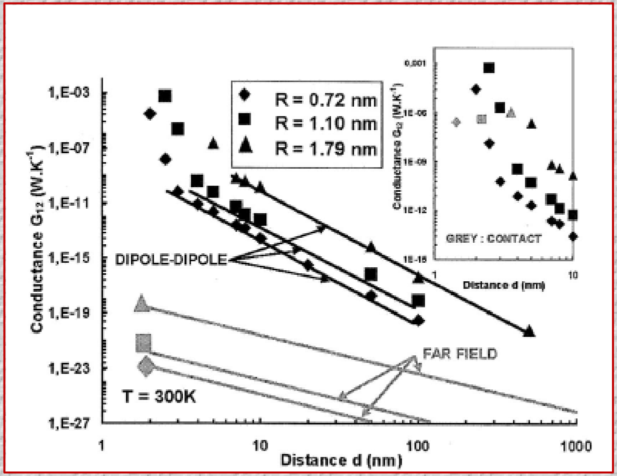


A.Pérez, J.M.Rubi., L. Lapas, Phys. Rev. B 77, 155417 (2008)

$$G_{12}^{dip}(T_0) = \frac{3}{8\pi^3}\left(\int_0^\infty \Theta'(\omega,T_0)\alpha''_{(1)}\alpha''_{(2)}\,d\omega\right) d^{-6}$$

$$G_{12}^{qd}(T_0) = \frac{1}{2\pi^3}\int_0^\infty \Theta'(\omega,T_0)\left\{45\left(\alpha''_{(1)}\beta''_{(2)} + \alpha''_{(2)}\beta''_{(1)}\right) d^{-8} + \frac{15}{4}\,\beta''_{(1)}(\omega)\beta''_{(2)}(\omega) d^{-10}\right\} d\omega$$





Dipolar approximation: d>8R

Domingues *et al*.,PRL, 94, 085901 (2005)

Equilibrium photon gas

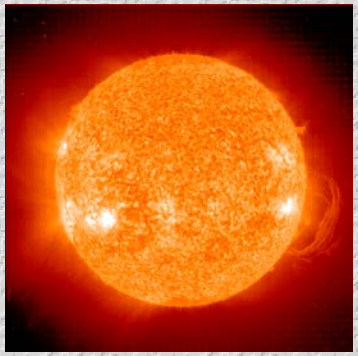
$$S_0 = k_B N \ln \Omega$$

microstates

Energy conservation

$$N_\omega = \frac{1}{\exp\left(\frac{\hbar\omega}{kT}\right) - 1}$$

Planck distribution



TdS=dE

$$J_{eq} = \sigma T^4$$

Stefan-Boltzmann

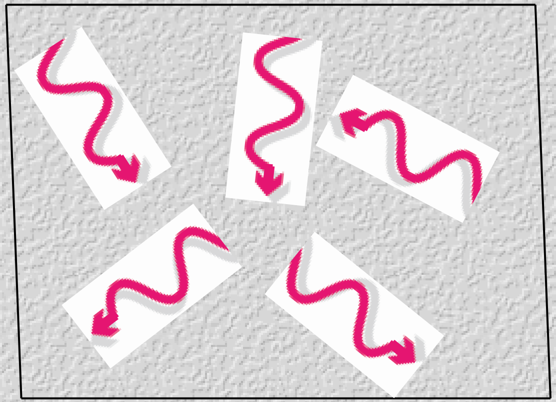
Planck's theory is not valid when length scales are comparable to the wave length of thermal radiation

Planck's radiation law

N: photons in a box with frequency quantum states

N_ω : photons with frequency ω

g_ω : quantum states



Single configuration:

x: photon
|…|: state

xxx|x|xx|xxxx|xxx|xx

Bosons: no restriction on the numeber of particles in each level

Ω: number of microstates; combinatorial problem

$$\Omega_{BE} = \prod_{\omega} \frac{(N_\omega + g_\omega - 1)!}{N_\omega!(g_\omega - 1)!}$$

