The multipolar hamiltonian to model quantum metamaterials in the visible range

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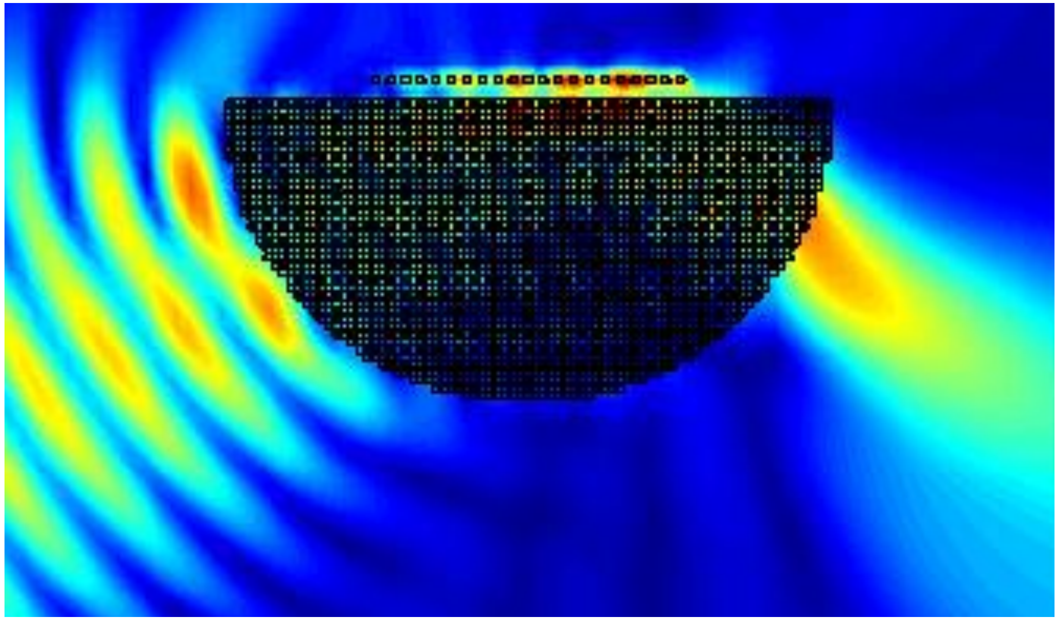

Quantum metamaterials
& quantum technology workshop
Spetses – Greece – 20th-25th of june 2016

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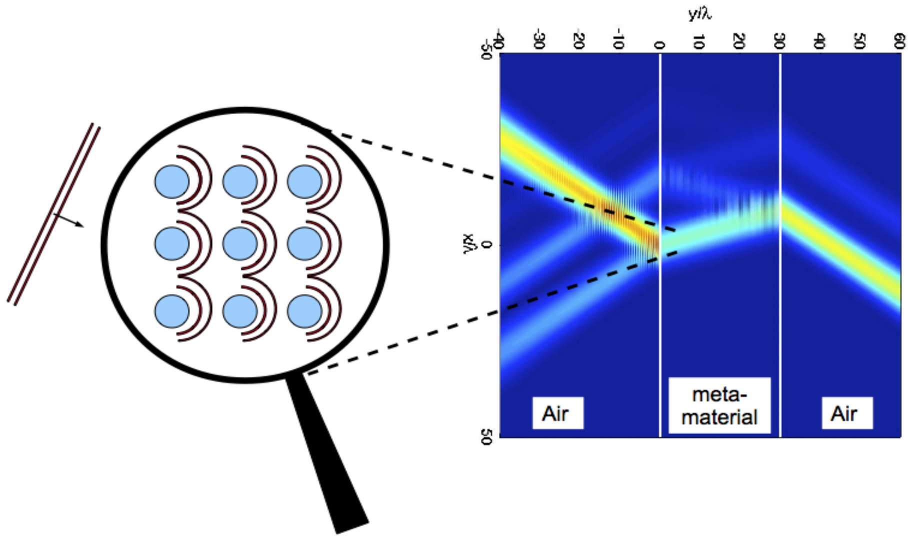
Metamaterials = effective properties



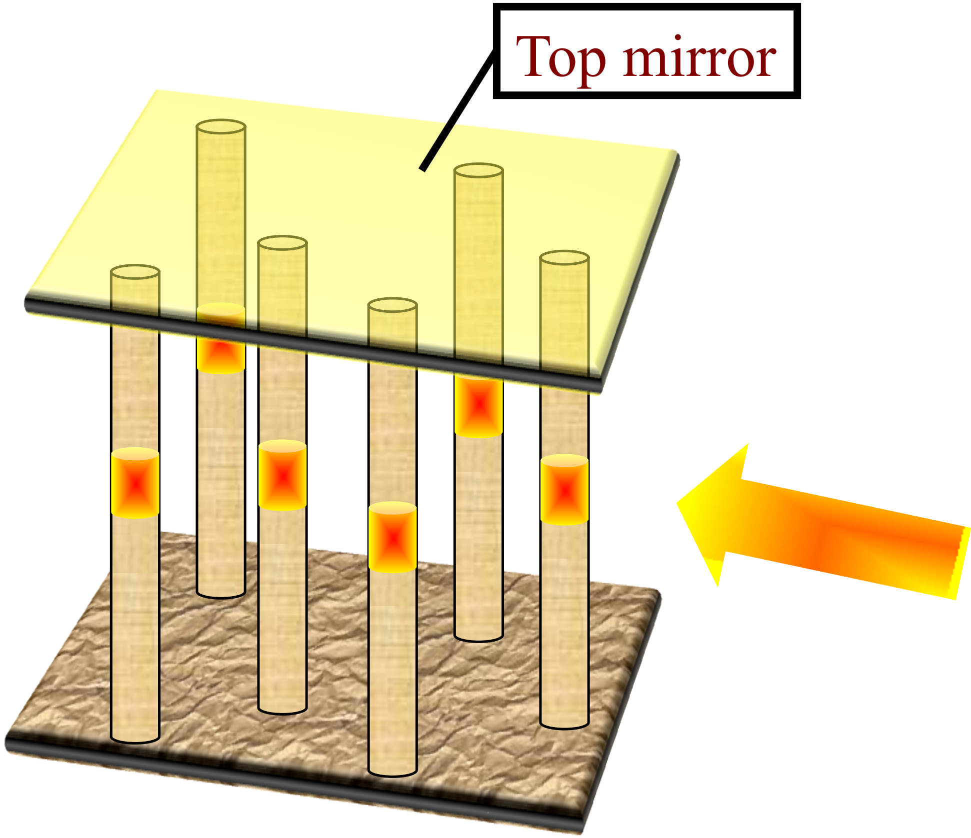
Heterogeneous materials :
@ microscopic scale $d \ll \lambda$

Appear like an homogeneous medium
@ macroscopic scale

with *effective* optical properties
That result from collective effects
@ microscopic scale

Not found in Nature:
Negative permeability @ the optical frequencies
=> Good but not required.

Dielectric metamaterials with quantum dots



Metamaterials based on:
Dielectric cylinders
(periodic shaping or not)

