Thermodynamics of atoms in non-trivial environments

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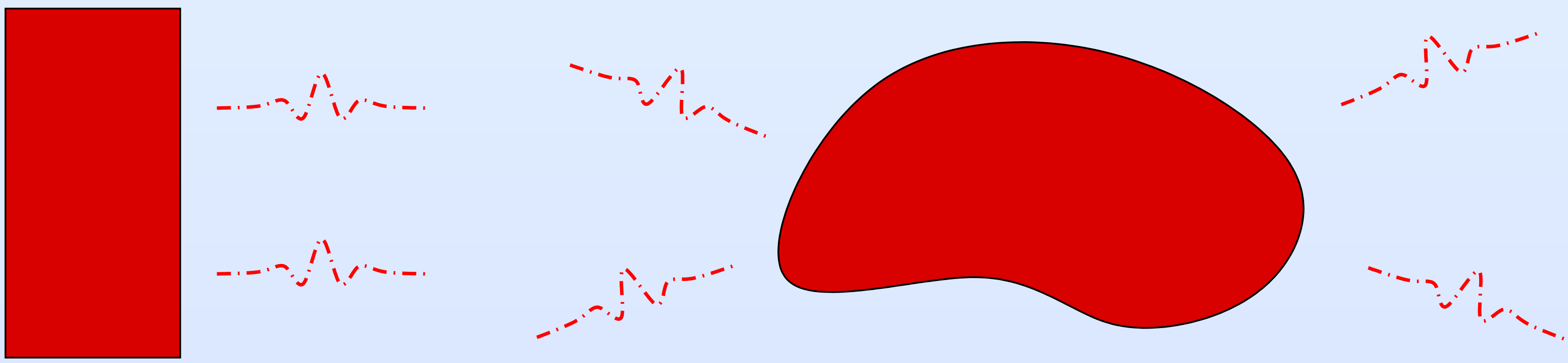
Content

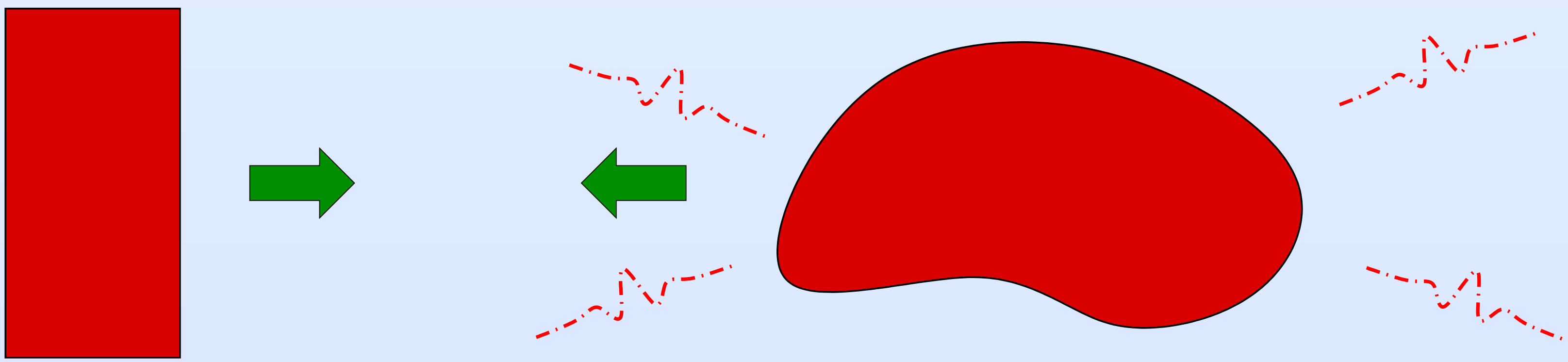
QED effects: Zero vs finite temperature



Zero temperature:

- $\langle \hat{\boldsymbol{E}}^2 \rangle_0 \neq 0$

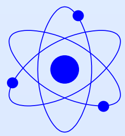
QED effects: Zero vs finite temperature

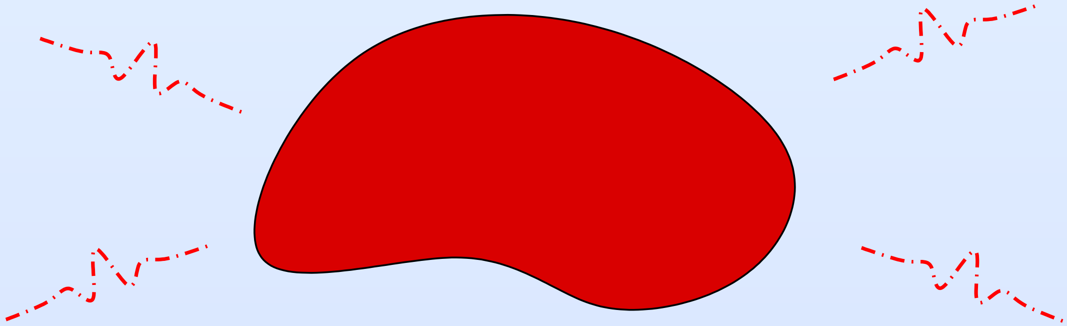


Zero temperature:

- $\langle \hat{\boldsymbol{E}}^2 \rangle_0 \neq 0 \;\; \rightarrow$ Casimir force

QED effects: Zero vs finite temperature

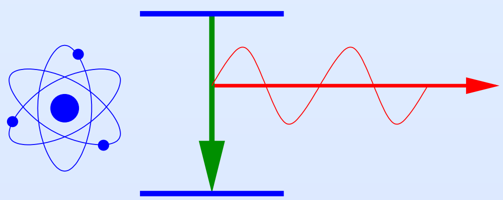


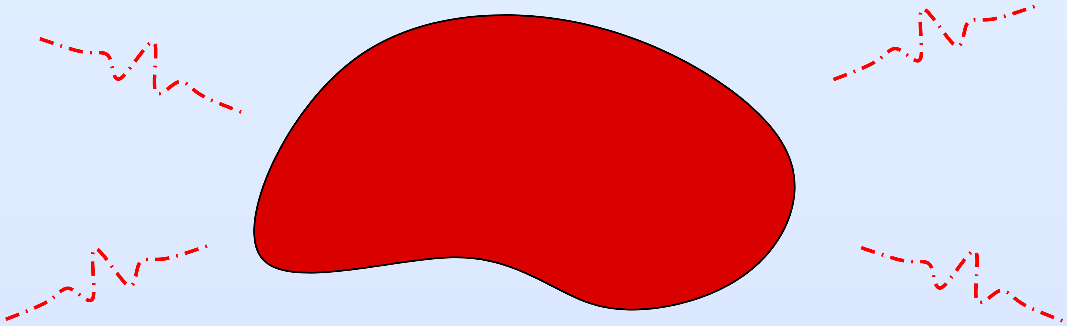


Zero temperature:

- $\langle \hat{\boldsymbol{E}}^2 \rangle_0 \neq 0 \;\; \rightarrow$ Casimir force
- Excited atom

