Dynamics, Thermalization and Cooling of a Simple Quantum System in Environments Out of Thermal Equilibrium

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B. Bellomo, R. Messina and M. Antezza, EPL **100**, 20006 (2012)

B. Bellomo, R. Messina, D. Felbacq and M. Antezza, arXiv: 1205.6089 (2012)

16/11/2012, LKB-ENS, Paris (France)

Introduction

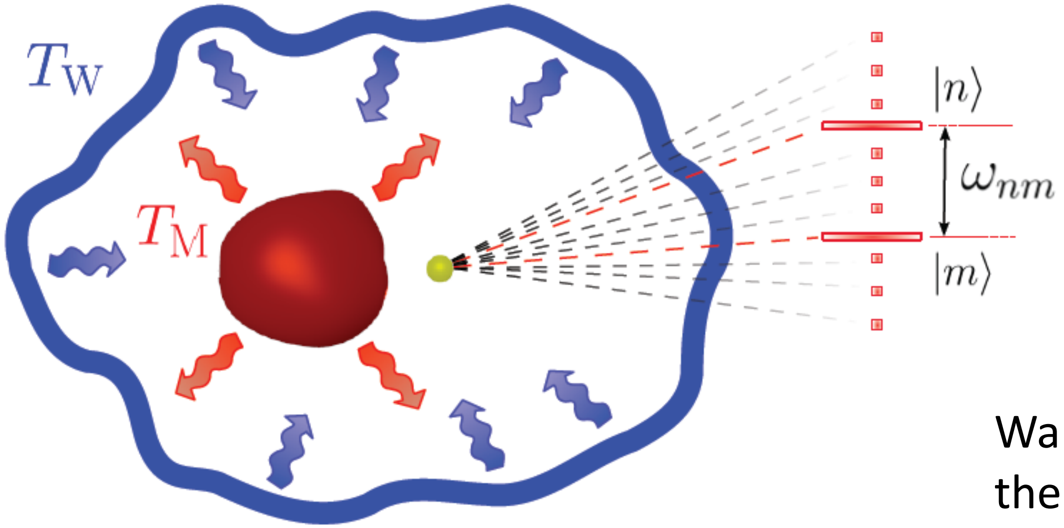
Thermalization of classical and quantum systems driven by changes of external parameters may offer a great variety of relaxation phenomena, typically studied for many-body systems

What does happen to an elementary, one-body quantum system in an environment driven out of thermal equilibrium?

Out of thermal equilibrium great richness: quantum gases, biology, Casimir forces, heat transfer,…

We study the internal evolution of an atomic system (real atoms, quantum dots, …) by means of its density matrix

Physical configuration: a *N*-level system placed close to a body



Body M of arbitrary geometry and dielectric permittivity

Body temperature T_M different from that of the surrounding walls T_W

Walls of irregular shape very far from both the body and the atom: universal isotropic black-body radiation in absence of the body

Multipolar-coupling Hamiltonian

$$H_I = -\mathbf{D} \cdot \mathbf{E}(\mathbf{R})$$

E(R) : total electromagnetic field at the atomic position

D: Atomic electric-dipole operator

$$\mathbf{D}(t) = \sum_{m,n} \left(\mathbf{d}_{mn} |m\rangle\langle n| e^{-i\omega_{nm}t} + \mathbf{d}^*_{mn} |n\rangle\langle m| e^{i\omega_{nm}t} \right)$$ where $$\mathbf{d}_{mn} = \langle m|\mathbf{D}|n\rangle$$

Free Hamiltonians $$H_A = \sum_{n=1}^{N} \hbar\omega_n |n\rangle\langle n| \qquad H_B = \int d^3\mathbf{r} \int_0^\infty d\omega \hbar\omega b^\dagger(\mathbf{r},\omega) b(\mathbf{r},\omega)$$

bosonic operators

Open quantum system approach: master equation

Starting point: $$\frac{d}{dt}\rho_{\rm tot}(t) = -\frac{i}{\hbar}[H_I(t), \rho_{\rm tot}(t)]$$ → $\rho(t) = \mathrm{Tr}_B\, \rho_{\rm tot}(t)$

Derivation of atomic master equation (weak coupling)

Born, Markovian and rotating-wave approximations

$$\frac{d}{dt}\rho(t) = -i\Big[\sum_n \omega_n|n\rangle\langle n| + \sum_{m,n} S(-\omega_{nm})|m\rangle\langle m| + \sum_{m,n} S(\omega_{nm})|n\rangle\langle n|, \rho(t)\Big]$$
$$+\sum_{m,n}\Gamma(-\omega_{nm})\Big(\rho_{mm}|n\rangle\langle n| - \frac{1}{2}\{|m\rangle\langle m|, \rho(t)\}\Big)$$
$$+\sum_{m,n}\Gamma(\omega_{nm})\Big(\rho_{nn}|m\rangle\langle m| - \frac{1}{2}\{|n\rangle\langle n|, \rho(t)\}\Big),$$

$S(\pm\omega)$: Lamb-shifts not influencing the dynamics of populations (ρ_{ii}) and modulus of coherences ($|\rho_{ij}|$)

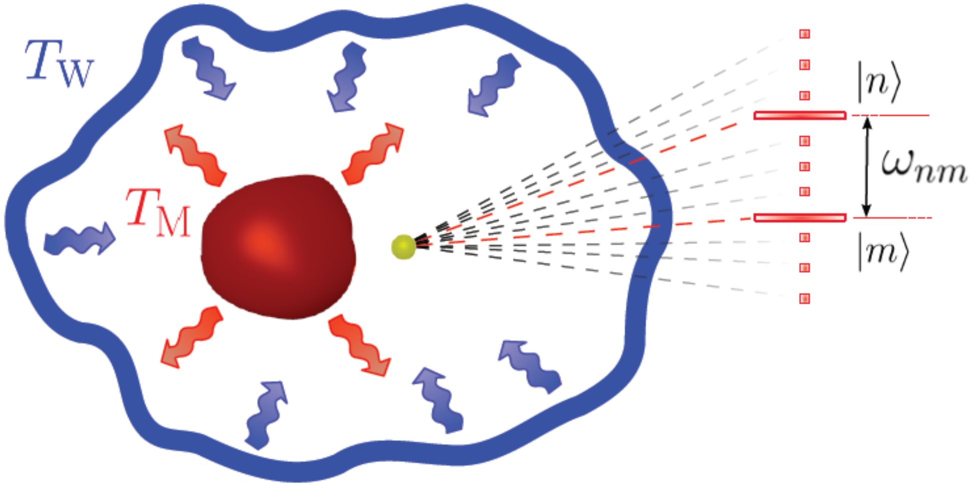
Transition rates

$$\Gamma(-\omega_{nm}) = \sum_{i,j}\gamma_{ij}(-\omega_{nm})[\mathbf{d}_{mn}]_i[\mathbf{d}_{mn}]_j^*,$$
$$\Gamma(\omega_{nm}) = \sum_{i,j}\gamma_{ij}(\omega_{nm})[\mathbf{d}_{mn}]_i^*[\mathbf{d}_{mn}]_j.$$