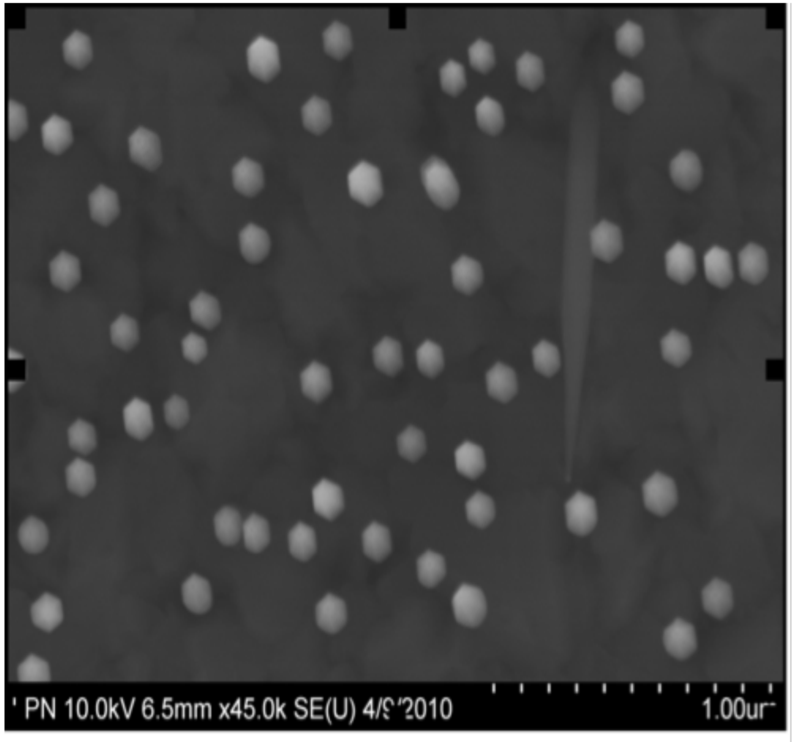
Quantum metamaterials:
Quantum dots

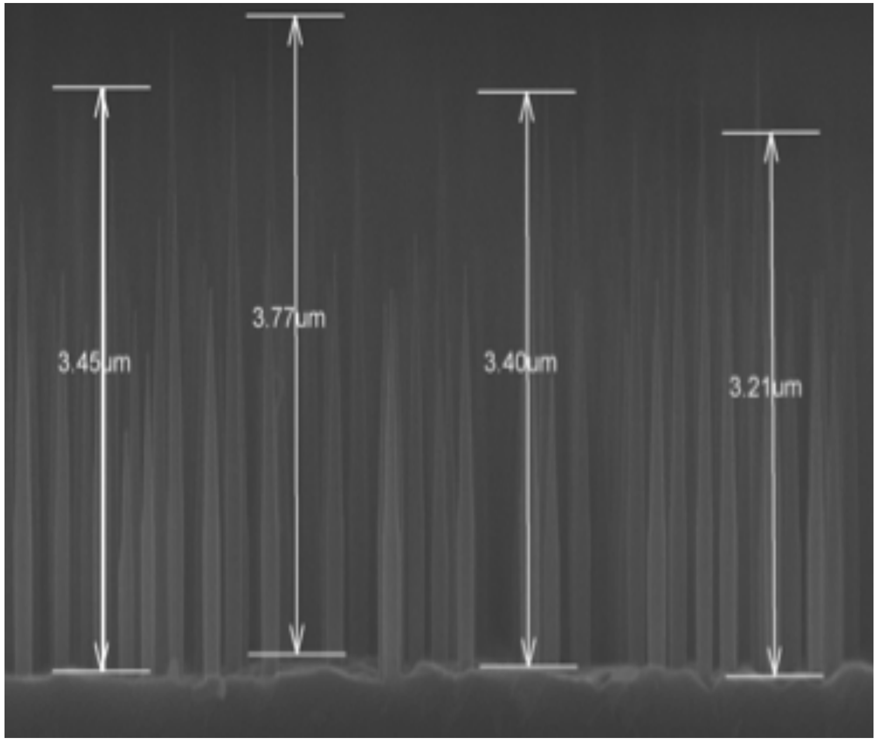
=> How Quantum dots modify light propagation?

Simplifications:
2D geometry
spatial confinement

InP nanowires growth: J. C Harmand (LPN)

A possible realisation

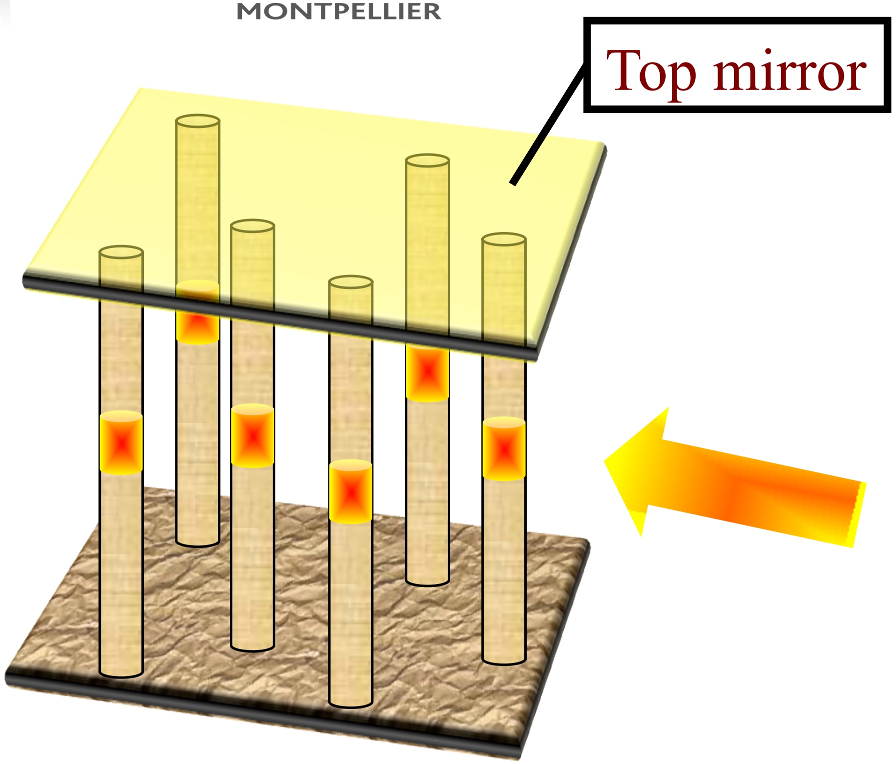


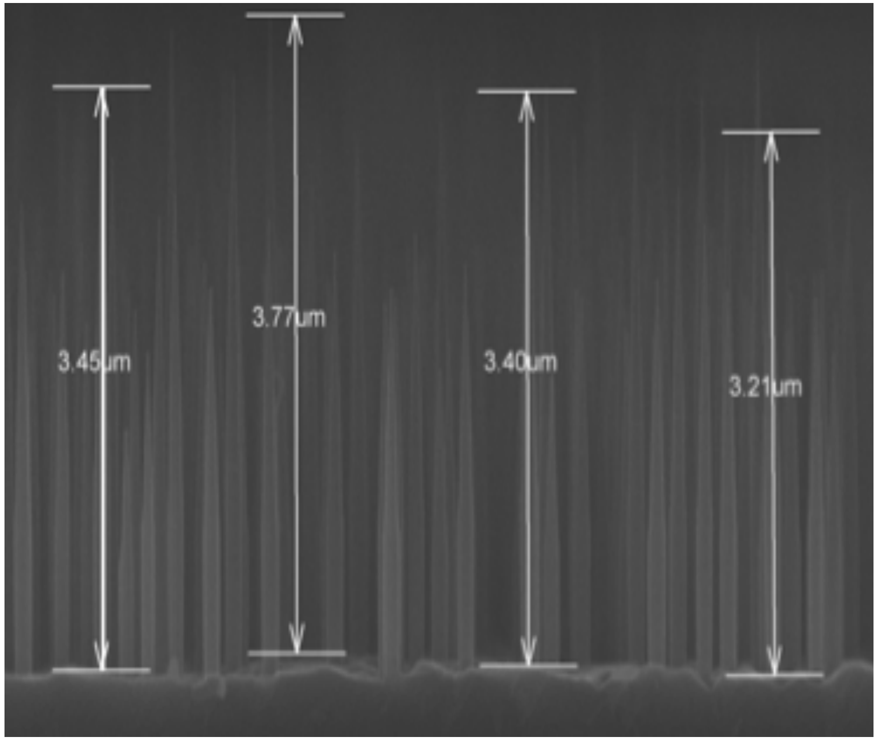


Nanorods: InP refractive index ~3.17 @ 1.5 µm

Quantum dots: InAsP the emitting wavelength is in the near-IR ~1.5 µm

InP nanowires growth: J. C Harmand (LPN)





Diameters: ~ 100 nm +/- 10 nm but can be adjusted from 50 nm to 500 nm during growth