Planck radiation law from thermodynamics

i) Maximizing the number of microstates:

$$\ln \Omega_{BE} = \sum \ln (N_\nu + g_\nu)! - \sum \ln N_\nu! - \sum \ln g_\nu!$$

$$N_\nu = \frac{g_\nu}{e^{\beta h\nu} - 1}$$

β?

ii) Condition: energy is constant

$$\sum N_\nu h\nu = U = \text{const}$$

$$N_\nu = \frac{8\pi V}{c^3} \frac{\nu^2}{e^{h\nu/kT} - 1}$$

iii) Boltzmann entropy

$$dS = k\, d \ln \Omega_{BE} = k \sum \ln \left(1 + \frac{g_\nu}{N_\nu}\right) dN_\nu$$

$$dS = k\beta\, dU$$

$$dS/dU = 1/T$$

$$\beta = \frac{1}{kT}$$

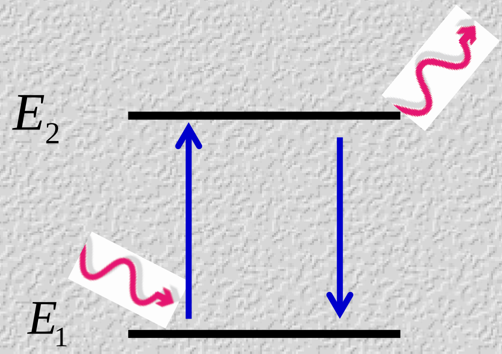
Plank radiation law from kinetics

Atoms in a radiation field

i) Absorption of photons

$$\frac{dN(1\rightarrow 2)}{dt} = B_{12}N_1\,u(\nu_{12})$$

$$\nu_{12} = E_2 - E_1$$



ii) Emission of photons

$$\frac{dN(2\rightarrow 1)}{dt} = A_{21}N_2 + B_{21}N_2\,u(\nu_{12})$$

Spontaneous

Radiation field

Detailed balance

$$B_{21} = B_{12}$$

Thermal equilibrium:

$$\frac{dN(1\rightarrow 2)}{dt} = \frac{dN(2\rightarrow 1)}{dt}$$

$$\frac{N_2}{N_1} = e^{-h\nu_{12}/\tau}$$

$$u(\nu_{12}) = \frac{(A_{21}/B_{12})}{e^{h\nu_{12}/\tau} - 1}$$

Wien displacement law

$$u(\nu) = \alpha\nu^3 f(\nu/\tau)$$

$$\frac{A_{21}}{B_{12}} = \alpha\nu^3$$

$$u(\nu_{12}) = \frac{\alpha\nu^3}{e^{h\nu/\tau} - 1}$$

Nanothermodynamics

Nanosystems: fluctuations are important
One has to adopt a probabilistic description

-D. Reguera, J.M. Rubi and J.M. Vilar, J. Phys. Chem. B (2005)
-J.M. Rubi, Scientific American, Nov., 40 (2008)
http://www.ffn.ub.es/webmrubi

Photons, phonons, electrons,….:

$\Gamma(x, p)$

$n(\Gamma, t)$

$\frac{\partial n}{\partial t}$? → kinetics ⇒ (Flux of particles, Heat flux, Energy flux, etc.)

Second law: entropy

$$dQ = T\delta s = -\mu\delta n$$

$$\frac{\partial s}{\partial t} = -\frac{\mu}{T}\frac{\partial n}{\partial t} = \Delta(\frac{\mu}{T}J) - \frac{1}{T}J\Delta\mu$$

entropy production

$$\frac{\partial n}{\partial t} = -\Delta J$$

$$J = -\frac{L}{T}(\mu_2 - \mu_1)$$

Linear

$$J = -\frac{L}{T}\Delta\mu \approx -kLe^{-\frac{\mu}{kT}}\Delta e^{\frac{\mu}{kT}}$$

$$J = -l(e^{\frac{\mu_2}{kT}} - e^{\frac{\mu_1}{kT}})$$

Nonlinear (Arrhenius)