QED effects: Zero vs finite temperature

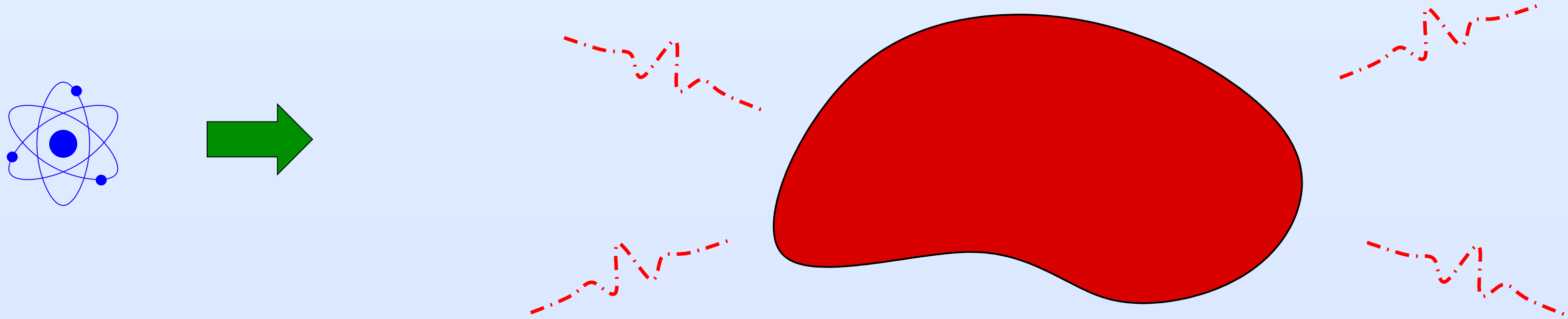




Zero temperature:

- $\langle \hat{\boldsymbol{E}}^2 \rangle_0 \neq 0$ → Casimir force
- Excited atom → Spontaneous emission

QED effects: Zero vs finite temperature



Zero temperature:

- $\langle \hat{\boldsymbol{E}}^2 \rangle_0 \neq 0$ $\rightarrow$ Casimir force
- Excited atom $\rightarrow$ Spontaneous emission
- $\langle \hat{\boldsymbol{E}}^2 \rangle_0 \neq 0$, $\langle \hat{\boldsymbol{d}}^2 \rangle \neq 0$ $\rightarrow$ Casimir–Polder force

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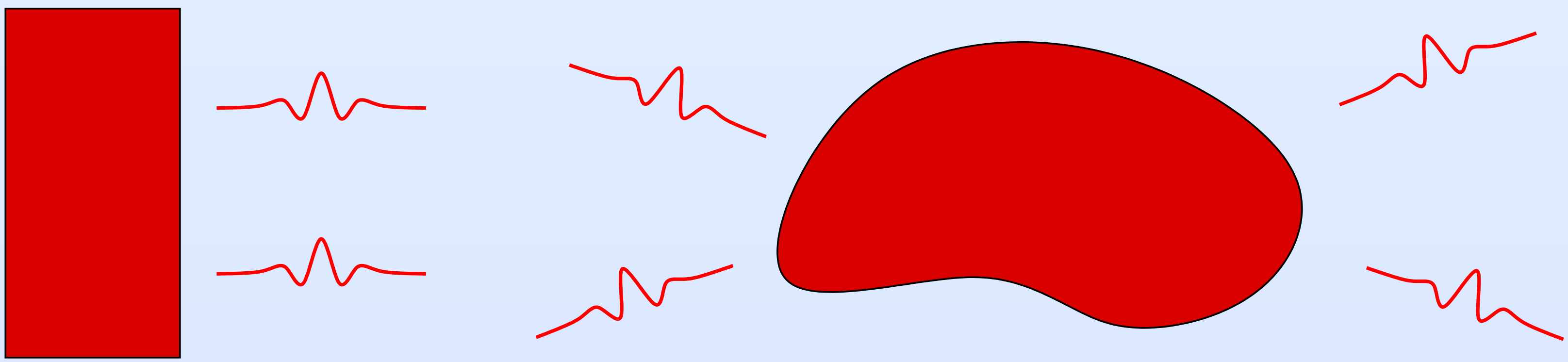

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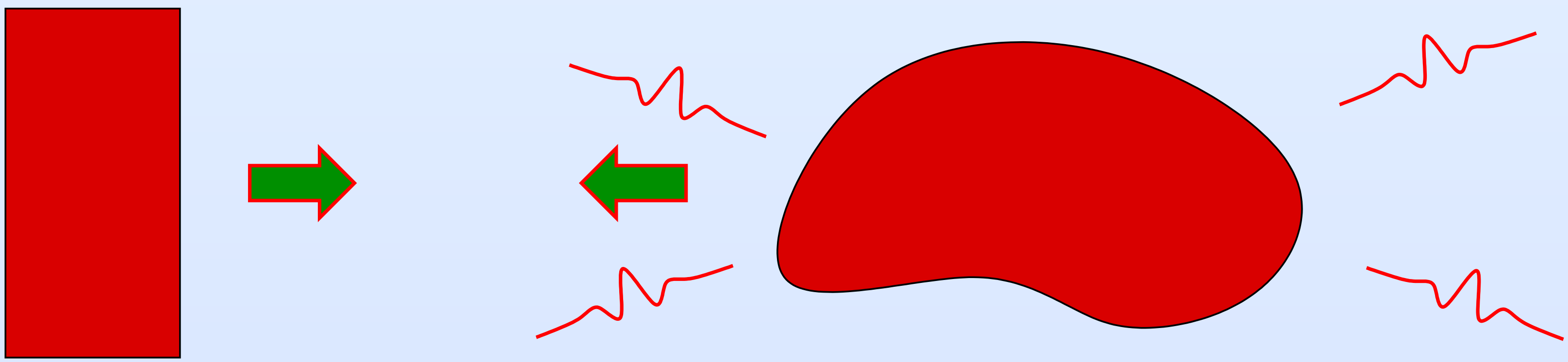
Finite temperature:

- $\langle \hat{\boldsymbol{E}}^2 \rangle_T \neq 0$

QED effects: Zero vs finite temperature



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- $\langle \hat{\boldsymbol{E}}^2 \rangle_T \neq 0$ $\rightarrow$ Thermal Casimir force

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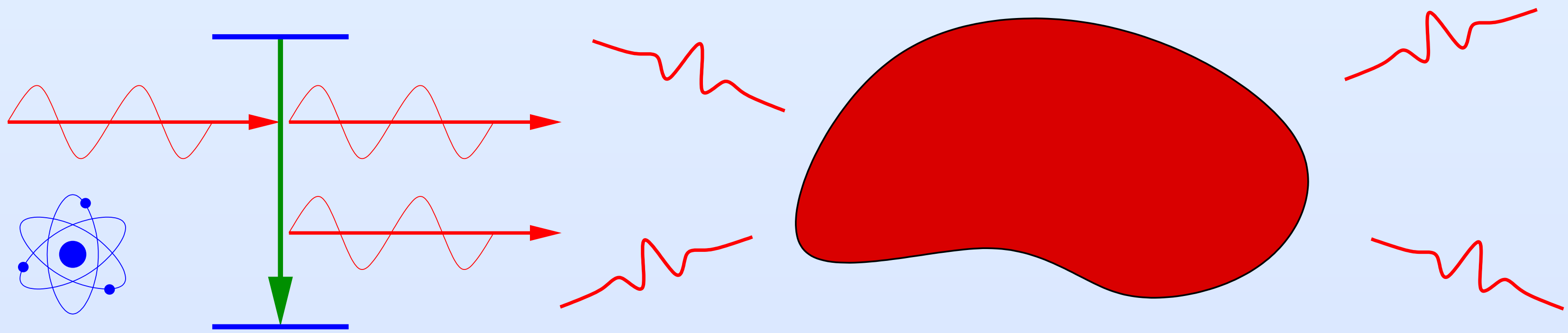