Length: ~ 3 – 4 µm *up to 10 µm*

Defaults free = very good optical properties

Random or periodic arrangement

Encapsulated in resist, top metallic mirror

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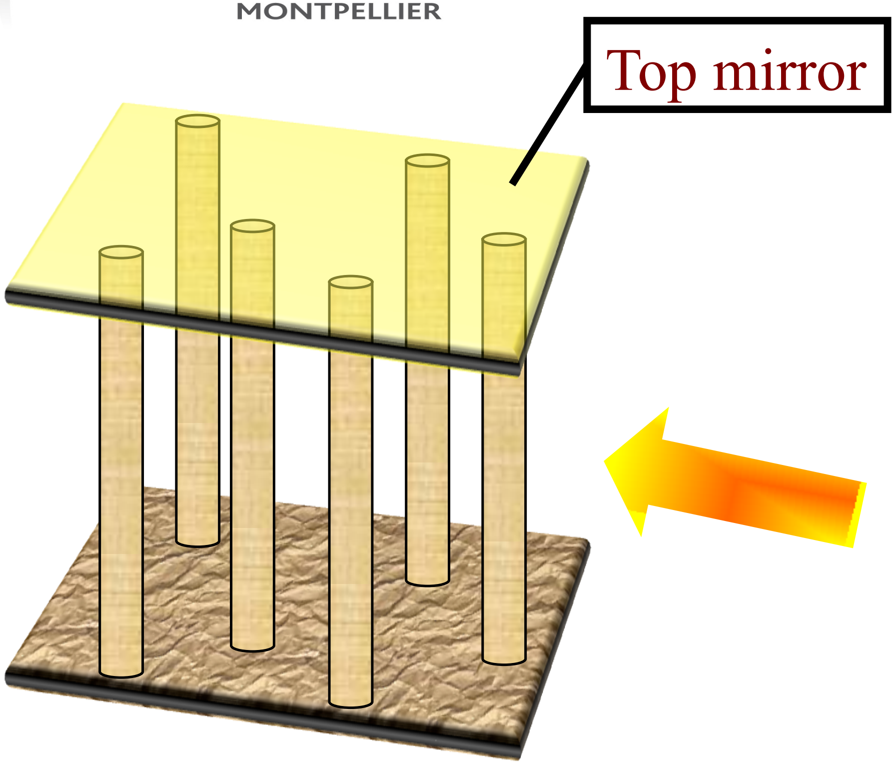
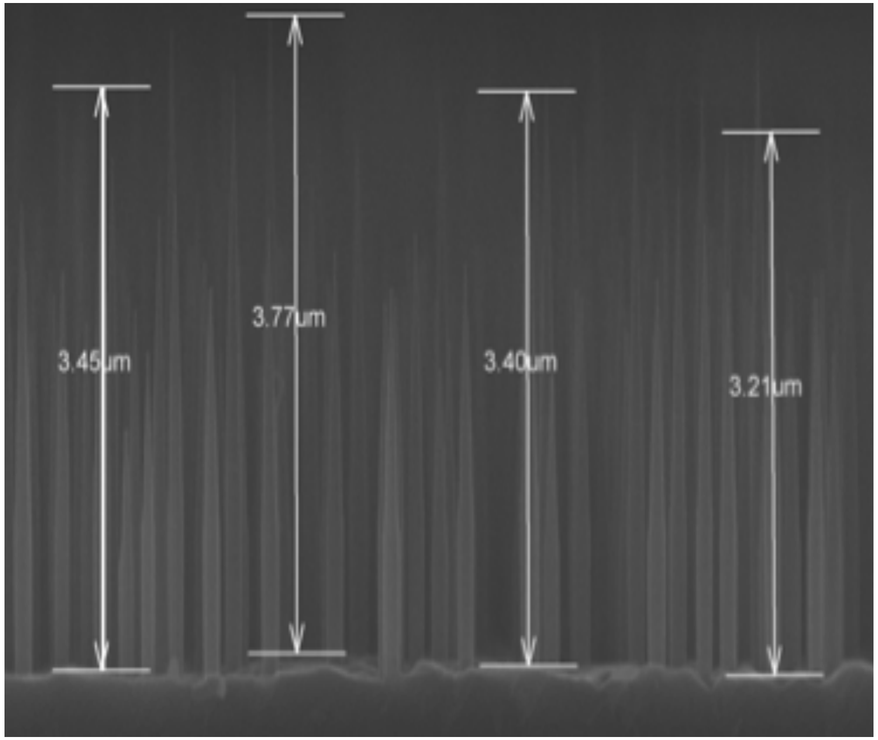
« Classical » metamaterials: effective optical properties

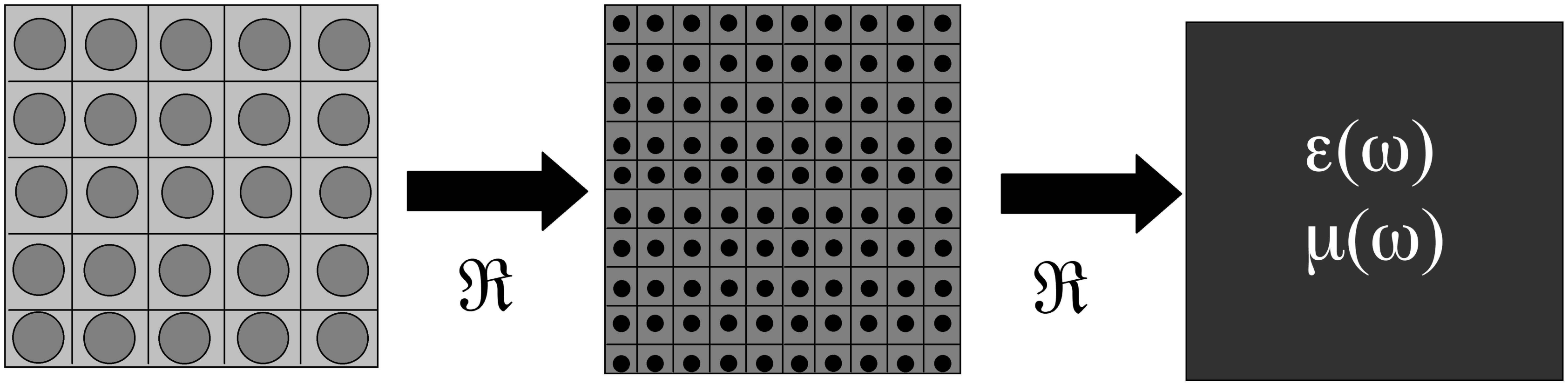




How to find the effective optical properties of an ensemble of nanorods?

Transmission of an incident beam?

Homogeneization theory



The renormalisation transform is defined by:

size divided by η

Permittivity multiply by η^2 $\longrightarrow$ **Constant optical diameter**

Wavelength been constant

How does this transform modify the band structure ?

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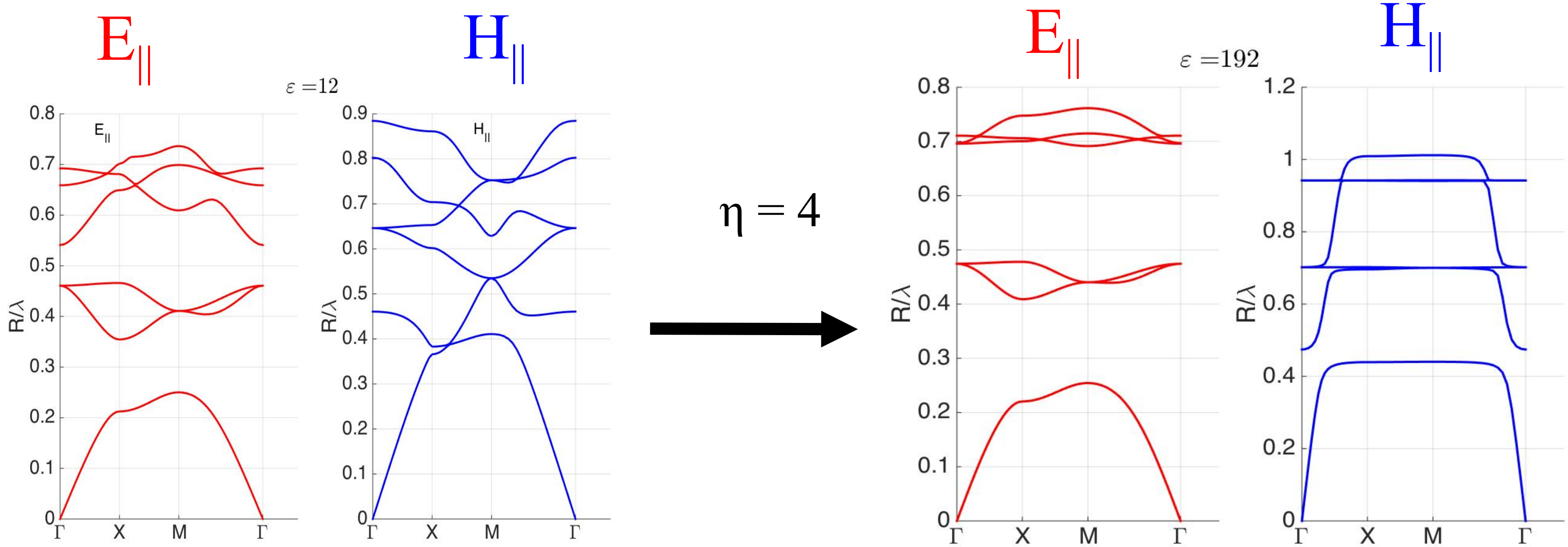
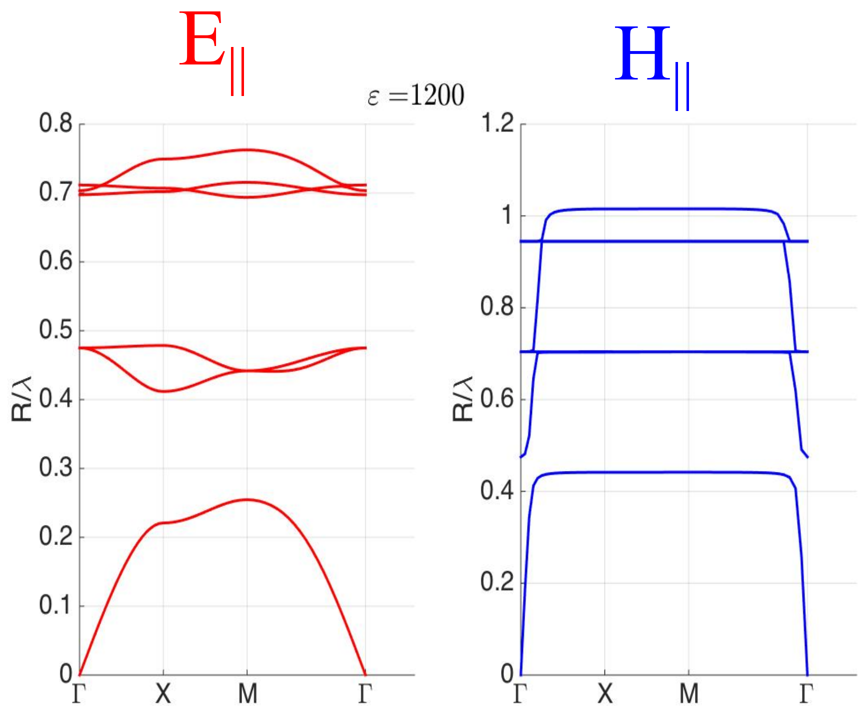
Bloch diagrams