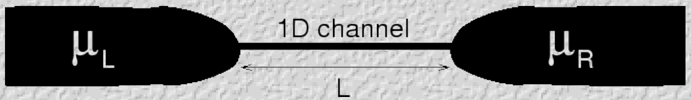
i) Boltzmann (BGK):

$$\mu = kT \ln \frac{n}{n_0} + \mu_0$$

$$\frac{\partial n}{\partial t} = -\frac{L}{T}(\mu - \mu_0) \approx -\frac{1}{\tau}(n - n_0)$$

$$\tau^{-1} = \frac{L}{Tn_0}$$

ii) Mesoscopic conductors (Landauer):



$$I = I^{>} - I^{<} = \frac{2q^2}{h} M \frac{\mu_L - \mu_R}{q}$$

iii) Photons

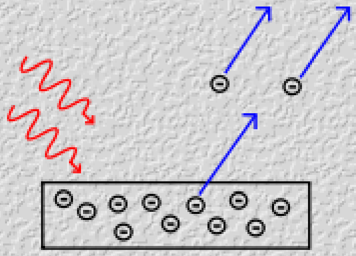
$$J_{st}(\omega) = -D_L(\omega) D_R(\omega)\left[n(\omega, T_R) - n(\omega, T_L)\right]$$

$$n(\omega, T) = \frac{1}{\exp(\hbar\omega / kT) - 1}$$

T_L T_R

$$J_{st} = \frac{\hbar}{4\pi^3 c^3} \int d\omega d\vec{\Omega}_p \omega^3 J_{st}(\omega) = \sigma(T_R^4 - T_L^4)$$

iv) Thermal emission, adsorption (Langmuir), electrokinetic phenomena (Butler-Volmer): Activated processes.



Entropy

Statistics:

JMR, Sci. Am, November, 2008

$$S(t) = -k_B \int n(\mathbf{\Gamma},t) \ln \frac{n(\mathbf{\Gamma},t)}{\Omega} d\mathbf{\Gamma} + S_0$$

$$\delta S = -k_B \int \delta n(\mathbf{\Gamma},t) \ln \frac{n(\mathbf{\Gamma},t)}{\Omega} d\mathbf{\Gamma}$$

$$\mu(\mathbf{\Gamma},t) = \frac{k_B T}{N} \ln \frac{n(\mathbf{\Gamma},t)}{\Omega}$$

Thermodynamics:

$$\delta S = -N \int \frac{\mu(\mathbf{\Gamma},t)}{T} \delta n(\mathbf{\Gamma},t) d\mathbf{\Gamma}$$

Entropy production

$$\frac{\partial S}{\partial t} = -\int \mathbf{J}\left(\mathbf{\Gamma},t\right) \cdot \frac{\partial}{\partial \mathbf{\Gamma}} \frac{N\mu(\mathbf{\Gamma},t)}{T} d\mathbf{\Gamma}$$

$$\mathbf{J}\left(\mathbf{\Gamma},t\right) = -L(\mathbf{\Gamma}) \frac{\partial}{\partial \mathbf{\Gamma}} \frac{N\mu(\mathbf{\Gamma},t)}{T}$$

Onsager coefficient

$$\mathbf{J}\left(\mathbf{\Gamma},t\right) = -D\frac{\partial}{\partial \mathbf{\Gamma}} \Omega \exp\left(\frac{N\mu(\mathbf{\Gamma},t)}{k_B T}\right) = -D \frac{\partial}{\partial \mathbf{\Gamma}} n(\mathbf{\Gamma},t).$$

$$J(t) = -D_L D_R \left[n(\mathbf{p}_L,t) - n(\mathbf{p}_R,t)\right]$$

$$\frac{\partial}{\partial t} n(\mathbf{\Gamma},t) = \frac{\partial}{\partial \mathbf{\Gamma}} \cdot D(\mathbf{\Gamma}) \frac{\partial}{\partial \mathbf{\Gamma}} n(\mathbf{\Gamma},t)$$