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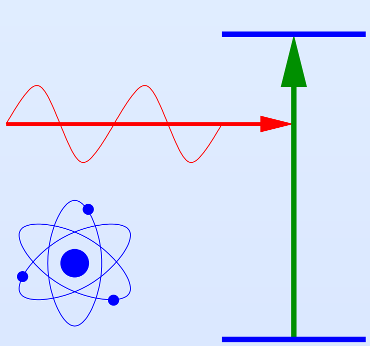
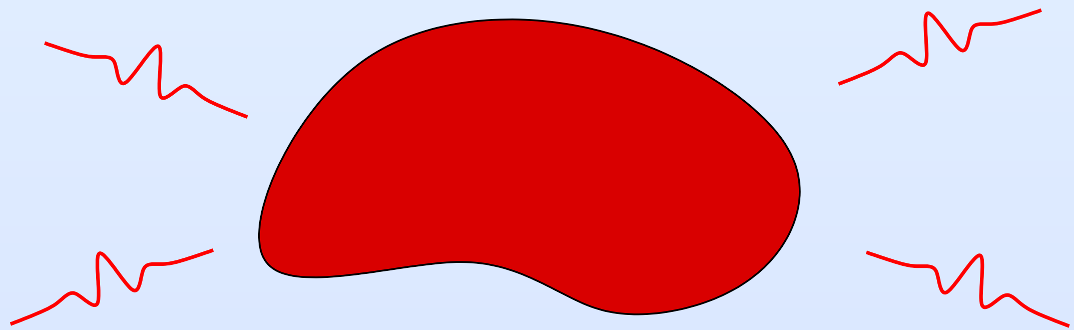
Finite temperature:

- $\langle \hat{\boldsymbol{E}}^2 \rangle_T \neq 0$ $\rightarrow$ Thermal Casimir force
- Nonequilibrium atom $\rightarrow$ (Stimulated) emission,

QED effects: Zero vs finite temperature





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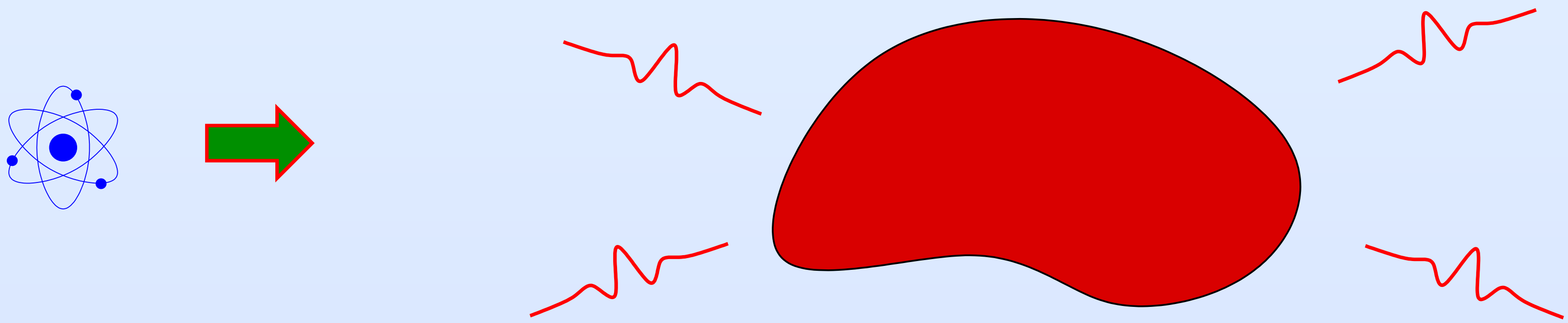
- Nonequilibrium atom $\rightarrow$ (Stimulated) emission, absorption

QED effects: Zero vs finite temperature



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- $\langle \hat{\boldsymbol{E}}^2 \rangle_T \neq 0$, $\langle \hat{\boldsymbol{d}}^2 \rangle \neq 0 \to$ Thermal Casimir–Polder force

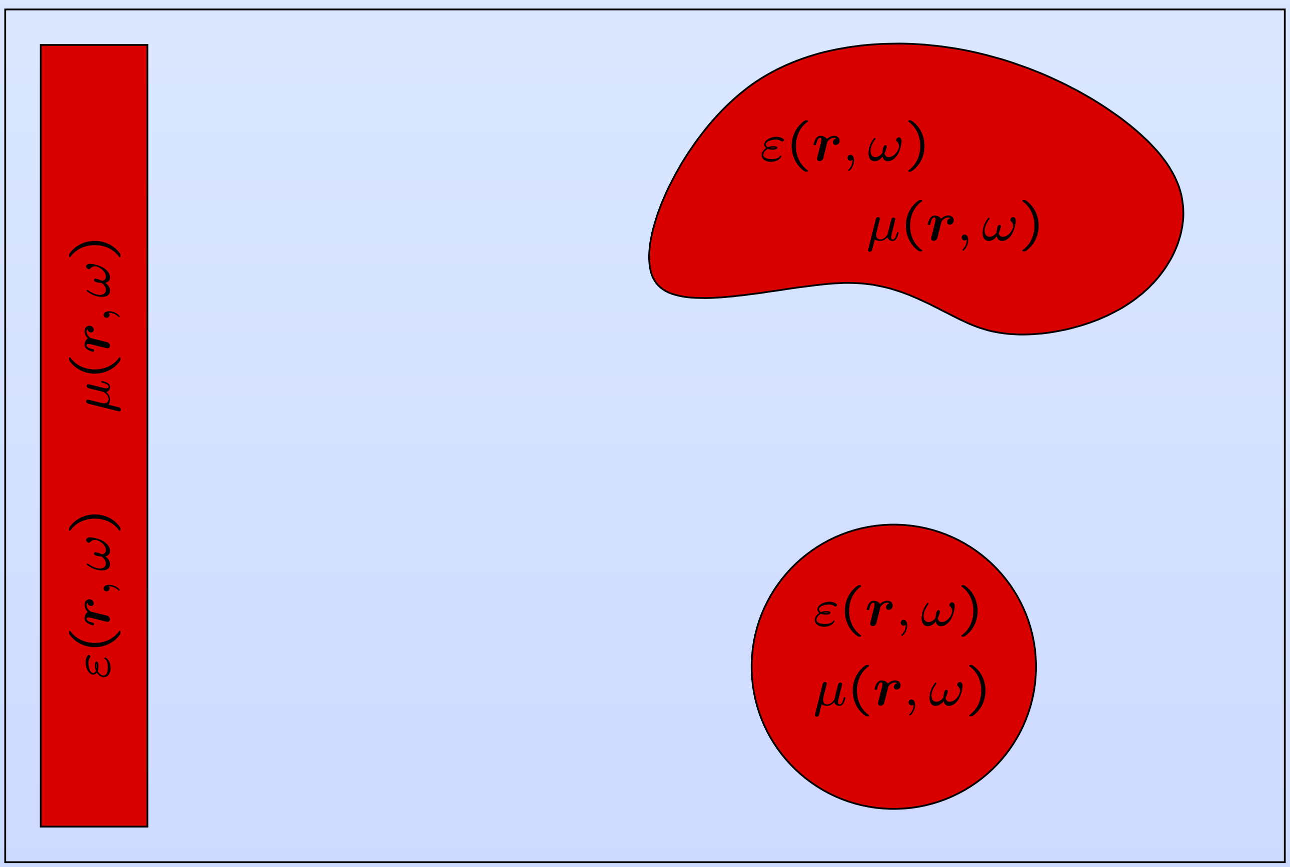
Theoretic background:

Macroscopic QED

Field quantisation

Green tensor of macroscopic Maxwell equations:

$$\left[\boldsymbol{\nabla}\times\frac{1}{\mu(\boldsymbol{r},\omega)}\boldsymbol{\nabla}\times-\frac{\omega^2}{c^2}\varepsilon(\boldsymbol{r},\omega)\right]\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)=\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')$$



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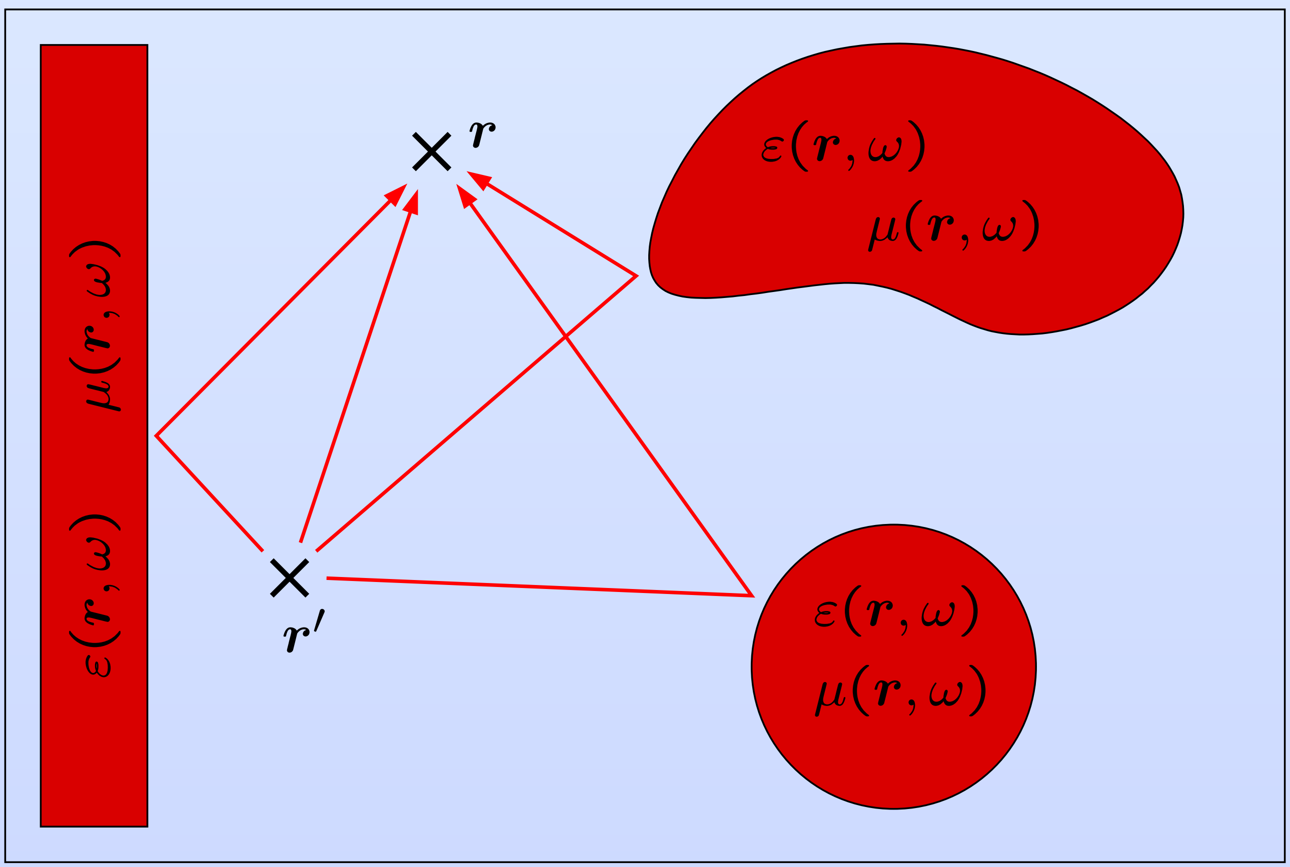
Physical interpretation:

$$\underline{\hat{\boldsymbol{E}}}(\boldsymbol{r},\omega)=i\omega\mu_0\int\mathrm{d}^3r'\,\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)\cdot\underline{\hat{\boldsymbol{j}}}(\boldsymbol{r}',\omega)$$



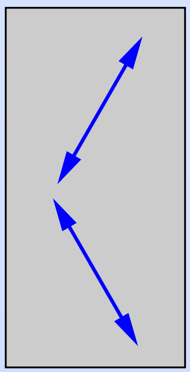
Noise current density:

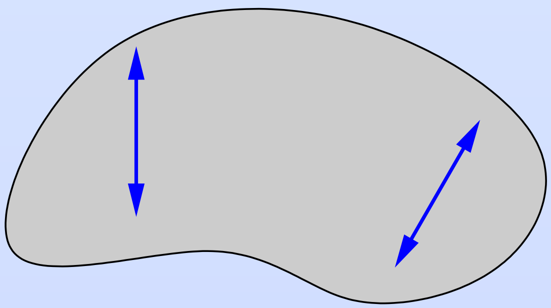
$$\underline{\hat{\boldsymbol{j}}}_{\mathsf{N}}(\boldsymbol{r},\omega) = -i\omega\underline{\hat{\boldsymbol{P}}}_{\mathsf{N}}(\boldsymbol{r},\omega) + \boldsymbol{\nabla}\times\underline{\hat{\boldsymbol{M}}}_{\mathsf{N}}(\boldsymbol{r},\omega)$$

$$= \omega\sqrt{\frac{\hbar\varepsilon_0}{\pi}\operatorname{Im}\varepsilon(\boldsymbol{r},\omega)}\,\hat{\boldsymbol{f}}_e(\boldsymbol{r},\omega) + \boldsymbol{\nabla}\times\sqrt{\frac{\hbar}{\mu_0\pi}\frac{\operatorname{Im}\mu(\boldsymbol{r},\omega)}{|\mu(\boldsymbol{r},\omega)|^2}}\,\hat{\boldsymbol{f}}_m(\boldsymbol{r},\omega)$$

Bosonic dynamical variables:

$$\left[\hat{f}_{\lambda i}(\mathbf{r},\omega),\hat{f}^{\dagger}_{\lambda' j}(\mathbf{r}',\omega')\right] = i\hbar\delta_{\lambda\lambda'}\delta_{ij}(\mathbf{r}-\mathbf{r}')\delta(\omega-\omega'), \qquad \lambda,\lambda'\in\{e,m\}$$