Bloch diagrams



$$\mu_{\text{eff}}(\omega) = 1 + \sum_n \frac{\omega^2}{\lambda_n \varepsilon_i^{-1} c^2 - \omega^2} \left(\int_D \phi_n(y) dy \right)^2$$

The $E_{||}$ Bloch spectrum is unchanged by the renormalisation transform

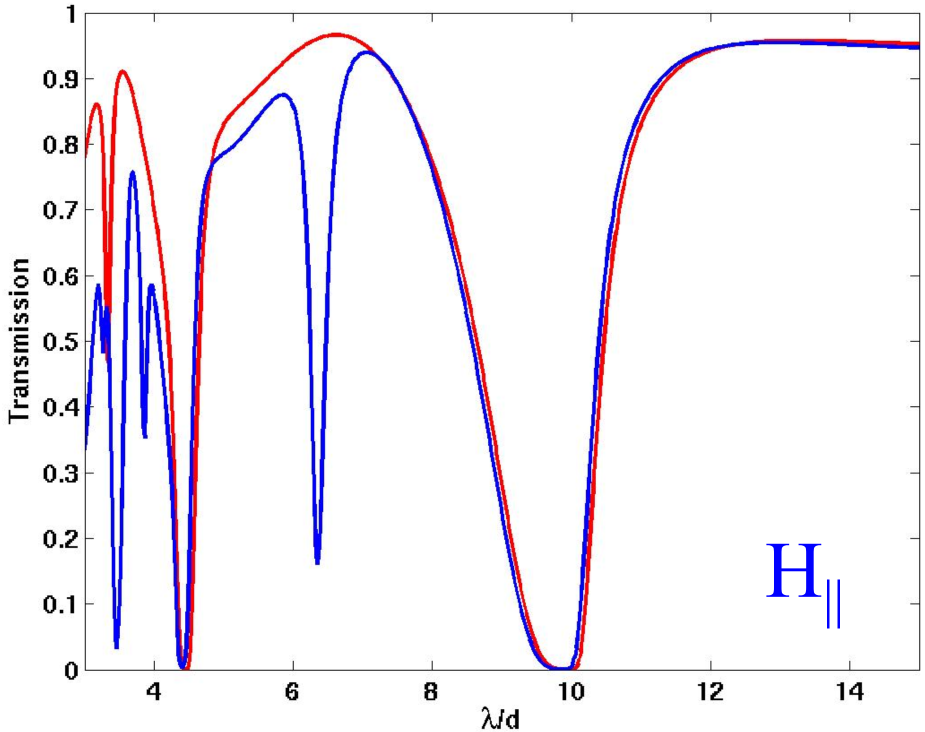
homogenization result near the Γ point

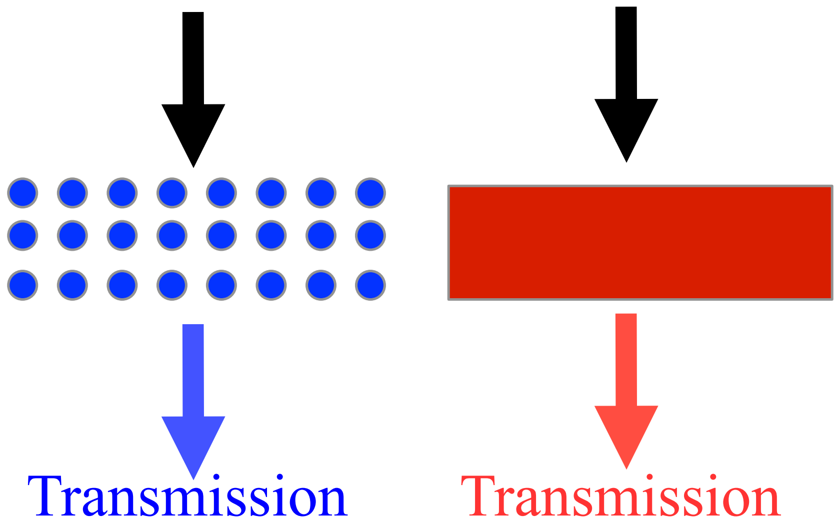
K.Vynck, D. Felbacq, Phys. Rev. Lett. **102**, 133901 (2009)

The $H_{||}$ Bloch spectrum converges towards that of a homogeneous medium with resonances
Homogeneization result everywhere with artificial magnetism

D. Felbacq, G. Bouchitté, Phys. Rev. Lett. **94**, 183902 (2005)

Light transmission through the rods





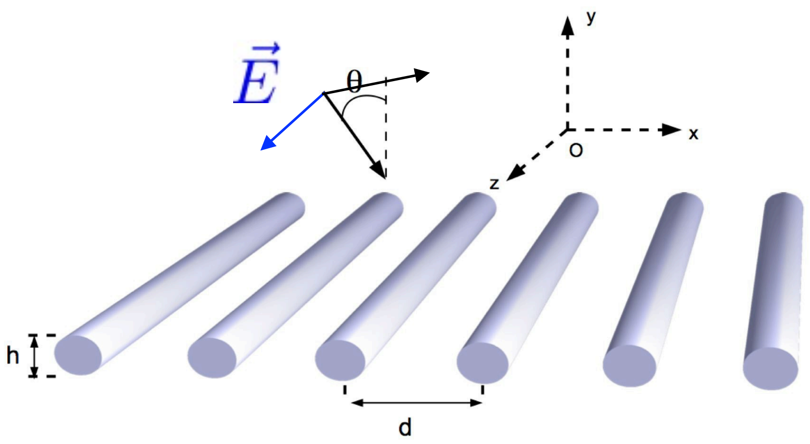
Blue: heterogeneous structure

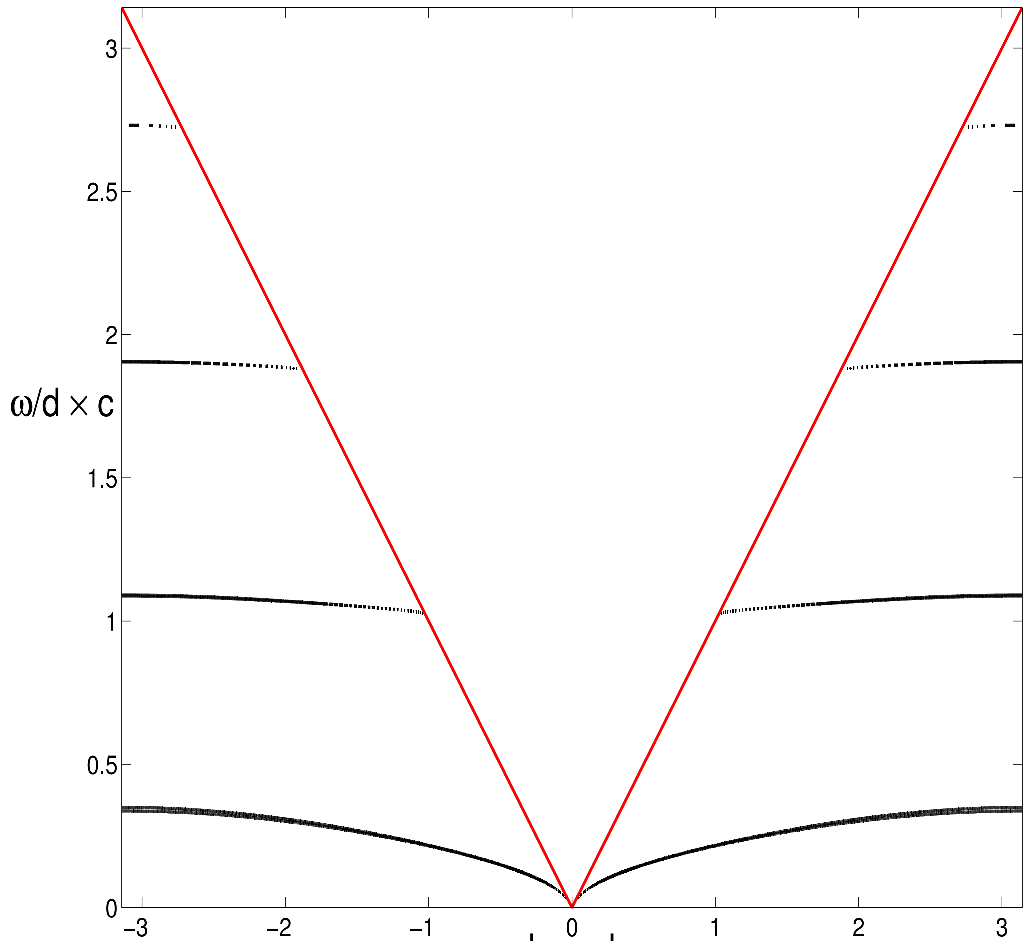
Red: homogenized structure => effective optical index