Non-equilibrium Stefan-Boltzmann law

$$J_{st}(\omega) = -D_L(\omega)D_R(\omega)\left[n(\omega,T_R) - n(\omega,T_L)\right]$$

$$n(\omega,T) = \frac{1}{\exp\left(\hbar\omega / kT\right) - 1}$$

$$J_{st} = \frac{\hbar}{4\pi^3 c^3}\int d\omega d\vec{\Omega}_p \omega^3 J_{st}(\omega) = \sigma(T_R^4 - T_L^4)$$

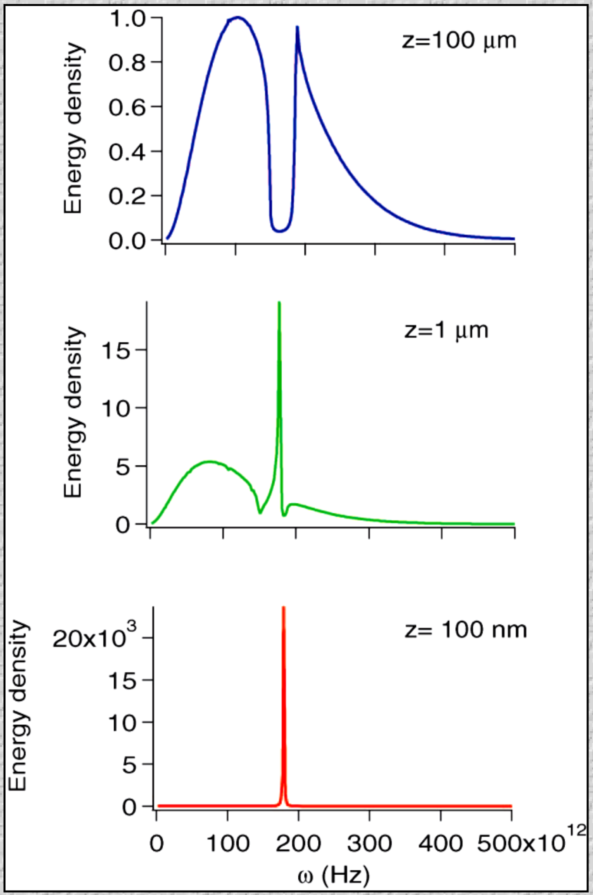
Shorter distances, no longer valid

Near-field thermodynamics

ELECTROMAGNETIC WAVES CONFINED IN A VERY NARROW GAP

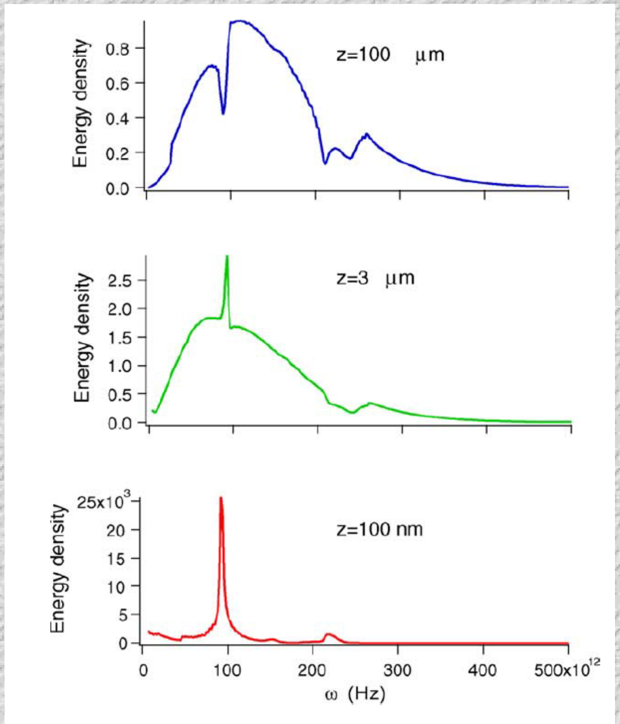
When the distance diminishes, thermal radiation becomes a highly directional beam of coherent radiation.