Key ingredient: correlation functions of the EM field

$$\gamma_{ij}(\omega) = \frac{1}{\hbar^2}\int_{-\infty}^{\infty} ds\, e^{i\omega s}\langle E_i(\mathbf{R},t)E_j(\mathbf{R},t-s)\rangle$$

Correlation functions out of thermal equilibrium



For a given set (ω; k; p), modes of the field propagating in the two directions

$$\begin{cases} E^+ = E^{(M)+} + \mathcal{T}E^{(W)+} + \mathcal{R}E^{(W)-} \\ E^- = E^{(W)-} \end{cases}$$

$\mathcal{R}$ and $\mathcal{T}$: standard reflection and transmission scattering operators, associated to the right side of the body

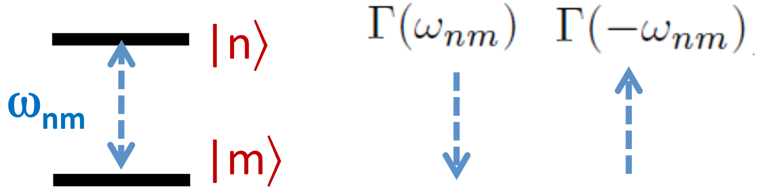
Correlation functions out equilibrium

Total field correlators obtained by mean of the correlators of the fields emitted by each source

Source fields characterized by treating each source independently as if it was at thermal equilibrium at its own temperature and thus applying the fluctuation-dissipation theorem

R. Messina and M. Antezza, Europhys. Lett. **95**, 61002 (2011); Phys. Rev. A **84**, 042102 (2011)

Transition rates: thermal equilibrium



Vacuum spontaneous emission rate

$$\Gamma_0(\omega_{nm}) = \frac{\omega_{nm}^3 |\mathbf{d}_{mn}|^2}{3\pi\epsilon_0\hbar c^3}$$

$$\begin{pmatrix} \Gamma(\omega_{nm}) \\ \Gamma(-\omega_{nm}) \end{pmatrix} = \Gamma_0(\omega_{nm})\left[\alpha_{\mathrm{W}}(\omega_{nm}) + \alpha_{\mathrm{M}}(\omega_{nm})\right] \begin{pmatrix} 1 + n(\omega_{nm}, t) \\ n(\omega_{nm}, t) \end{pmatrix}$$

Factorization: **Vacuum** **Matter** **Thermal**

α_W and α_M functions depend on the properties of the body and of the atom (geometry, dielectric permittivity, …)

Average number of photons: $n(\omega, T) = \left(e^{\frac{\hbar\omega}{k_B T}} - 1\right)^{-1}$

α functions for an arbitrary body

General expressions for an arbitrary body

$$\alpha_{\mathrm{W}}(\omega_{nm}) = \frac{3\pi c}{2\omega}\sum_{p,p'}\sum_{i,j}\frac{[\mathbf{d}_{mn}]_i^*[\mathbf{d}_{mn}]_j}{|\mathbf{d}_{mn}|^2}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\int\frac{d^2\mathbf{k}'}{(2\pi)^2}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\langle p,\mathbf{k}|\Big[e^{-i(k_z-k_z'^*)z}[\hat{\epsilon}_p^-(\mathbf{k},\omega)]_i[\hat{\epsilon}_{p'}^-(\mathbf{k}',\omega)]_j^*\mathcal{P}_{-1}^{(\mathrm{pw})}$$
$$+ e^{i(k_z+k_z'^*)z}[\hat{\epsilon}_p^+(\mathbf{k},\omega)]_i[\hat{\epsilon}_{p'}^-(\mathbf{k}',\omega)]_j^*\mathcal{R}\mathcal{P}_{-1}^{(\mathrm{pw})} + e^{-i(k_z+k_z'^*)z}[\hat{\epsilon}_p^-(\mathbf{k},\omega)]_i[\hat{\epsilon}_{p'}^+(\mathbf{k}',\omega)]_j^*\mathcal{P}_{-1}^{(\mathrm{pw})}\mathcal{R}^\dagger$$
$$+ e^{i(k_z-k_z'^*)z}[\hat{\epsilon}_p^+(\mathbf{k},\omega)]_i[\hat{\epsilon}_{p'}^+(\mathbf{k}',\omega)]_j^*\Big(\mathcal{T}\mathcal{P}_{-1}^{(\mathrm{pw})}\mathcal{T}^\dagger + \mathcal{R}\mathcal{P}_{-1}^{(\mathrm{pw})}\mathcal{R}^\dagger\Big)\Big]|p',\mathbf{k}'\rangle,$$

$$\alpha_{\mathrm{M}}(\omega_{nm}) = \frac{3\pi c}{2\omega}\sum_{p,p'}\sum_{i,j}\frac{[\mathbf{d}_{mn}]_i^*[\mathbf{d}_{mn}]_j}{|\mathbf{d}_{mn}|^2}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\int\frac{d^2\mathbf{k}'}{(2\pi)^2}e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\langle p,\mathbf{k}|e^{i(k_z-k_z'^*)z}$$
$$\times [\hat{\epsilon}_p^+(\mathbf{k},\omega)]_i[\hat{\epsilon}_{p'}^+(\mathbf{k}',\omega)]_j^*\Big(\mathcal{P}_{-1}^{(\mathrm{pw})} - \mathcal{R}\mathcal{P}_{-1}^{(\mathrm{pw})}\mathcal{R}^\dagger + \mathcal{R}\mathcal{P}_{-1}^{(\mathrm{ew})} - \mathcal{P}_{-1}^{(\mathrm{ew})}\mathcal{R}^\dagger - \mathcal{T}\mathcal{P}_{-1}^{(\mathrm{pw})}\mathcal{T}^\dagger\Big)|p',\mathbf{k}'\rangle$$

where $\langle p,\mathbf{k}|\mathcal{P}_n^{(\mathrm{pw/ew})}|p',\mathbf{k}'\rangle = k_z^n\langle p,\mathbf{k}|\Pi^{(\mathrm{pw/ew})}|p',\mathbf{k}'\rangle$

At thermal equilibrium α_W and α_M functions sum each other producing cancellations

Instead, out of thermal equilibrium…

Transition rates: out of thermal equilibrium

$$\begin{pmatrix} \Gamma(\omega_{nm}) \\ \Gamma(-\omega_{nm}) \end{pmatrix} = \Gamma_0(\omega_{nm})\left[\alpha_{\mathrm{W}}(\omega_{nm}) + \alpha_{\mathrm{M}}(\omega_{nm})\right] \begin{pmatrix} 1 + n_{\mathrm{eff}}^{(nm)} \\ n_{\mathrm{eff}}^{(nm)} \end{pmatrix}$$

No factorization!