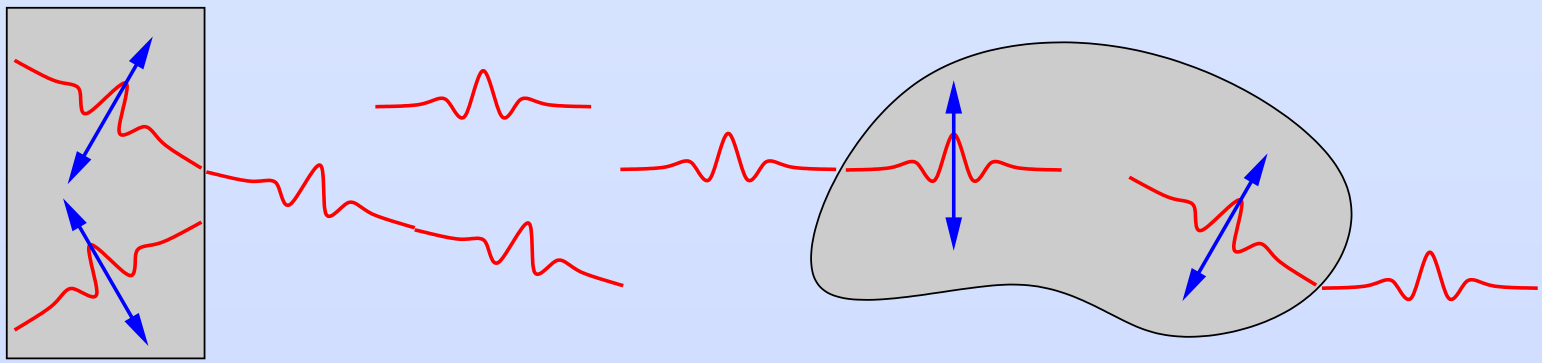


D.T. Ho, S.Y.B., J. Kästel, L. Knöll, S. Scheel, D.-G. Welsch, PRA **68**, 043816 (2003)

Quantised electric field in linear, causal media:

$$\hat{\boldsymbol{E}}(\mathbf{r}) = \sum_{\lambda=e,m} \int_0^\infty \mathrm{d}\omega \int \mathrm{d}^3 r' \, \mathbf{G}_\lambda(\boldsymbol{r}, \boldsymbol{r}', \omega) \cdot \hat{\boldsymbol{f}}_\lambda(\boldsymbol{r}', \omega) + \mathrm{H.c.}$$

$$\mathbf{G}_{e,m}(\boldsymbol{r}, \boldsymbol{r}', \omega) = \mathrm{i}\,\frac{\omega}{c}\sqrt{\frac{\hbar}{\pi\varepsilon_0}} \times \begin{cases} \frac{\omega}{c}\sqrt{\mathrm{Im}\,\varepsilon(\boldsymbol{r}', \omega)}\,\mathbf{G}(\boldsymbol{r}, \boldsymbol{r}', \omega) \\ \sqrt{\frac{\mathrm{Im}\,\mu(\boldsymbol{r}', \omega)}{|\mu(\boldsymbol{r}', \omega)|^2}}\left[\boldsymbol{\nabla}' \times \mathbf{G}(\boldsymbol{r}', \boldsymbol{r}, \omega)\right]^{\mathsf{T}} \end{cases}$$



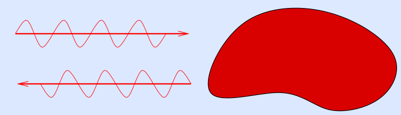
D.T. Ho, S.Y.B., J. Kästel, L. Knöll, S. Scheel, D.-G. Welsch, PRA **68**, 043816 (2003)

Hamiltonian

$$\boxed{\hat{H} = \hat{H}_{\mathsf{F}} + \hat{H}_{\mathsf{A}} + \hat{H}_{\mathsf{AF}}}$$

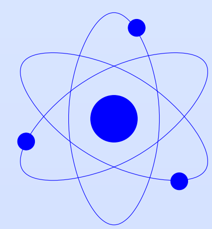
Body–field Hamiltonian:

$$\hat{H}_{\mathsf{F}} = \sum_{\lambda=e,m} \int \mathrm{d}^3 r \int_0^\infty \mathrm{d}\omega\, \hbar\omega\, \hat{\boldsymbol{f}}_\lambda^\dagger(\boldsymbol{r},\omega)\cdot\hat{\boldsymbol{f}}_\lambda(\boldsymbol{r},\omega)$$



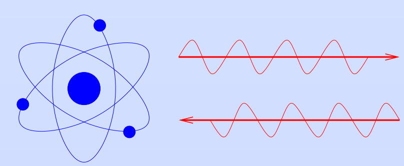
Atomic Hamiltonian:

$$\hat{H}_{\mathsf{A}} = \sum_\alpha \frac{\hat{\boldsymbol{p}}_\alpha^2}{2m_\alpha} + \frac{1}{2\varepsilon_0}\int \mathrm{d}^3 r \hat{\boldsymbol{P}}_{\mathsf{A}}^2(\boldsymbol{r})$$



Electric-dipole interaction:

$$\hat{H}_{\mathsf{AF}} = -\hat{\boldsymbol{d}}\cdot\hat{\boldsymbol{E}}(\boldsymbol{r}_{\mathsf{A}})$$



S.Y.B., D.T. Ho, L. Knöll, D.-G. Welsch, PRA **70**, 052117 (2004)

Imperial College London

Thermal Fields

Thermal density matrix: $\hat{\rho}_T = \dfrac{\mathrm{e}^{-\hat{H}_\mathsf{F}/(k_\mathrm{B}T)}}{\mathrm{tr}[\mathrm{e}^{-\hat{H}_\mathsf{F}/(k_\mathrm{B}T)}]}$

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Dynamical variables: $n(\omega) = \frac{1}{\mathrm{e}^{\hbar\omega/(k_{\mathsf{B}}T)} - 1}$

$$\left\langle \hat{\boldsymbol{f}}_\lambda^\dagger(\boldsymbol{r},\omega)\hat{\boldsymbol{f}}_{\lambda'}(\boldsymbol{r}',\omega')\right\rangle = n(\omega)\delta_{\lambda\lambda'}\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')\delta(\omega-\omega')$$

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Fluctuation–Dissipation theorem:

$$\left\langle \tfrac{1}{2}\Big[\Delta\hat{\boldsymbol{P}}_\mathsf{N}(\boldsymbol{r},\omega)\Delta\hat{\boldsymbol{P}}^\dagger_\mathsf{N}(\boldsymbol{r}',\omega')\Big]_+\right\rangle = c(\omega,\omega')\,\mathrm{Im}[\varepsilon_0\varepsilon(\boldsymbol{r},\omega)]\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')$$

$$\left\langle \tfrac{1}{2}\Big[\langle\Delta\hat{\boldsymbol{M}}_\mathsf{N}(\boldsymbol{r},\omega)\Delta\hat{\boldsymbol{M}}^\dagger_\mathsf{N}(\boldsymbol{r}',\omega')\Big]_+\right\rangle = c(\omega,\omega')\,\mathrm{Im}[\kappa_0\kappa(\boldsymbol{r},\omega)]\boldsymbol{\delta}(\boldsymbol{r}-\boldsymbol{r}')$$

$$\left\langle \tfrac{1}{2}\Big[\Delta\hat{\boldsymbol{E}}(\boldsymbol{r},\omega)\Delta\hat{\boldsymbol{E}}^\dagger(\boldsymbol{r}',\omega')\Big]_+\right\rangle_T = c(\omega,\omega')\mu_0\omega^2\,\mathrm{Im}\,\mathbf{G}(\boldsymbol{r},\boldsymbol{r}',\omega)$$

$$c(\omega,\omega') = \frac{\hbar}{2\pi}\Big[n(\omega)+\tfrac{1}{2}\Big]\delta(\omega-\omega')$$