The narrow gap acts as a resonant cavity



Spectrum of electromagnetic energy for different detection distances above surface of silicon carbide normalized by its maximum value in far field at T= 300 K. (J.-J. Greffet and C. Henkel, 2007)

Electromagnetic energy density above a plane interface separating glass (amorphous, optical phonons poorly defined) at T = 300 K from vacuum at T = 0 K



Photon Kinetics

$$J = \left(\frac{D_{pp} D_{xx}}{D_{xp}} - D_{px} \right) \frac{\partial n}{\partial x}$$

$$J = \frac{\hbar}{\tau^*}(n_2 - n_1)$$

$$\tau^*(t) = \int n\tau(n)\, d\Gamma$$

$$i)\ d >> \lambda_T\ ; black\ body$$

$$ii)\ d \leq \lambda_T$$

$$\Delta x \Delta p \geq h$$

$$\Delta p \geq \frac{h}{d};\ \ \Delta E \geq h\frac{Kc}{d} \equiv h\omega_R$$

Heat flux results from the contribution of
Different modes

A. Perez, L. Lapas, J.M. Rubi, PRL, 103, 048301 (2009)

Input of the theory $\Rightarrow$ $\tau^*(t) \rightarrow \tau^*(\omega)$

Elastic:

$$\frac{1}{\tau^*(\omega)} \sim \frac{1}{\tau_0}$$

Inelastic:

Lognormal DOS $\Rightarrow$
$$\frac{1}{\tau^*(\omega)} \sim \frac{1}{\tau_0} \frac{(\omega/\omega_0)\, e^{\left[-\ln^2(\omega/\omega_0)/2\sigma^2\right]}}{\sqrt{2\pi}\sigma}$$

$Fitting\ \ parameters: \omega_0, \sigma$

Y. V. Denisov, A.P. Rylev, JEPT Lett. 52, 411 (1990)

-Statistical model which can describe collective motions.
-Stems from the existence of a hierarchy of relaxations mechanisms in the material
-The energy consists of a large number of contributions; central limit theorem