Vacuum — **Matter and Thermal**

effective number of photons!

$$n_{\mathrm{eff}}^{(nm)} = \frac{n(\omega_{nm}, T_{\mathrm{W}})\alpha_{\mathrm{W}}(\omega_{nm}) + n(\omega_{nm}, T_{\mathrm{M}})\alpha_{\mathrm{M}}(\omega_{nm})}{\alpha_{\mathrm{W}}(\omega_{nm}) + \alpha_{\mathrm{M}}(\omega_{nm})}$$

$$n(\omega_{nm}, T_{\min}) < n_{\mathrm{eff}}^{(nm)} < n(\omega_{nm}, T_{\max})$$

$$\begin{cases} T_{\min} = \min(T_{\mathrm{M}}, T_{\mathrm{W}}) \\ T_{\max} = \max(T_{\mathrm{M}}, T_{\mathrm{W}}) \end{cases}$$

Transition rates confined by their values at thermal equilibrium at $T_{\min}$ and $T_{\max}$

Effective temperatures

The decay rates of each transition have the same value they would have if the temperatures of the body and of the environment were equal to the same:

$$T_{\text{eff}}^{(nm)} = \frac{\hbar\omega_{nm}}{k_B}\left[\log\left(1 + n_{\text{eff}}^{(nm)}{}^{-1}\right)\right]^{-1}$$

being, in general

$$T_{\text{eff}}^{(nm)} \neq T_{\text{eff}}^{(n'm')}$$

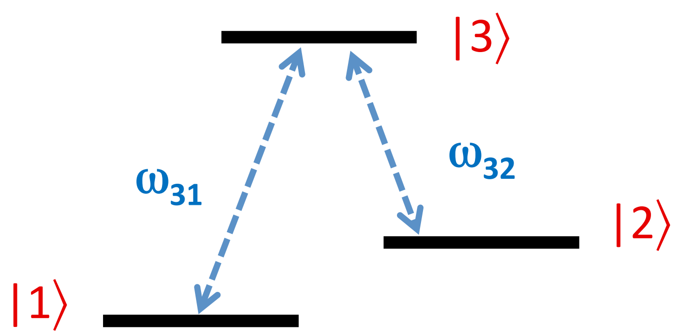
To each transition we can associate an effective temperature comprised between T_W and T_M

$$T_{\text{min}} < T_{\text{eff}}^{(nm)} < T_{\text{max}}$$

The various transitions *feel* **different temperatures** whose values depend on the system-body distance, on the geometry of the body and on the interplay of all such parameters with the resonances of the body dielectric function.

Thermalization dynamics can be readily interpreted in terms of effective temperatures

Steady states: three-level system (thermal equilibrium)



The atom thermalizes to a diagonal state whose populations are given by ratios of functions of various transition rates

At thermal equilibrium →

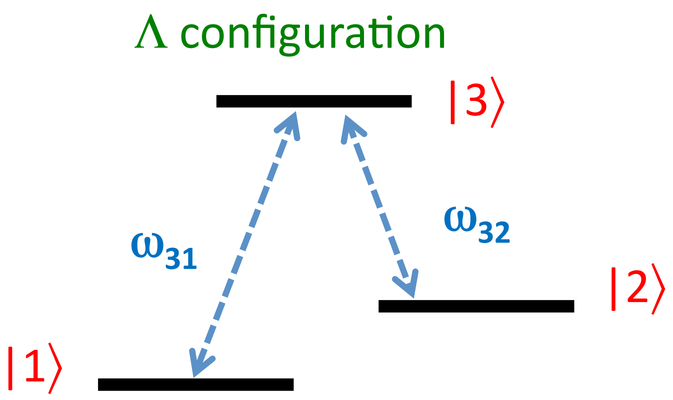
Steady populations: thermal state

$$\begin{pmatrix} \rho_{11}(\infty) \\ \rho_{22}(\infty) \\ \rho_{33}(\infty) \end{pmatrix} = \frac{1}{Z} \begin{pmatrix} n(\omega_{32},T)(1+n(\omega_{31},T)) \\ n(\omega_{31},T)(1+n(\omega_{32},T)) \\ n(\omega_{31},T)n(\omega_{32},T) \end{pmatrix}$$

$$Z = 3n(\omega_{31},T)n(\omega_{32},T) + n(\omega_{31},T) + n(\omega_{32},T)$$

Peculiar cancellation of α_W and α_M, so that the result becomes universal and independent on the atom-body distance and body's properties: steady populations depend only on the ratios $h\omega_{nm}/k_B T$

Steady states: three-level system (out equilibrium)



Out of thermal equilibrium ($T_W \neq T_M$)

Steady populations

$$\begin{pmatrix} \rho_{11}(\infty) \\ \rho_{22}(\infty) \\ \rho_{33}(\infty) \end{pmatrix} = \frac{1}{Z} \begin{pmatrix} n_{\text{eff}}^{(32)}(1+n_{\text{eff}}^{(31)}) \\ n_{\text{eff}}^{(31)}(1+n_{\text{eff}}^{(32)}) \\ n_{\text{eff}}^{(31)} n_{\text{eff}}^{(32)} \end{pmatrix}$$

$$Z = 3n_{\text{eff}}^{(31)} n_{\text{eff}}^{(32)} + n_{\text{eff}}^{(31)} + n_{\text{eff}}^{(32)}$$

Steady populations depend on α_W and α_M , that

is on properties of the body and of the atom

Steady state is **not in general a thermal-state**

Emergence of various interesting and counter-intuitive dynamical features!!

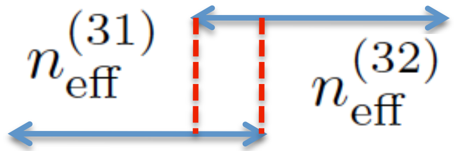
Playing with effective temperatures

By varying the various parameters one can control separately effective temperatures

Inversion of population ordering of the two lowest energy states |1> and |2>

Required condition: $n_{\rm eff}^{(32)} < n_{\rm eff}^{(31)}$ that is $\omega_{32}/T_{\rm eff}^{(32)} > \omega_{31}/T_{\rm eff}^{(31)}$