No fitting parameters

Low transmission = negative permittivity

Single line: metasurface



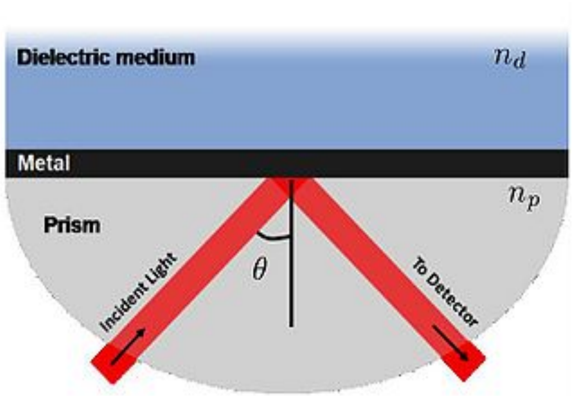


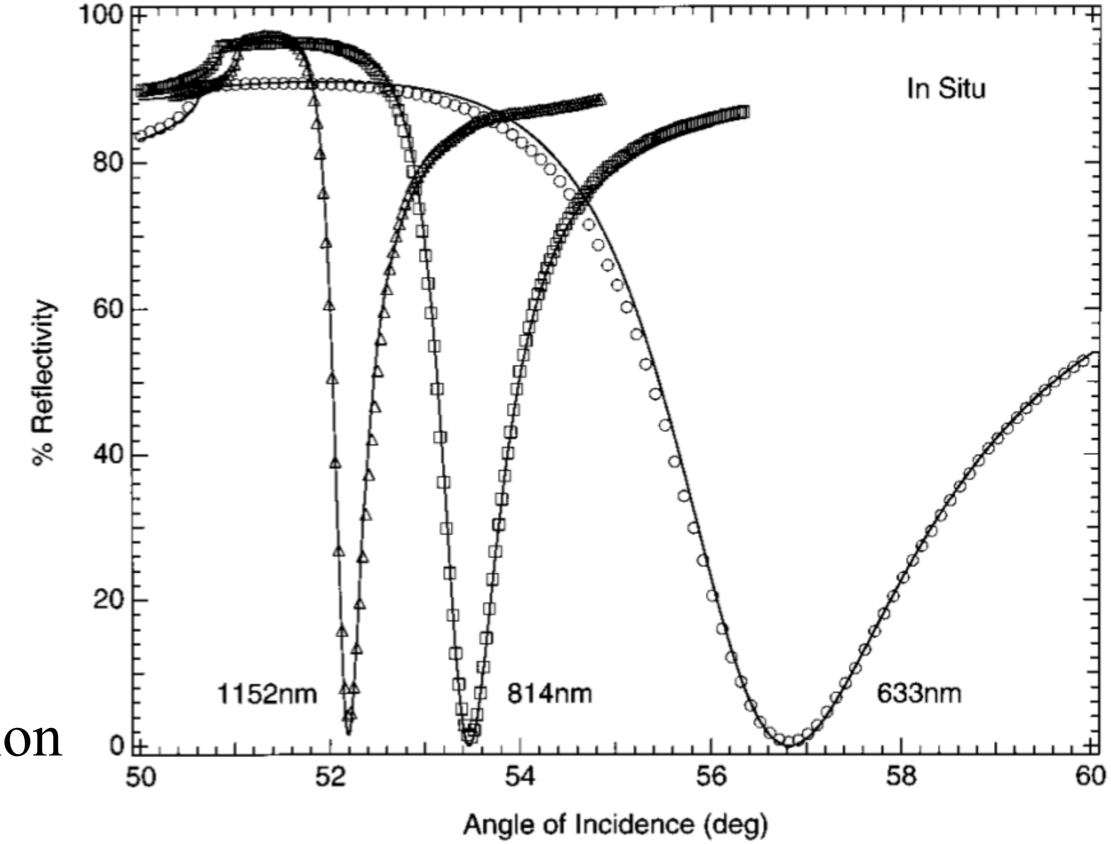
Bloch modes in the structure :

Non-propagating modes :

Propagation in x -direction
Evanescent in y-direction
Surface mode in $E_{||}$ polarisation

Plasmonics and surface modes





Surface plasmon resonance:

Excitation of a collective oscillation of the electrons in metal

Energy is dissipated in metals through Joule losses

Only in $H_{||}$ excitation

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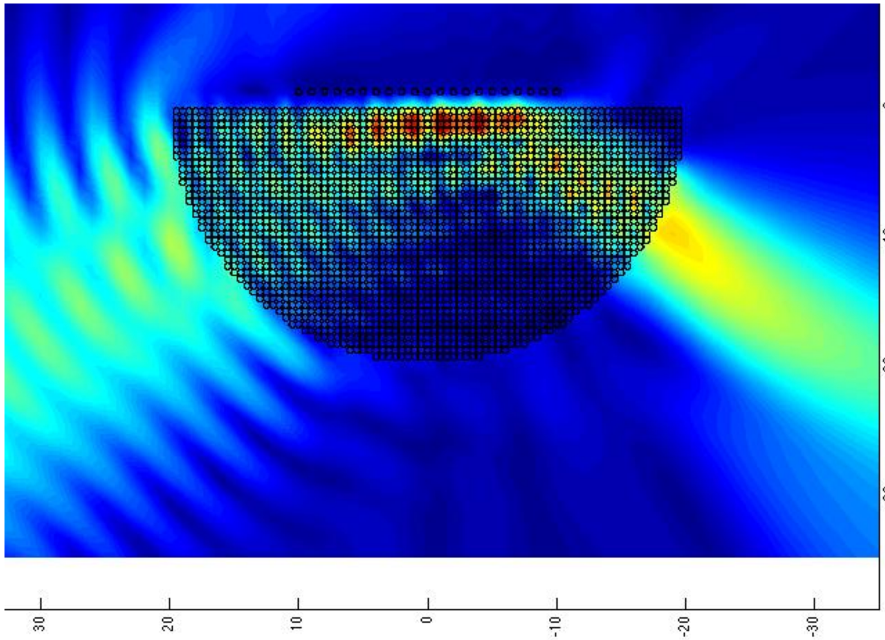
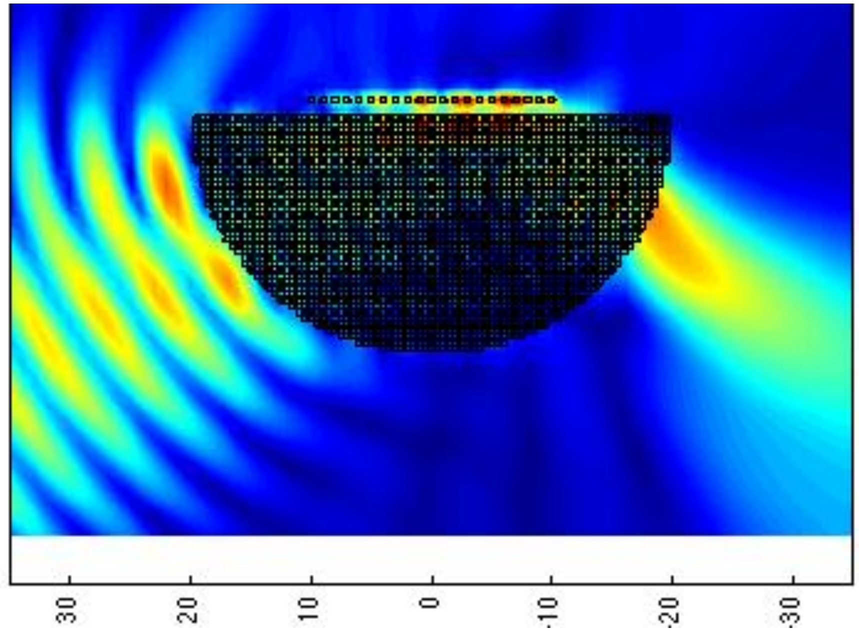
Exciting the evanescent modes