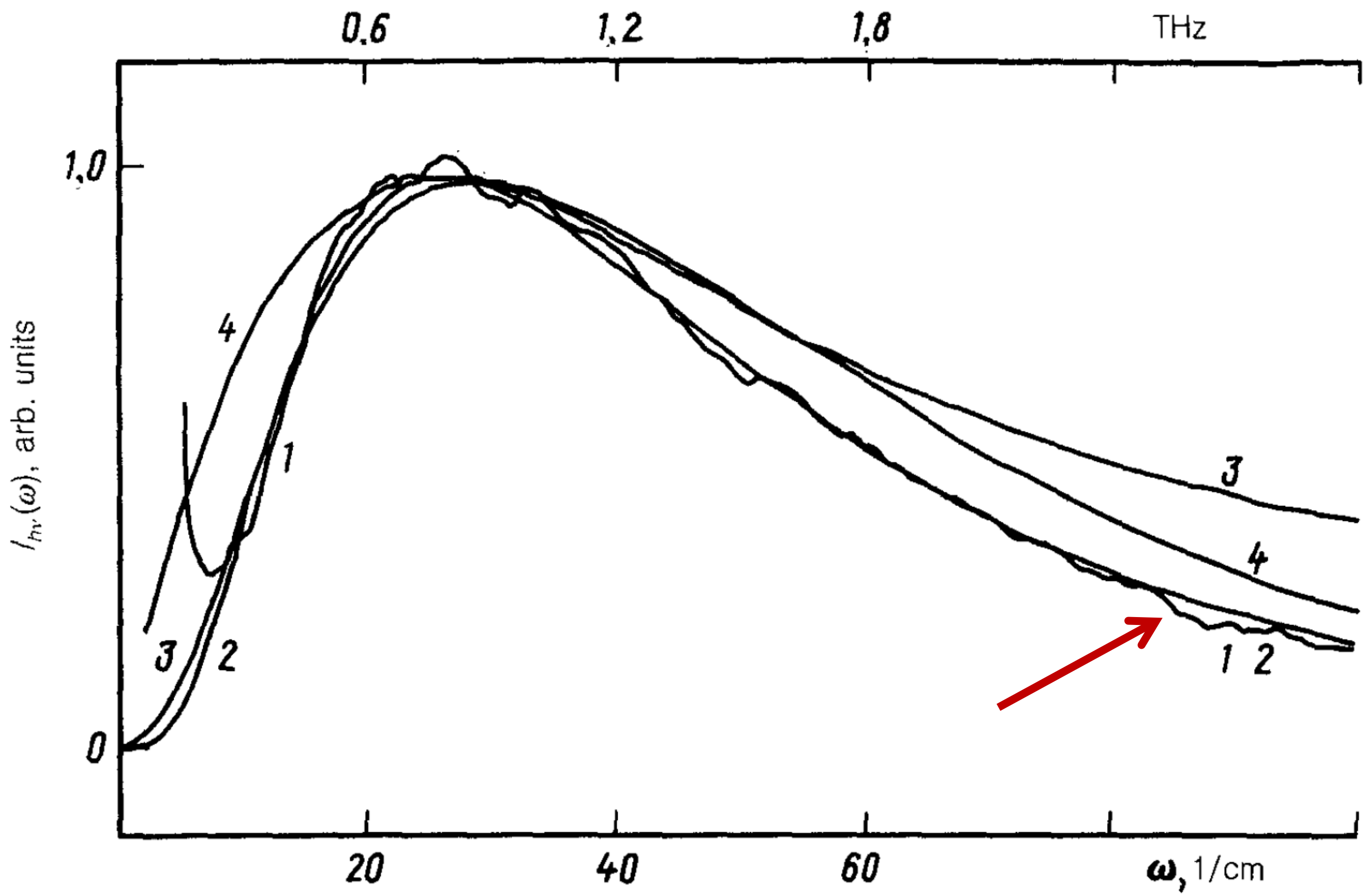


FIG. 1. *1*—Low-frequency depolarized vibrational spectrum of glassy B_2O_3; *2–4*—approximations of this spectrum; *2*—$I(\omega) = (n(\omega)+1)\omega \exp[-\{\ln(\omega/\omega_0)\}^2]$; *3*—$I(\omega) = (n(\omega)+1)\omega^3/(\omega^2+\omega_1^2)^2$; *4*—$I(\omega) = (n(\omega)+1)\omega^2 \exp[-(\omega/\omega_2)]$.

Yu. V. Denisov and A.P. Rylev, JETP Lett. 52 (1990), 411.

Heat transfer coefficient

$$H(T_0) \equiv Q/(T_1 - T_2)$$

$$Q = \int c\hbar\tau^*(\omega)^{-1}\left[N(\omega,T_1) - N(\omega,T_2)\right] g(\omega)\, d\omega$$

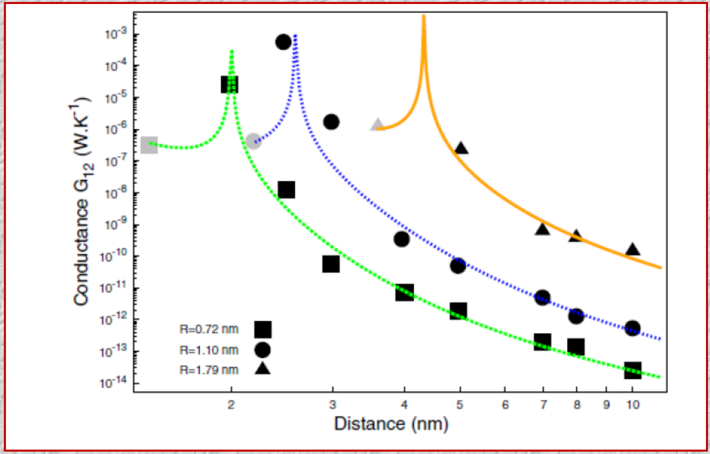
$$H(d,T_0) = \frac{k_B}{\tau_o' d^2}\left[1 + \frac{(2\pi)^{1/2}\nu c}{\sigma\omega_0 d}\exp\left\{-\left[\frac{\ln(2\pi\nu c/\omega_0 d)}{\sqrt{2}\sigma}\right]^2\right\}\right]\left(\frac{h\nu c/2k_B T_0 d}{\sinh(h\nu c/2k_B T_0 d)}\right)^2,$$