This can happen if $n(\omega_{32}, T_{\rm min}) < n(\omega_{31}, T_{\rm max})$

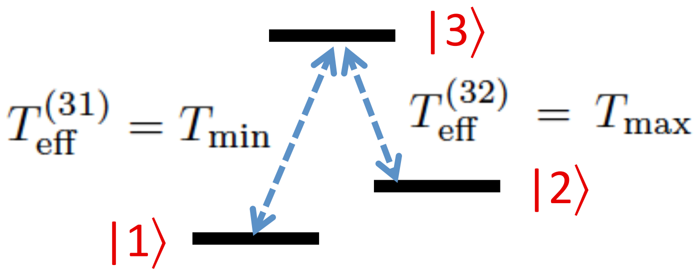


Steady populations can go outside their values at equilibrium

The maximum of $\rho_{11}(\infty)$, obtained when

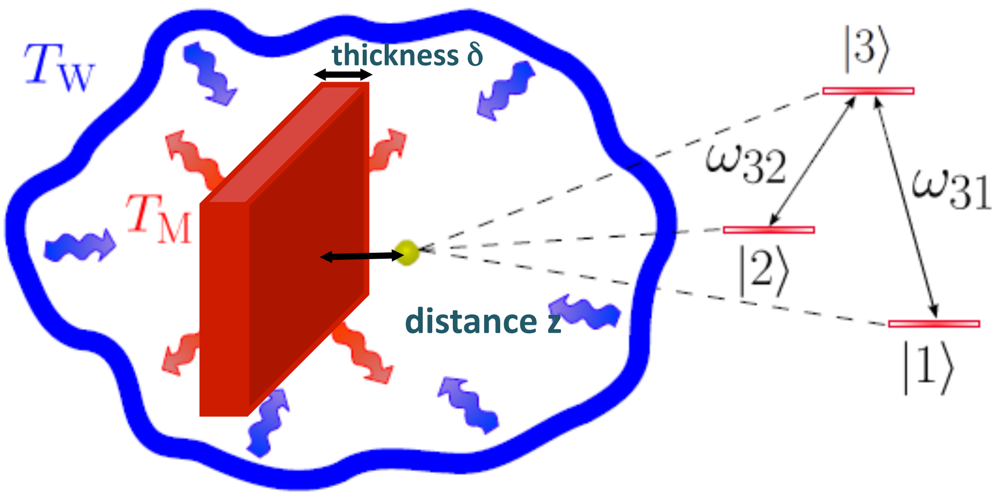
$n_{\rm eff}^{(32)} = n(\omega_{32}, T_{\rm max})$ $n_{\rm eff}^{(31)} = n(\omega_{31}, T_{\rm min})$

is larger than its value when $T_W = T_M = T_{min}$:



One can also obtain $T_{\rm eff}^{(32)} = T_{\rm eff}^{(31)}$. In this case the steady atomic state is a thermal one even if the full system is out of thermal equilibrium.

Specific example: atom in front of a slab



Dielectric permittivity of SiC

Drude-Lorentz model

$$\epsilon(\omega) = \epsilon_{\inf} \frac{\omega^2 - \omega_l^2 + i\Gamma\omega}{\omega^2 - \omega_r^2 + i\Gamma\omega}$$

Resonances: ω_r = 1.495 10^{14} rad/s

Surface phonon: ω_p = 1.787 10^{14} rad/s

Relevant length scale: $c/\omega_r \approx 2$ μm

Relevant temperature: $\hbar\,\omega_r / k_B \approx 1140$ K

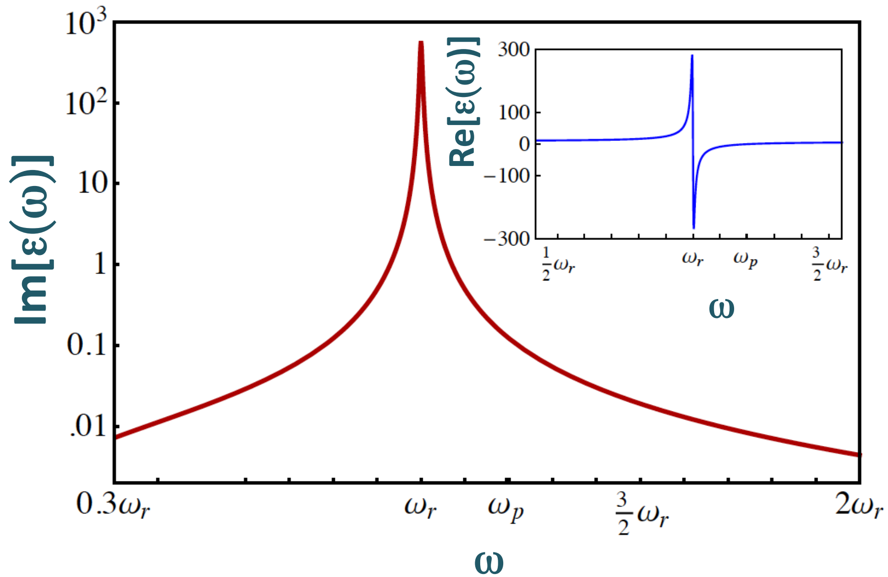
Slab: simple expressions for $\mathcal{R}$ and $\mathcal{T}$: analytic results for α_W and α_M

$$\alpha_W(\omega_{nm}) = \frac{\mathbb{1} + \mathbf{B}(\omega_{nm}) + 2\mathbf{C}(\omega_{nm})}{2} \cdot \tilde{\mathbf{d}}_{nm}$$

$$\alpha_M(\omega_{nm}) = \frac{\mathbb{1} - \mathbf{B}(\omega_{nm}) + 2\mathbf{D}(\omega_{nm})}{2} \cdot \tilde{\mathbf{d}}_{nm}$$

where $\mathbb{1} = (1,1,1)$

$$\tilde{\mathbf{d}}_{nm} = (|[\mathbf{d}_{nm}]_x|^2, |[\mathbf{d}_{nm}]_y|^2, |[\mathbf{d}_{nm}]_z|^2)/|\mathbf{d}_{nm}|^2$$



At thermal equilibrium B(ω) disappears

Specific example: atom in front of a slab

$$\mathrm{M}_1^\phi = (1,1,0) \qquad \mathrm{M}_2^\phi = \frac{c^2}{\omega^2}(\phi|k_z|^2, \phi|k_z|^2, 2k^2)$$

Fresnel coefficients

Propagative sector

$$\mathrm{B}(\omega) = \frac{3c}{4\omega}\sum_p \int_0^{\frac{\omega}{c}} \frac{k\,dk}{k_z} \mathrm{M}_p^+(k)\left(|\rho_p(k,\omega)|^2 + |\tau_p(k,\omega)|^2\right)$$

$$\mathrm{C}(\omega) = \frac{3c}{4\omega}\sum_p \int_0^{\frac{\omega}{c}} \frac{k\,dk}{k_z} \mathrm{M}_p^-(k)\,\mathrm{Re}\left(\rho_p(k,\omega)e^{2ik_z z}\right)$$

Evanescent sector

$$\mathrm{D}(\omega) = \frac{3c}{4\omega}\sum_p \int_{\frac{\omega}{c}}^{+\infty} \frac{k\,dk}{\mathrm{Im}(k_z)} e^{-2\,\mathrm{Im}(k_z)z} \mathrm{M}_p^+(k)\,\mathrm{Im}(\rho_p(k,\omega))$$