OFF-resonance excitation



ON-resonance excitation

Surface mode in $E_{||}$ polarisation (TE-polarization)

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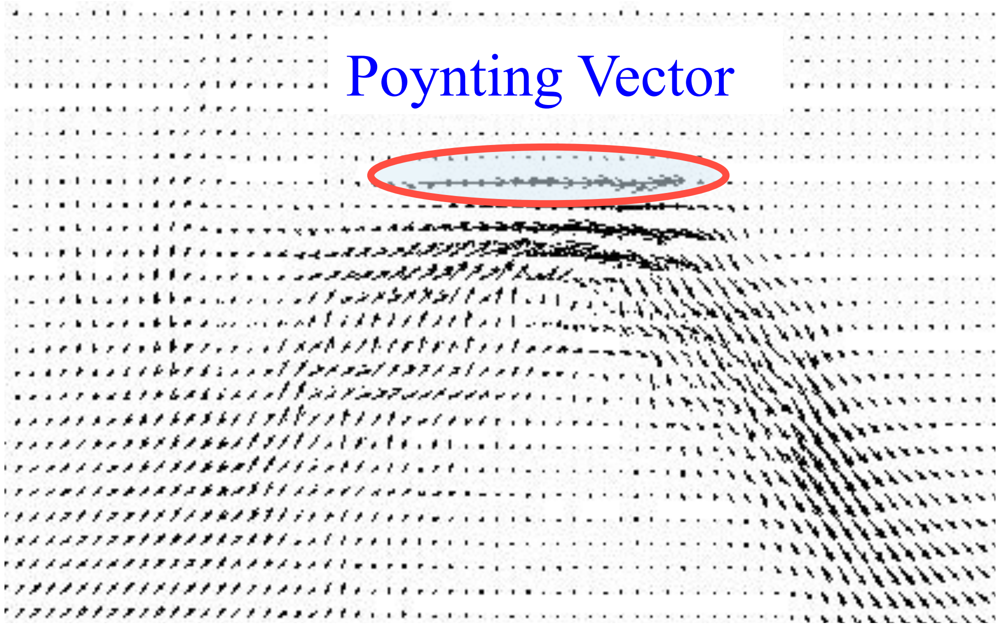
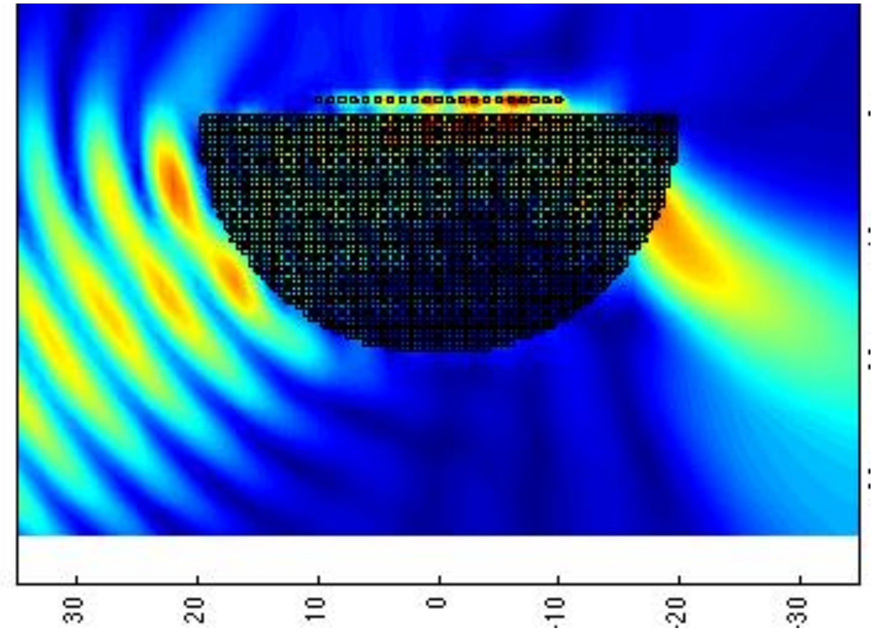
Exciting the evanescent modes



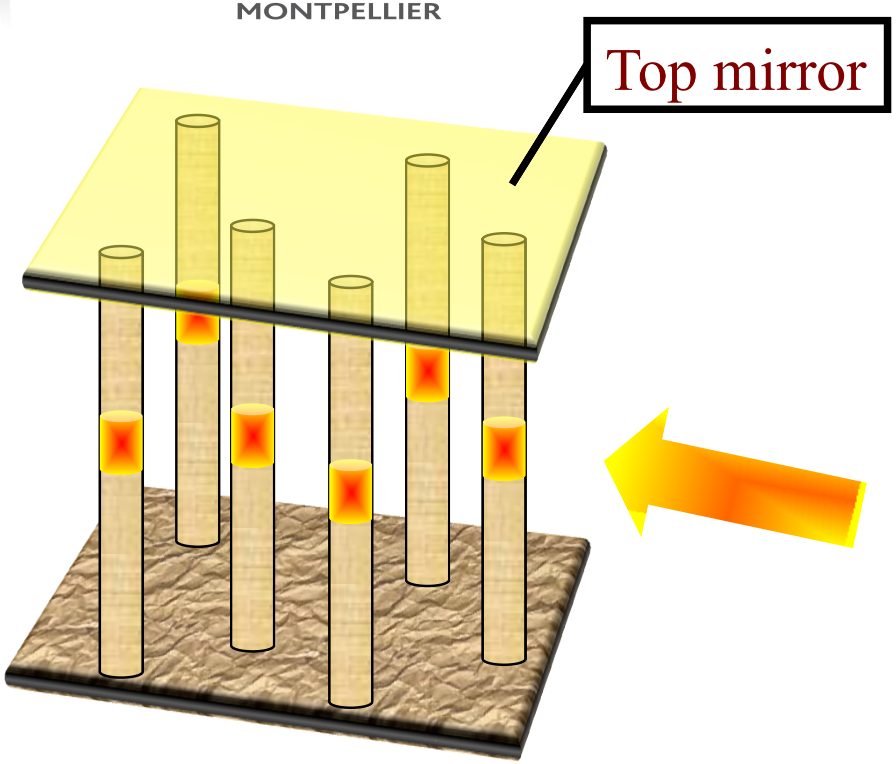
ON-resonance excitation

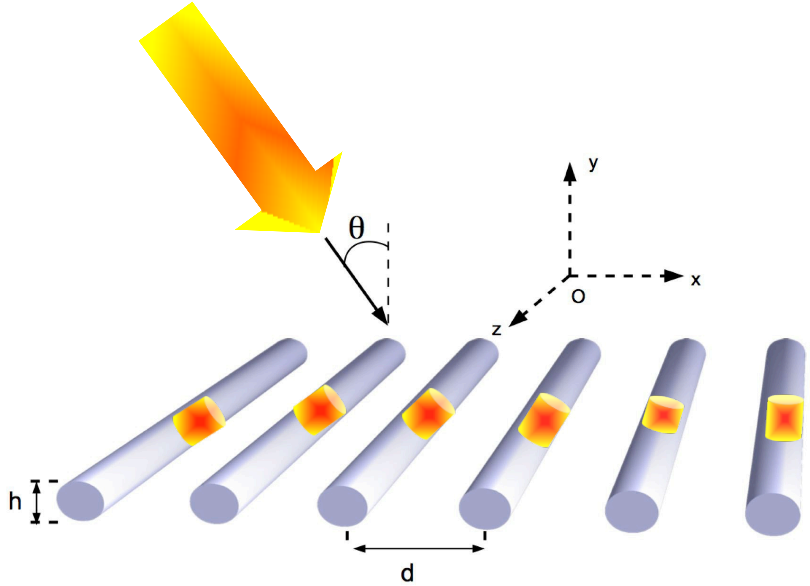


ON-resonance excitation

Surface mode in $E_{||}$ polarisation (TE-polarization)

Quantum metamaterials





First effect: superradiance

Quantum description of quantum dots: quantum hamiltonian

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The usual assumptions

Heisenbert picture => Operators vary with time
Wave-functions are constant with time