Atomic dynamics

Transition rates at finite temperature

Coupled atom–field dynamics: $\hat{A}_{mn} = |m\rangle\langle n|$, $\hat{\boldsymbol{f}}_\lambda(\boldsymbol{r},\omega)$

$$\dot{\hat{A}}_{mn} = \mathrm{i}\omega_{mn}\hat{A}_{mn} + \frac{\mathrm{i}}{\hbar}\sum_k\sum_\lambda\int \mathrm{d}^3r\int_0^\infty \mathrm{d}\omega\Big(\boldsymbol{d}_{nk}\hat{A}_{mk} - \boldsymbol{d}_{km}\hat{A}_{kn}\Big)\cdot\Big[\mathbf{G}_\lambda(\boldsymbol{r}_A,\boldsymbol{r},\omega)\cdot\hat{\boldsymbol{f}}_\lambda(\boldsymbol{r},\omega) + \mathrm{H.\,c.}\Big]$$

$$\dot{\hat{\boldsymbol{f}}}_\lambda(\boldsymbol{r},\omega) = -\mathrm{i}\omega\hat{\boldsymbol{f}}_\lambda(\boldsymbol{r},\omega) + \frac{\mathrm{i}}{\hbar}\sum_{m,n}\boldsymbol{d}_{mn}\cdot\mathbf{G}^*_\lambda(\boldsymbol{r}_A,\boldsymbol{r},\omega)\hat{A}_{mn}$$

Solve: Eliminate field, Markov approximation, $\langle\hat{A}_{mn}\rangle = \sigma_{nm}$

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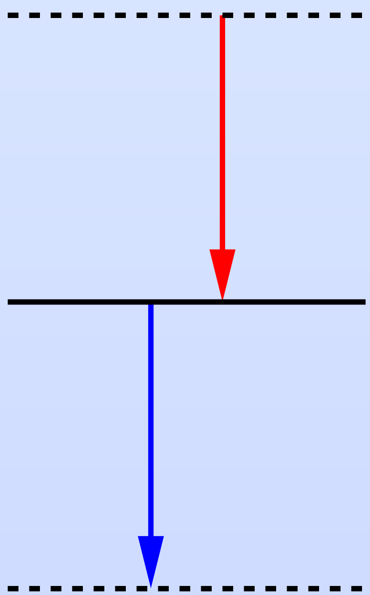
Zero temperature:

$$\dot{\sigma}_{mm} = -\sum_{k<m}\Gamma_{mk}\sigma_{mm} + \sum_{k>m}\Gamma_{km}\sigma_{kk}$$

$$\Gamma_{mk} = \frac{2\mu_0}{\hbar}\,\tilde{\omega}^2_{mk}\boldsymbol{d}_{mk}\cdot\mathrm{Im}\,\mathbf{G}(\boldsymbol{r}_A,\boldsymbol{r}_A,\tilde{\omega}_{mk})\cdot\boldsymbol{d}_{km}$$



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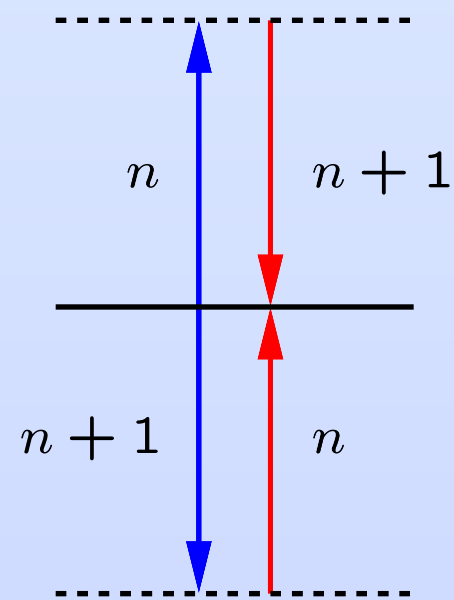

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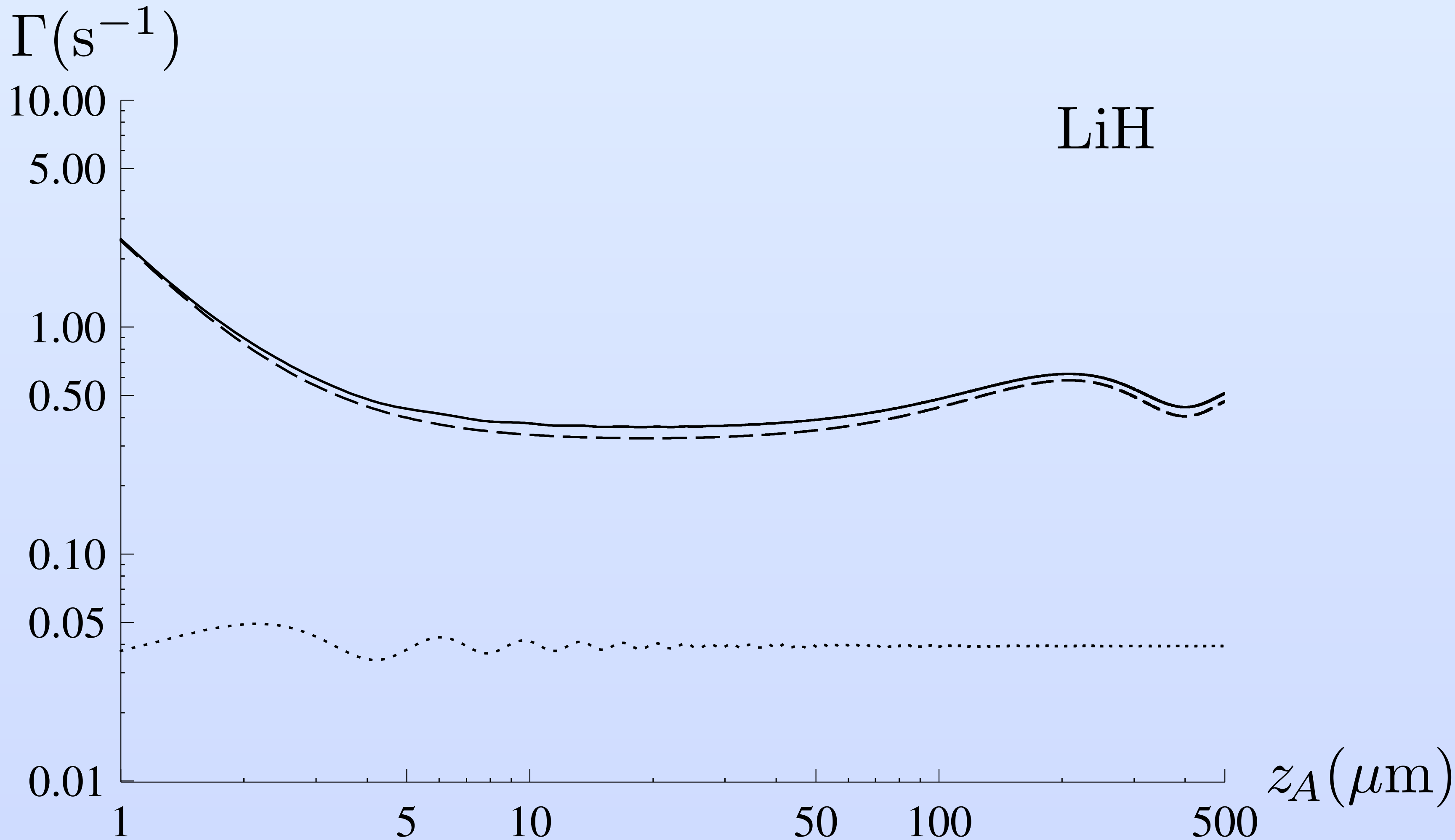
Steady state: $\sigma_{T,mm} = \mathrm{e}^{-\tilde{E}_m/(k_\mathrm{B}T)}\Big/\Big[\sum_k \mathrm{e}^{-\tilde{E}_k/(k_\mathrm{B}T)}\Big]$