B is distance-independent and depends on the slab thickness δ

C and **D** depend both on δ and on the atom-slab distance z

For z → ∞ : **C** and **D** tend to 0, **B** remains finite and less than one

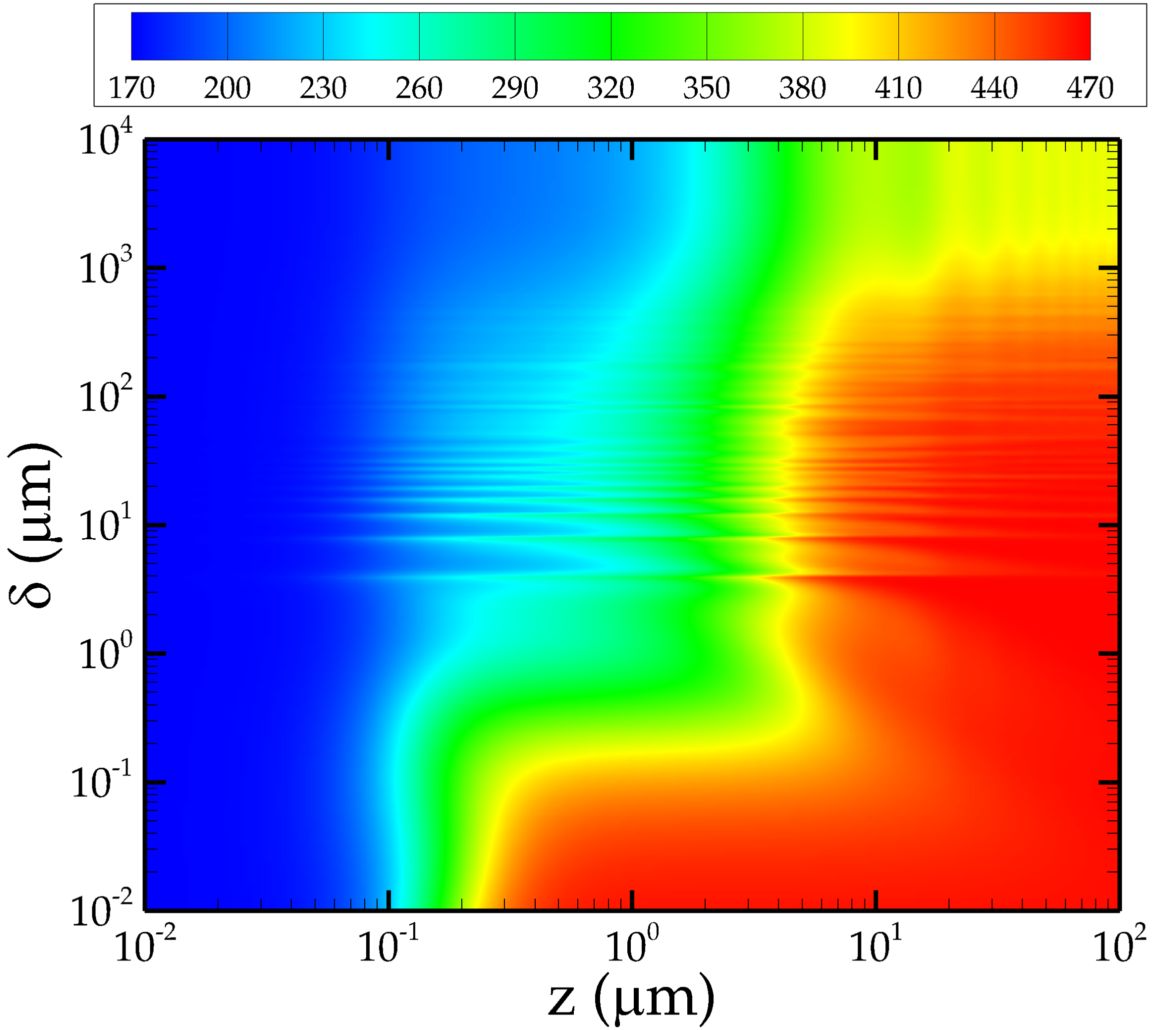
for z → 0 : **C** remains finite and **D** diverges (its TM contribution) as

$$\mathbf{D}(\omega, z \to 0) \simeq \frac{3c^3}{16\omega^3 z^3}\,\mathrm{Im}\left(\frac{\varepsilon(\omega)-1}{\varepsilon(\omega)+1}\right)(2,2,1)$$

For small z: α_M dominates because of **the divergence of evanescent slab-field (D)**

For large z: $\alpha_W > \alpha_M$ and their values are determined by a **propagative contribution (B)**

Effective temperature for a given transition



Isotropic dipoles. $\omega = 0.5\ \omega_r$

T_W **= 470 K,** T_M **= 170 K**

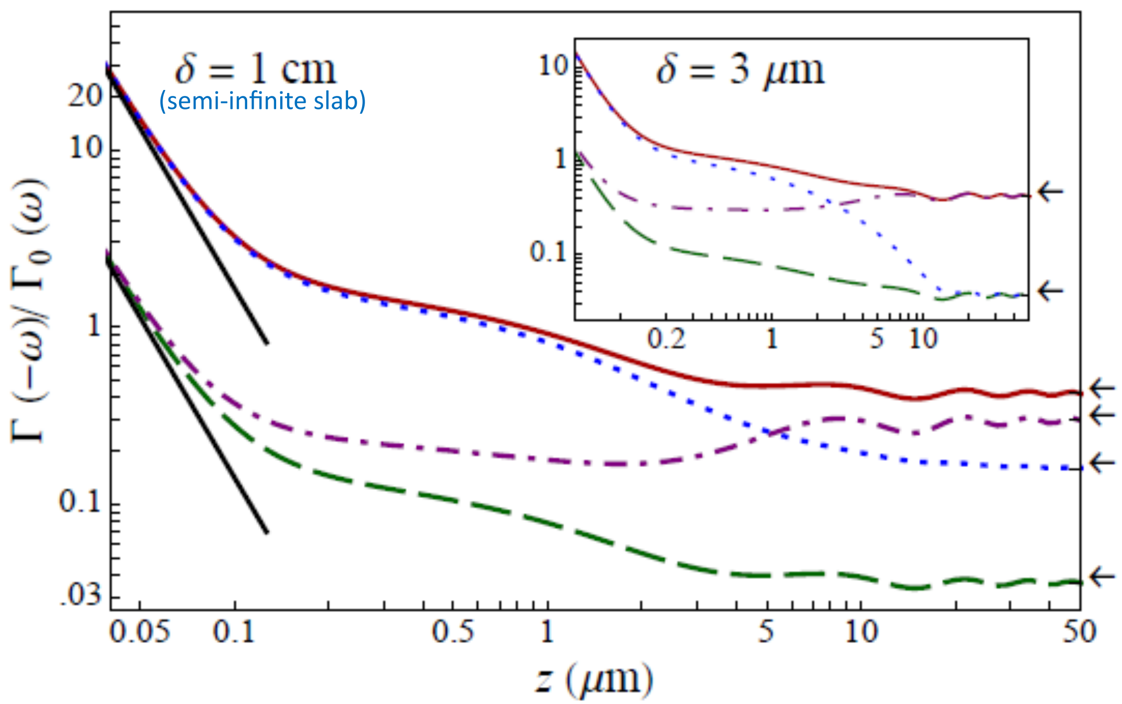
For small *z*, for any thickness δ, the atomic temperature always tends to T_M , because of the divergence of **D**

By increasing z, there are oscillations connected to **C**

For large distances the value of T_{eff} depends on the interplay between δ and z.