Time evolution => Heisenberg equation

$$i\hbar\dot{\hat{O}} = [\hat{O}, \hat{H}]$$

$\hat{H}$ = Minimal-coupling hamiltonian in the Coulomb gauge

Hamiltonian without approximations
(not restricted to *or* by the dipole approximation)

The minimal-coupling hamiltonian in the Coulomb gauge

$$\hat{H}_C = \frac{1}{2m}[\hat{p} - q\hat{A}(\hat{r},t)]^2 + V(\hat{r}) \qquad (1)$$

$$+ \int [\frac{1}{2}\varepsilon_0 \hat{E^{\perp}}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)]d\vec{x} \qquad (2)$$

Describes an electric charge q in a binding potential + e.m. field

(1) Charge energy: Kinetic energy + potential energy (nucleus + other electric charges)

(2) Electromagnetic field energy: free electromagnetic field energy

$div(\hat{A}) = 0$ The Coulomb gauge condition

Commutators in the Coulomb gauge

$$\hat{H}_C = \frac{1}{2m}[\hat{p} - q\hat{A}(\hat{r},t)]^2 + V(\hat{r}) \quad (1)$$

$$+ \int [\frac{1}{2}\varepsilon_0 \hat{E^{\perp}}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)]d\vec{x} \quad (2)$$

$$\boxed{[\hat{A}_i(\vec{x},t), -\varepsilon_0 \hat{E}_j^{\perp}(\vec{y},t)] = i\hbar\delta^T_{i,j}(\vec{x}-\vec{y})}$$

Transverse component of the electric field $div(\hat{E}^{\perp}) = 0$

Only two degrees of freedom are quantized
=> perpendicular direction propagation $\vec{k}.\hat{E}^{\perp}(\vec{k}) = 0$

Inconvenient of the minimal-coupling hamiltonian

$$\hat{H}_C = \frac{1}{2m}[\hat{p} - q\hat{A}(\hat{r},t)]^2 + V(\hat{r}) + \int [\frac{1}{2}\varepsilon_0 \hat{E^{\perp}}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)] d\vec{x}$$

light/matter coupling arises through the potential vector

physical fields (electric, magnetic field)

Microscopic description of charge dynamics

atoms/molecules/qdots are neutral

less microscropic description,

atoms through their multipolar moments (dipolar, quadrupolar moment etc…)

In the literature: The Power-Zienau-Woolley Hamiltonian

~~Coupling light/matter arises through potential vector~~
physical fields (electric, magnetic field)

~~Microscopic description of charge dynamics~~
atoms through their multipolar moments

In the literature: a hamiltonian known as the multipolar hamiltonian or the *Power-Zienau-Woolley* hamiltonian meets these requirements

Derive from the minimal-coupling hamiltonian in the Coulomb gauge from a gauge transformation

The two starting points are equivalent
=> They give the same physical results but one starting point may be more convenient

The Power-Zienau-Woolley hamiltonian

$$
\begin{aligned}
H_{pzw} &= \frac{1}{2m}[\hat{p}_{pzw} + q\int_0^1 udu\ \hat{r}_{pzw} \times \vec{B}(u\hat{r}_{pzw}, t)]^2 + V(\hat{r}_{pzw}) \\
&+ \int d\vec{x}\ [\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x}, t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x}, t)] \\
&- \int d\vec{x}\ \frac{1}{\varepsilon_0}\hat{P^{\perp}}(\vec{x}, t).\hat{D}(\vec{x}, t) \\
&+ \int d\vec{x}\ \frac{\hat{P^{\perp}}^2(\vec{x}, t)}{2\varepsilon_0}
\end{aligned}
$$

$$\hat{P}^{\perp} = q\hat{r}\int_0^1 du\delta^T(\vec{x} - u\hat{r})$$ Polarization field

$$\vec{P}(\vec{x}) = q\vec{r}\delta(\vec{x} - \vec{r})$$ Classical definition

$$\hat{D} = \varepsilon_0\hat{E}^{\perp} + \hat{P}^{\perp}$$ Displacement field

The Power-Zienau-Woolley hamiltonian: dipolar approximation

$$
\begin{aligned}
H_{pzw} &= \frac{1}{2m}\hat{p}_{pzw}^2 + V(\hat{r}_{pzw}) && (1)\\
&+ \int d\vec{x}\,[\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)] && (2)\\
&- \int d\vec{x}\,\frac{1}{\varepsilon_0}\hat{P^\perp}(\vec{x},t).\hat{D}(\vec{x},t) && (3)\\
&+ \int d\vec{x}\,\frac{\hat{P^\perp}^2(\vec{x},t)}{2\varepsilon_0} && (4)
\end{aligned}
$$

$$\hat{P}^\perp(\vec{x}) = q\hat{r}\delta^T(\vec{x}-\hat{r})$$

(1) The free particle hamiltonian

(2) Electromagnetic field hamiltonian *(free ?)*

(3) Interaction term

(4) P-square term: self-interaction term *(neglected)*

Power-Zienau-Woolley hamiltonian: its advantages

$$
\begin{aligned}
H_{pzw} &= \frac{1}{2m}\hat{p}^2_{pzw} + V(\hat{r}_{pzw}) && (1)\\
&+ \int d\vec{x}\, [\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)] && (2)\\
&- \int d\vec{x}\, \frac{1}{\varepsilon_0}\hat{P^\perp}(\vec{x},t).\hat{D}(\vec{x},t) && (3)\\
&+ \int d\vec{x}\, \frac{\hat{P^\perp}^2(\vec{x},t)}{2\varepsilon_0} && (4)
\end{aligned}
$$

Exact: derived form the Coulomb gauge hamiltonian through a gauge transformation

Robust result: Same results from 3 differents starting point

Coulomb gauge hamiltonian => unitary transformation

Classical Lagrangian => gauge transformation on vector/scalar potential

Lagrangian density (2^{nd} quantization) => gauge transformation

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The Power-Zienau-Woolley hamiltonian: original papers

$$
\begin{aligned}
\hat{H}_{pzw} = \hat{H}_C^{(2)} &= \frac{1}{2m}[\hat{p}_{pzw} + q\int_0^1 udu\ \hat{r}_{pzw} \times \vec{B}(u\hat{r}_{pzw}, t)]^2 + V(\hat{r}_{pzw}) \\
&+ \int d\vec{x}\ [\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x}, t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x}, t)] \\
&- \int d\vec{x}\ \frac{1}{\varepsilon_0}\hat{P^\perp}(\vec{x}, t).\hat{D}(\vec{x}, t) \\
&+ \int d\vec{x}\ \frac{\hat{P^\perp}^2(\vec{x}, t)}{2\varepsilon_0}
\end{aligned}
$$

COULOMB GAUGE IN NON-RELATIVISTIC QUANTUM ELECTRO-DYNAMICS AND THE SHAPE OF SPECTRAL LINES

By E. A. POWER AND S. ZIENAU

University College London

Cited: ~ 460 times

The Power-Zienau-Woolley hamiltonian: original papers

$$
\begin{aligned}
\hat{H}_{pzw} = \hat{H}_C^{(2)} &= \frac{1}{2m}[\hat{p}_{pzw} + q\int_0^1 udu\ \hat{r}_{pzw} \times \vec{B}(u\hat{r}_{pzw}, t)]^2 + V(\hat{r}_{pzw}) \\
&+ \int d\vec{x}\ [\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x}, t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x}, t)] \\
&- \int d\vec{x}\ \frac{1}{\varepsilon_0}\hat{P^\perp}(\vec{x}, t).\hat{D}(\vec{x}, t) \\
&+ \int d\vec{x}\ \frac{\hat{P^\perp}^2(\vec{x}, t)}{2\varepsilon_0}
\end{aligned}
$$

Proc. Roy. Soc. Lond. A. **319**, 549–563 (1970)
Printed in Great Britain

The interaction of molecular multipoles with the electromagnetic field in the canonical formulation of non-covariant quantum electrodynamics

By P. W. Atkins and R. G. Woolley
Physical Chemistry Laboratory, South Parks Road, Oxford

Cited: ~ 130 times

The Power-Zienau-Woolley hamiltonian: Highly cited result

$$\begin{aligned}\hat{H}_{pzw} = \hat{H}_C^{(2)} &= \frac{1}{2m}\hat{p}_{pzw}^2 + V(\hat{r}_{pzw}) \\ &+ \int d\vec{x}\,[\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)] \\ &- \int d\vec{x}\,\frac{1}{\varepsilon_0}\hat{P^\perp}(\vec{x},t).\hat{D}(\vec{x},t) \\ &+ \int d\vec{x}\,\frac{\hat{P^\perp}^2(\vec{x},t)}{2\varepsilon_0}\end{aligned}$$

Highly used result:

- Cold atoms (PhysRevA.**51**.*3896;* PhysRevA.**56**.*905*)
- Light quantization in medium (Quantum optics by Vogel, Welsch)
- Metamaterials (PhysRevB.**86**.*085116)*
- Near-Field optics (Quantum theory in the near-field by Keller)