Example: Heating of polar molecules

Scenario: Ground-state molecule at distance z_A from gold surface at $T = 273$K



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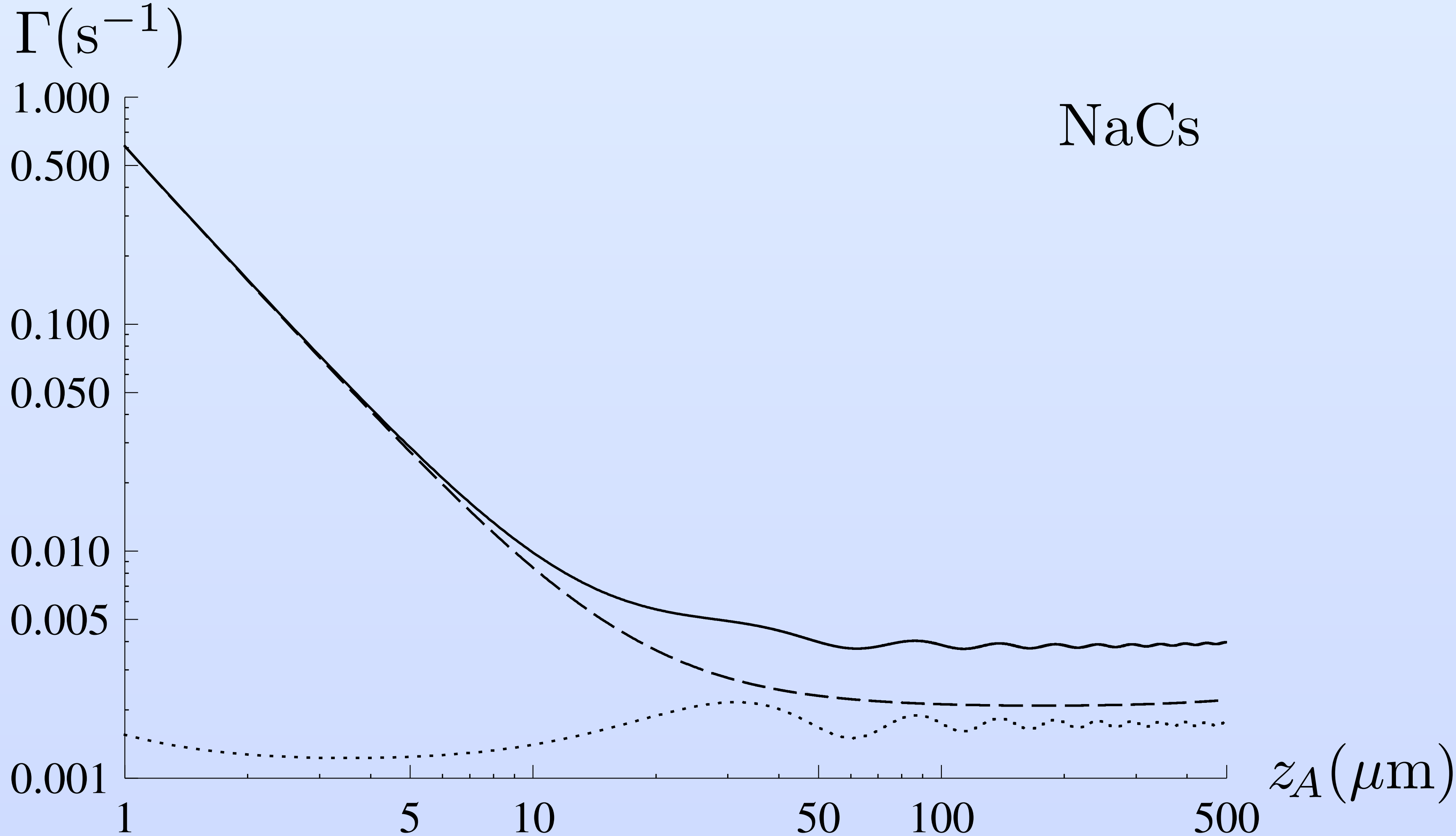
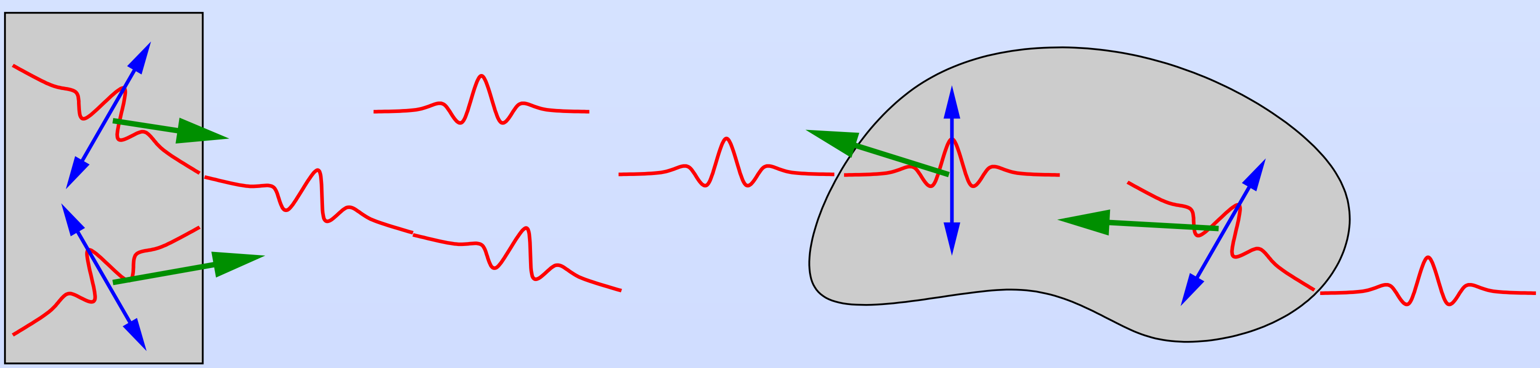


Casimir–Polder force

Lifshitz Theory

Average Lorentz force: Field in thermal state $\hat{\rho}_T$

$$\boldsymbol{F} = \int_V \mathrm{d}^3 r \left\langle \hat{\rho}(\boldsymbol{r}) \hat{\boldsymbol{E}}(\boldsymbol{r}') + \hat{\boldsymbol{j}}(\boldsymbol{r}) \times \hat{\boldsymbol{B}}(\boldsymbol{r}') \right\rangle_{\boldsymbol{r}' \to \boldsymbol{r}}$$



C. Raabe, D.-G. Welsch, PRA **71**, 013814 (2005); *ibid.* **73**, 063822 (2006)

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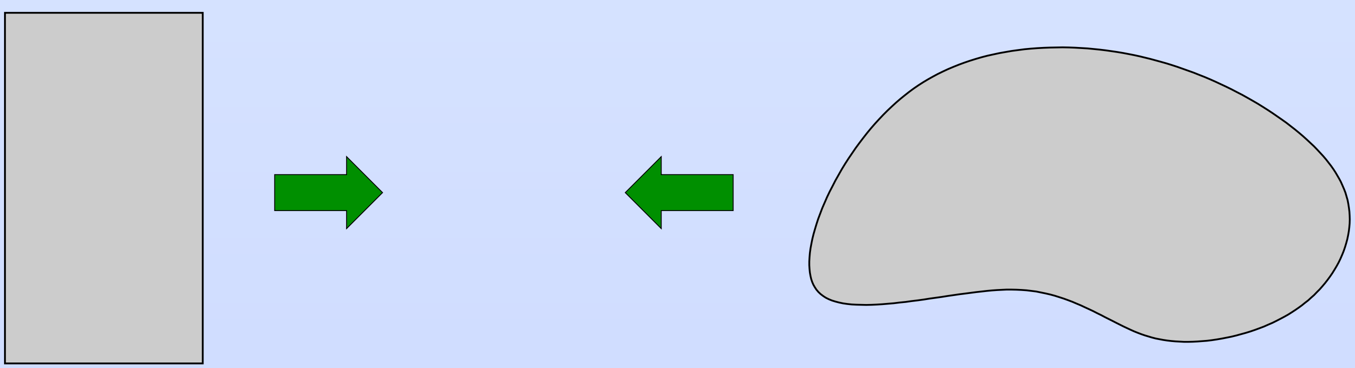
Casimir force: $\xi_N = 2\pi k_\mathrm{B} T N/\hbar$