The position of T_{eff} in the interval [T_{min} , T_{max}] is governed by the value of **B**

Analysis of transition rates



For both panels: $\omega = 0.5\ \omega_r$

$T_W = T_M = 470$ K (red continuous)

$T_W = 470$ K; $T_M = 170$ K (purple dot-dashed)

$T_W = 170$ K; $T_M = 470$ K (blue dotted)

$T_W = T_M = 170$ K (green dashed)

← indicate the asymptotic values

Panel a) asymptotic curves for small z (black continuous) for $T_W = T_M = 470$ K and $T_W = T_M = 170$ K ($\propto z^{-3}$)

For small *z,* slab thickness regulates the distances from the slab at which the evanescent field emitted by the slab dominates the atomic dynamics

For large z, both temperatures may contribute (for large δ) depending on the value of **B**

Crossing point delimits the two zones of influence.

Decay time two level system

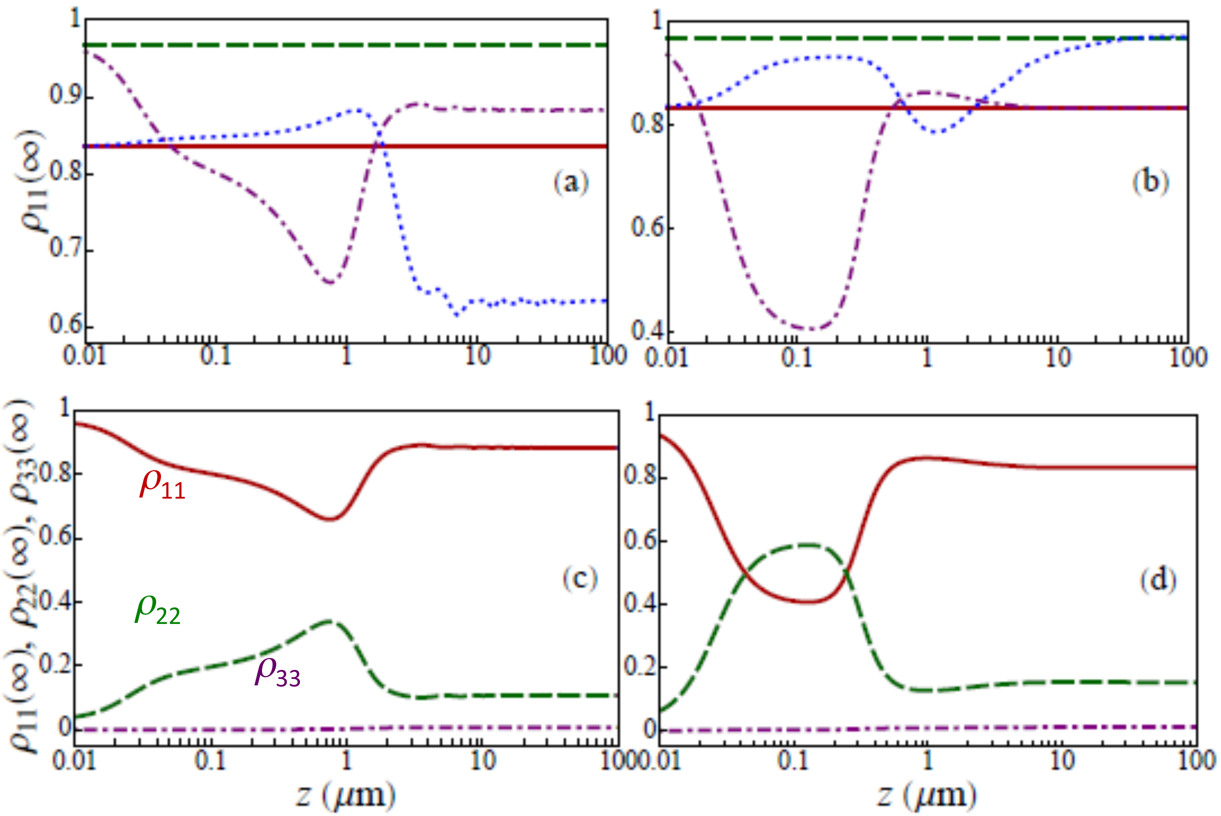
$$\tau_R = \left[\Gamma(-\omega_{nm}) + \Gamma(\omega_{nm})\right]^{-1}$$

At ω_r: $[10^{-7}, 10^{-3}]$ s

At ω_p: $[10^{-10}, 10^{-4}]$ s

dipole momentum $\approx 10^{-29}$ Cm

Steady populations



For all panels: $\omega_{32} = \omega_r$, $\omega_{31} = 2\,\omega_r$

$T_W = T_M$ = 470 K (red continuous)

T_W = 470 K; T_M = 170 K (purple dot-dashed)

T_W = 170 K; T_M = 470 K (blue dotted)

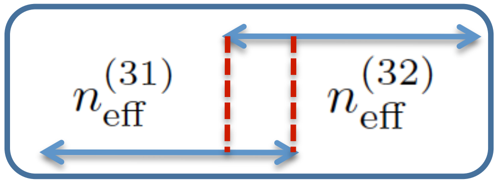
$T_W = T_M$ = 170 K (green dashed)

Panels: (c)-(d) T_W = 540 K, T_M = 270 K

Left column δ = 1 cm (semi-infinite slab)
Right column δ = 110 nm

Out equilibrium, steady populations depend on atomic and slab properties (z, δ, ε(ω))

Steady populations of |1> and |2> can go outside their values at equilibrium and be inverted in order



For small z, slab temperature T_M dominates. For large z, both temperatures may contribute

Purity

$$\Pi(\rho) = \mathrm{Tr}[\rho^2] = \sum_i \rho_{ii}^2 + 2\left(|\rho_{12}|^2 + |\rho_{13}|^2 + |\rho_{23}|^2\right)$$