$$T_0 = (T_1 + T_2)/2$$

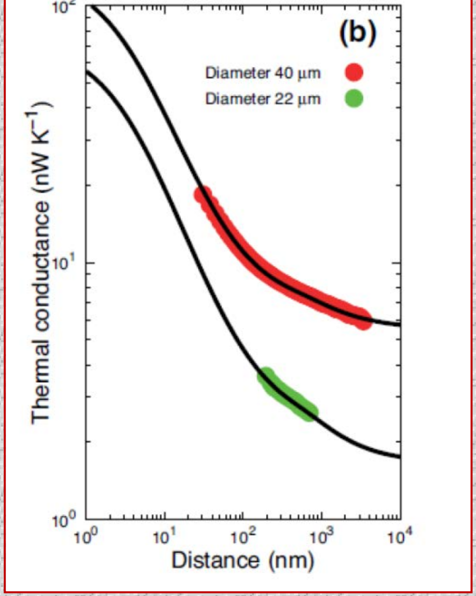
FF $H \sim T_0^3$

NF $H \sim T_0$

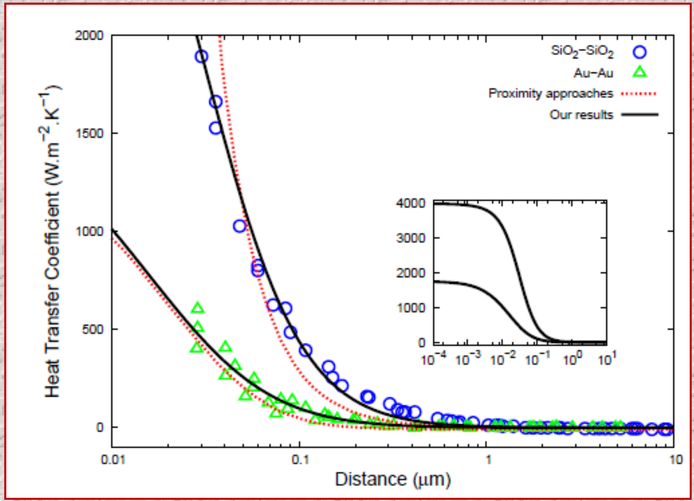
A. Perez, L. Lapas, J.M. Rubi, PRL, 103, 048301 (2009)



[10] G. Domingues, S. Volz, K. Joulain, and J.-J. Greffet, Phys. Rev. Lett. **94** (2005), 085901.



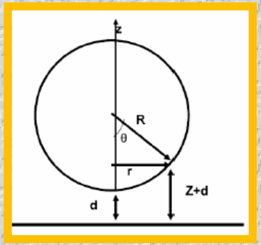
[6] E. Rousseau, A. Siria, G. Jourdan, S. Volz, F. Comin, J. Chevrier, and J.-J. Greffet, Nature Photon. **3** (2009), 514.



S. Shen, A. Mavrokefalos, P. Sambegoro, and G. Chen, Appl. Phys. Lett. 100, 233114 (2012).

$$G = (1/A)\int_0^R H[\tilde{d}(r), T_0]2\pi r dr$$

$$\tilde{d}(r) = d + b + R - \sqrt{R^2 - r^2}$$



A. Perez-Madrid, L. Lapas, J.M. Rubi, Plos One, 8, e58770 (2013)

Conclusions

- We have evaluated the heat transfer coefficient and the thermal conductance in a wide range of length scales, from the far-field to the near-field, giving a thermokinetic description of several experiments involving heat radiation through a very narrow gap.
- The thermokinetic theory presented may also be used in the study of other heat exchange processes such as those occurring in phonon systems and in the analysis of thermal contributions to Casimir forces.