$$\boldsymbol{F} = -2k_\mathrm{B}T \int_V \mathrm{d}^3 r \sum_N{}' \Big\{ \xi_N^2/c^2\, \boldsymbol{\nabla} \cdot \mathbf{G}^{(1)}(\boldsymbol{r}, \boldsymbol{r}, \mathrm{i}\xi_N) - \mathrm{tr}\Big[\mathbf{I} \times \Big(\boldsymbol{\nabla} \times \boldsymbol{\nabla} \times + \xi_N^2/c^2\Big) \mathbf{G}^{(1)}(\boldsymbol{r}, \boldsymbol{r}', \mathrm{i}\xi_N) \times \overleftarrow{\boldsymbol{\nabla}}'\Big]_{\boldsymbol{r}=\boldsymbol{r}'} \Big\}$$



C. Raabe, D.-G. Welsch, PRA **71**, 013814 (2005); *ibid.* **73**, 063822 (2006)

Lifshitz Theory

Average Lorentz force: Field in thermal state $\hat{\rho}_T$

$$\boldsymbol{F} = \int_V \mathrm{d}^3 r \left\langle \hat{\rho}(\boldsymbol{r}) \hat{\boldsymbol{E}}(\boldsymbol{r}') + \hat{\boldsymbol{j}}(\boldsymbol{r}) \times \hat{\boldsymbol{B}}(\boldsymbol{r}') \right\rangle_{\boldsymbol{r}' \to \boldsymbol{r}}$$

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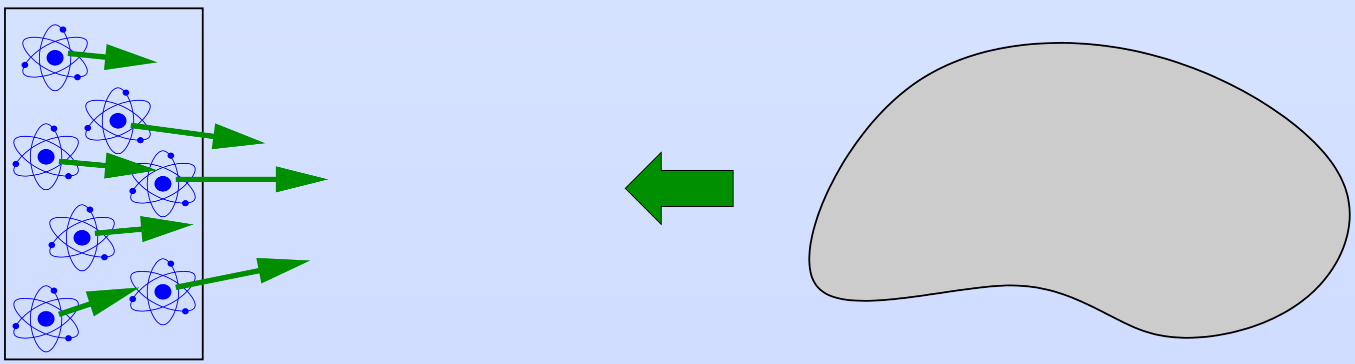

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Open questions: $\alpha = \alpha_0$? Dynamics? Resonant effects?

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Microscopic calculation

Average Lorentz force: Field in thermal state $\hat{\rho}_T$, atom in incoherent state $\hat{\sigma}$

$$\boldsymbol{F}(t) = \int_V \mathrm{d}^3 r \left\langle \hat{\rho}_A(\boldsymbol{r},t)\hat{\boldsymbol{E}}(\boldsymbol{r},t) + \hat{\boldsymbol{j}}_A(\boldsymbol{r},t) \times \hat{\boldsymbol{B}}(\boldsymbol{r},t) \right\rangle$$

S.Y.B, L. Knöll, D.-G. Welsch, Ho Trung Dung PRA **70**, 052117 (2004);
S.Y.B, S. Scheel, `quant-ph/0803.0738`

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Solve: Use atom–field dynamics (Markov approximation)

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$$\boxed{\boldsymbol{F}(\boldsymbol{r}_{\mathrm{A}},t) = \sum_m \sigma_{mm}(t)\boldsymbol{F}_m(\boldsymbol{r}_{\mathrm{A}})}$$

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Atom in eigenstate

Lifshitz result:

$$\boldsymbol{F}(\boldsymbol{r}_A) = -\mu_0 k_\mathrm{B} T \sum_N{}' \xi_N^2 \alpha(\mathrm{i}\xi_N) \boldsymbol{\nabla}_A \,\mathrm{tr}\, \mathbf{G}^{(1)}(\boldsymbol{r}_A, \boldsymbol{r}_A, \mathrm{i}\xi_N)$$

S.Y.B, S. Scheel, `quant-ph/0803.0738`

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Macroscopic result: $\hat{\sigma}(t_0) = |m\rangle\langle m|$, perturbative limit

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$$+ \frac{\mu_0}{3} \sum_{k<m} \omega_{mk}^2 [n(\omega_{mk}) + 1] |\boldsymbol{d}_{mk}|^2 \boldsymbol{\nabla}_A \operatorname{tr} \operatorname{Re} \mathbf{G}^{(1)}(\boldsymbol{r}_A, \boldsymbol{r}_A, \omega_{mk})$$

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Polarisability: $\alpha_m(\omega) = \lim_{\epsilon \to 0} \frac{2}{3\hbar} \sum_k \frac{\omega_{km} |\boldsymbol{d}_{mk}|^2}{\omega_{km}^2 - \omega^2 - \mathrm{i}\omega\epsilon}$

Resonant forces: Photon emission/absorption, opposite sign, different distance dependence

$\Rightarrow$ **Possible deviation from Lifshitz result!**

S.Y.B, S. Scheel, `quant-ph/0803.0738`

Fully thermalised atom

Steady-state force: $\hat{\sigma}(t \to \infty) = \hat{\sigma}_T$

$\to$ Cancellation of resonant forces

$$\boldsymbol{F}(\boldsymbol{r}_A, t \to \infty) = -\mu_0 k_\mathrm{B} T {\sum_N}' \xi_N^2 \alpha_T(\mathrm{i}\xi_N) \boldsymbol{\nabla}_A \operatorname{tr} \mathbf{G}^{(1)}(\boldsymbol{r}_A, \boldsymbol{r}_A, \mathrm{i}\xi_N)$$

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Polarisability: $\alpha_T(\omega) = \sum_m \sigma_{T,mm} \alpha_m(\omega)$

Resonant forces: Non-equilibrium effect

$\Rightarrow$ **Agreement with Lifshitz result if correctly intepreted!**

S.Y.B, S. Scheel, `quant-ph/0803.0738`

Summary

Atomic dynamics

- *Transition rates* for emission ($\propto n+1$) and absorption ($\propto n$)
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