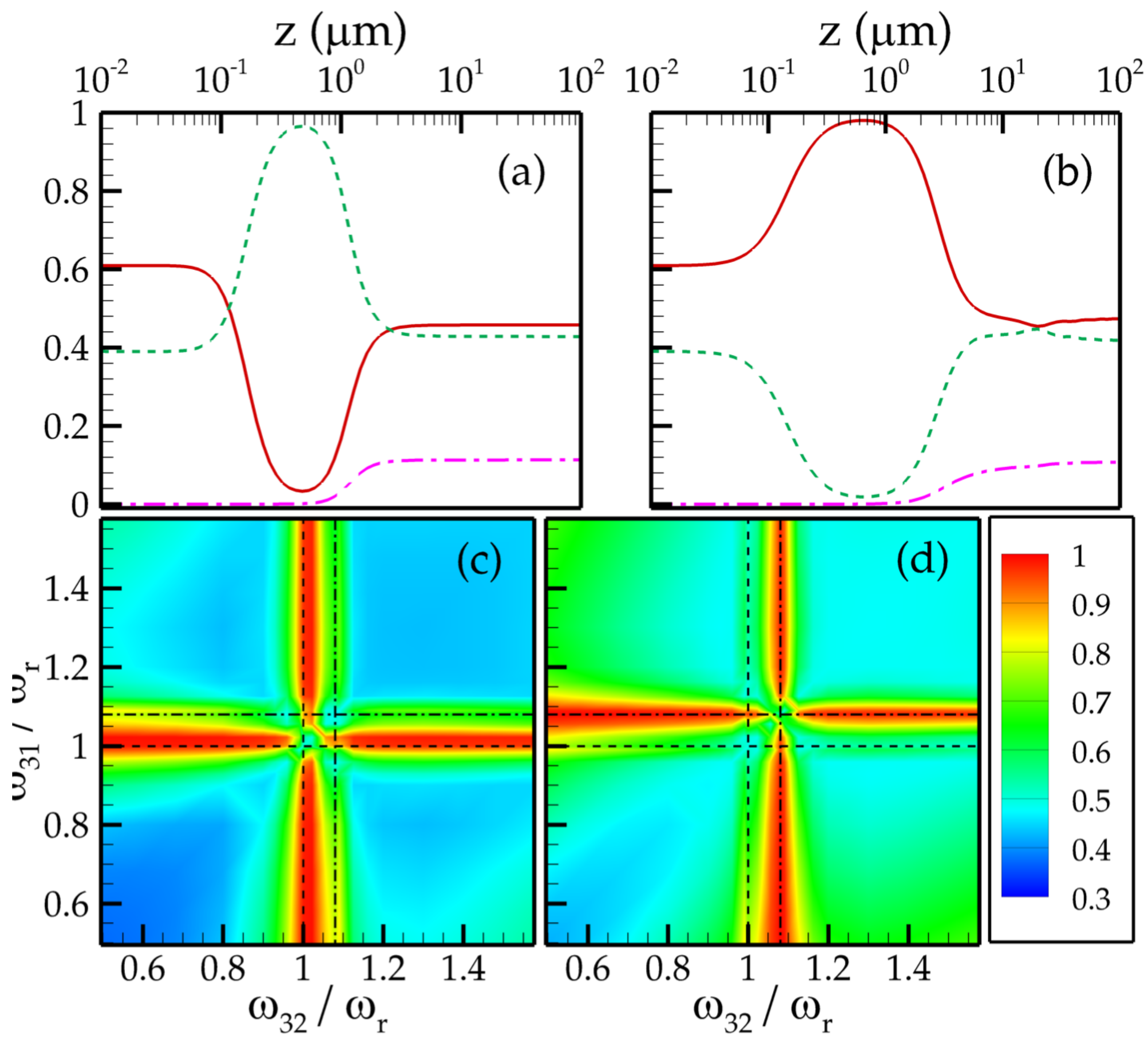
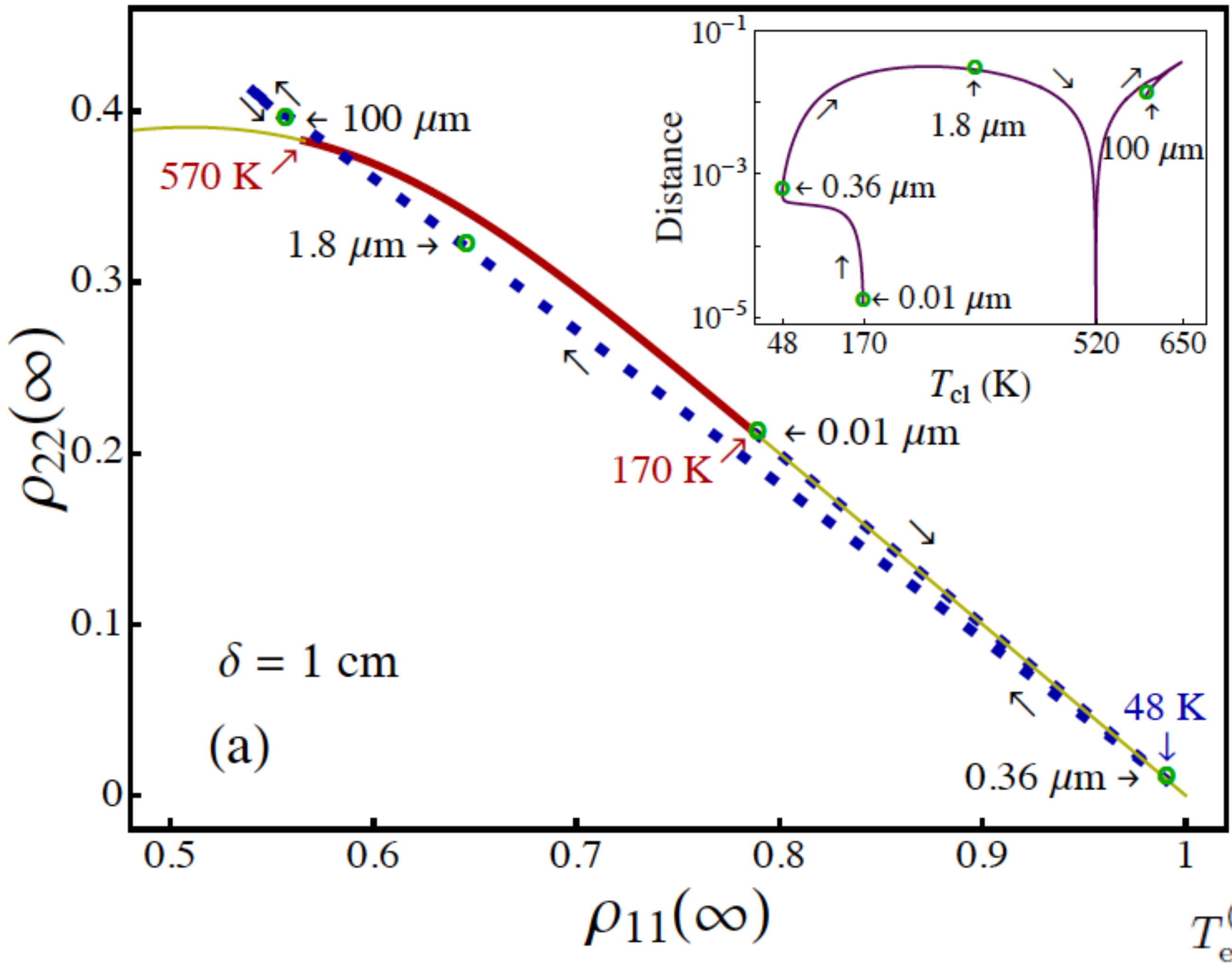


Figure 9: (color online). Steady populations (red solid line for $\rho_{11}(\infty)$, green dashed line for $\rho_{22}(\infty)$, purple dot-dashed line for $\rho_{33}(\infty)$) as a function of z for $\delta = 0.01\,\mu$m (a) and $\delta = 2\,\mu$m (b), being $(T_{\mathrm{W}}, T_{\mathrm{M}}) = (300, 50)\,$K, $\omega_{32} = 1.02\,\omega_r$ and $\omega_{31} = \omega_p$. Density plot of purity as a function of the two frequencies ω_{32} and ω_{31} for $z = 0.47\,\mu$m, $\delta = 0.01\,\mu$m (c) and $\delta = 2\,\mu$m (d). The black dotted lines correspond to ω_r and ω_p and highlight the zones where high values of purity are obtainable.

Atomic cooling out of thermal equilibrium



$\omega_{32} = \omega_r$, $\omega_{31} = \omega_p$

Thermal state : solid line

170 K < T < 570 K: red thick line

T<170 K and T>570 K: yellow thinner

Inset: distance from the closest thermal state as a function of its temperature

Distance = $\sqrt{\mathrm{Tr}(\rho-\sigma)^2}$

Distances between thermal states differing of 1 K, respectively at T = 48 K, 170K and 570K are: 1.3×10^{-3}; 1.8×10^{-3}; 3.4×10^{-4}.

Blue dotted line:
T_W = 570 K and T_M = 170 K

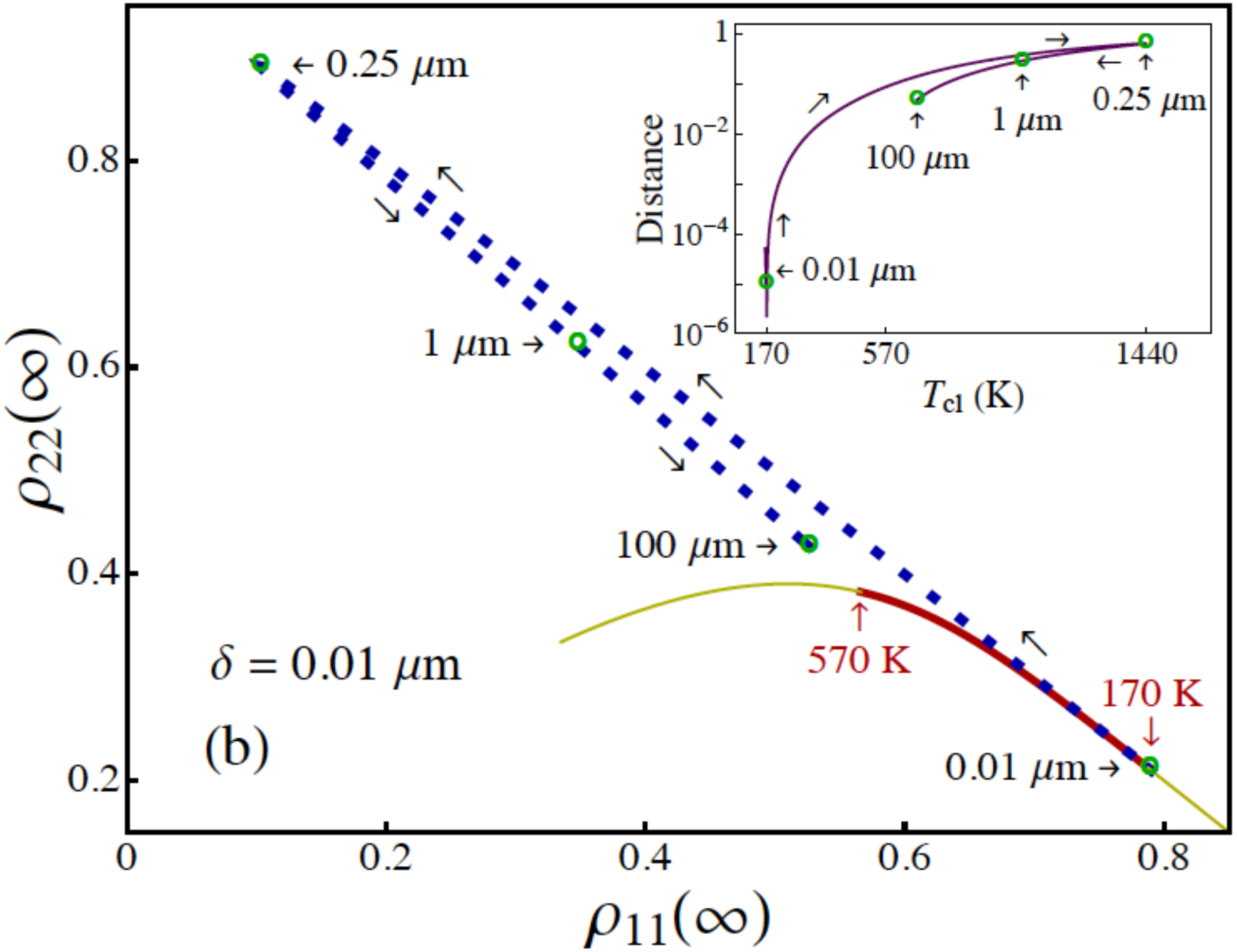
Strong dependence on z, δ, ε(ω)

at $z = 0.36\,\mu$m

$$T_{\rm eff}^{(32)} \approx 390\,\mathrm{K} \gg T_{\rm eff}^{(31)} \approx 178\,\mathrm{K}$$

Remarkable effect: starting from equilibrium configuration, by increasing the environmental temperature the atomic temperature can be decreased

Non-thermal states out of thermal-equilibrium



$\omega_{32} = \omega_r$, $\omega_{31} = \omega_p$

Thermal state : solid line

170 K < T < 570 K: red thick line

T<170 K and T>570 K: yellow thinner

Inset: distance from the closest thermal state as a function of its temperature.

Distance = $\sqrt{\mathrm{Tr}(\rho-\sigma)^2}$

Blue dotted line:

T_E = 570 K and T_M = 170 K

Strong dependence from z, δ, ε(ω)

One can exploit out of equilibrium configurations to obtain values for the steady populations very far from the ones at equilibrium

Conclusions

We have investigated **dynamics, lifetimes and thermalization mechanism of an elementary quantum system** (real or artificial atoms) interacting with a radiation **field out of thermal equilibrium**

We have shown that configurations out of thermal equilibrium can be exploited to obtain a **large variety of steady states, both thermal and non-thermal**, with populations that **can significantly differ** from their corresponding values at thermal equilibrium. Strong dependence on **atom-body distance, body geometry, dielectric response of the body and temperatures**

Three-levels: **Unexpected behaviors** such as ordering **inversion of the population** of the two lowest-energy atomic states can occur. We also predict a **new atomic-cooling mechanism based on steady configurations without any additional external laser source**

Our predictions suggest a **mechanism to produce and control, through the modification of external parameters, a variety of atomic states** which are stationary and obtained without any external laser source

Possible experimental tests ?