Maybe more than 1000 of papers used the PZW hamiltonian as a starting point…

The Power-Zienau-Woolley hamiltonian: a recent result

PRL **112,** 073601 (2014) PHYSICAL REVIEW LETTERS week ending 21 FEBRUARY 2014

Elimination of the *A*-Square Problem from Cavity QED

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(Received 2 October 2013; published 20 February 2014)

We generalize the Power-Zineau-Woolley transformation to obtain a canonical Hamiltonian of cavity quantum electrodynamics for arbitrary geometry of boundaries. This Hamiltonian is free from the *A*-square term and the instantaneous Coulomb interaction between distinct atoms. The single-mode models of cavity QED (Dicke, Tavis-Cummings, Jaynes-Cummings) are justified by a term by term mapping to the proposed microscopic Hamiltonian. As one straightforward consequence, the basis of no-go argumentations concerning the Dicke phase transition with atoms in electromagnetic fields dissolves.

$$H' = \sum_\alpha \frac{\mathbf{p}_\alpha'^2}{2m_\alpha} + \frac{1}{2\varepsilon_0}\int_D d^3r\mathbf{P}^2 - \frac{1}{\varepsilon_0}\int_D d^3r\mathbf{D}\cdot\mathbf{P} + H'_{\text{field}}, \tag{16}$$

Important for superradiance!

LABORATOIRE CHARLES COULOMB MONTPELLIER

The Power-Zienau-Woolley hamiltonian: a well-established result

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Photons et atomes. Cohen Tannoudji

Gauge Transformation: Classical level

$$div(\vec{B}) = 0 \Rightarrow \vec{B} = \vec{rot}\vec{A}$$

$$\vec{rot}\vec{E} = -\frac{\partial}{\partial t}\vec{B} \Rightarrow \vec{E} = -\frac{\partial}{\partial t}\vec{A} - \vec{\nabla}\phi$$

$$\vec{E} = -\frac{\partial}{\partial t}\vec{A} - \vec{\nabla}\phi$$

3 known values

4 unknowns values

1 scalar condition is needed => Gauge Conditions

$$div\vec{A} = 0$$

Coulomb gauge

$$div\vec{A} + \frac{1}{c}\frac{\partial\phi}{\partial t} = 0$$

Lorenz gauge

$$\vec{r}.\vec{A} = 0$$

Poincaré gauge

Interest of the Poincaré Gauge (Multipolar gauge)

$$div(\vec{B}) = 0 \Rightarrow \vec{B} = r\vec{o}t\vec{A} \qquad \vec{E} = -\frac{\partial}{\partial t}\vec{A} - \vec{\nabla}\phi$$

$$\vec{r}.\vec{A} = 0$$

$$\vec{A}(\vec{x},t) = -\vec{x} \times \int_0^1 du u \vec{B}(u\vec{x},t) \qquad \phi(\vec{x},t) = -\vec{x}.\int_0^1 du \vec{E}(u\vec{x},t)$$

The potentials express with the help of the physical fields

$$\phi(\vec{x},t) = -\vec{x}.\sum \frac{(\vec{z}.\vec{\nabla}_z)^n}{(n+1)!}\vec{E}(\vec{z},t)|_{\vec{z}=0}$$

Multipolar developpement

Gauge Transformation: Quantum level

$$\boxed{< \psi_1|H_1|\psi_1 >=< \psi_2|H_2|\psi_2 >}$$

Invariance of measurement through the gauge transformation

Gauge transformation induced by a transformation of the wavefunction

But

A transformation of the hamiltonian is needed to conserve the expected-values

$$\psi_p(\vec{x},t) = \exp[i\frac{q}{\hbar}\chi(\vec{r},\vec{A}_c,t)]\psi_c(\vec{x},t)$$

$$H_p = \exp[i\frac{q}{\hbar}\chi(\vec{r},\vec{A}_c,t)]H_c\exp[-i\frac{q}{\hbar}\chi(\vec{r},\vec{A}_c,t)] + \exp[i\frac{q}{\hbar}\chi(\vec{r},\vec{A}_c,t)]\frac{\partial}{\partial t}\exp[-i\frac{q}{\hbar}\chi(\vec{r},\vec{A}_c,t)]$$

$$U^\dagger(\vec{r},t) = \exp[i\frac{q}{\hbar}\chi(\vec{r},\vec{A}_c,t)]$$

Unitary transformation $\quad UU^\dagger = U^\dagger U = 1$

Concern the Schrödinger equation and the particle wavefunction

I) Electromagnetic energy?

$$\hat{H}_{pzw} = \hat{H}_C^{(2)} = \frac{1}{2m}\hat{p}^2_{pzw} + V(\hat{r}_{pzw})$$
$$\boxed{+ \int d\vec{x}\, [\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)]}$$
$$- \int d\vec{x}\, \frac{1}{\varepsilon_0}\hat{P^{\perp}}(\vec{x},t).\hat{D}(\vec{x},t)$$
$$+ \int d\vec{x}\, \frac{\hat{P^{\perp}}^2(\vec{x},t)}{2\varepsilon_0}$$

Neither the field-energy in vacuum nor in matter?

$$\frac{1}{2}\varepsilon_0\hat{E}^2 + \frac{1}{2\mu_0}\hat{B}^2 \qquad\qquad \frac{1}{2}\hat{D}.\hat{E} + \frac{1}{2}\hat{H}.\hat{B}$$

II) The interaction term?

$$\hat{H}_{pzw} = \hat{H}_C^{(2)} = \frac{1}{2m}\hat{p}_{pzw}^2 + V(\hat{r}_{pzw})$$

$$\boxed{\begin{aligned} &+ \int d\vec{x}\, [\frac{1}{2\varepsilon_0}\hat{D}^2(\vec{x},t) + \frac{1}{2\mu_0}\hat{B}^2(\vec{x},t)] \\ &- \int d\vec{x}\, \frac{1}{\varepsilon_0}\hat{P^\perp}(\vec{x},t).\hat{D}(\vec{x},t) \\ &+ \int d\vec{x}\, \frac{\hat{P^\perp}^2(\vec{x},t)}{2\varepsilon_0} \end{aligned}}$$

$$\vec{D} = \varepsilon_0\vec{E} + \vec{P}$$

Expressing the hamiltonian with E, P and B:

$$\begin{aligned} &\frac{1}{2\varepsilon_0}\hat{D}^2 + \frac{1}{2\mu_0}\hat{B}^2 - \frac{1}{\varepsilon_0}\hat{P}^\perp.\hat{D} + \frac{\hat{P}^{\perp 2}}{2\varepsilon_0} \\ &= \frac{1}{2}\varepsilon_0\hat{E}^{\perp 2} + \frac{1}{2\mu_0}\hat{B}^2 \end{aligned}$$

The interaction term disappears

III) Non gauge-invariance of the electromagnetic field?

Interaction Hamiltonian of quantum optics

J. Opt. Soc. Am. B/Vol. 1, No. 1/March 1984 — J. R. Ackerhalt and P. W. Milonni

$$\mathbf{E}_{\mathrm{NEW}} = U\mathbf{E}_{\mathrm{OLD}}U^{+} = \mathbf{E}_{\mathrm{OLD}} + 4\pi\mathbf{P}^{\perp}$$

Power-Zienau-Woolley:

gauge transformation = Unitary transformation

$$\hat{E}^{\perp} \rightarrow \hat{D}$$

Non-invariance of the electric field?

The error: the unitary transformation doesn't applied to the electromagnetic fields operators!

Derivation starting from a Lagrangian density

$$\begin{aligned}\mathcal{L} &= i\hbar\psi^\star(\vec{x},t)[\partial_t + \frac{iq}{\hbar}\varphi(\vec{x},t)]\psi(\vec{x},t)\\ &- \frac{\hbar^2}{2m}[\partial_\mu + \frac{iq}{\hbar}A_\mu(\vec{x},t)]\psi^\star(\vec{x},t)[\partial_\mu - \frac{iq}{\hbar}A_\mu(\vec{x},t)]\psi(\vec{x},t)\\ &- \psi^\star(\vec{x},t)V(\vec{x})\psi(\vec{x},t)\\ &+ \frac{1}{2}\varepsilon_0[(\partial_t\vec{A}(\vec{x},t) + \vec{\nabla}\varphi(\vec{x},t))]^2 - \frac{1}{2\mu_0}\vec{B}^2(\vec{x},t)] \qquad (5)\end{aligned}$$

Gauge invariant expression

Semiclassical: Schrödinger field, classical electromagnetic field

Quantum theory: Schrödinger operator, electromagnetic field operator operators acting on Fock space

The Hamiltonian density from the Lagrangian density

$$
\begin{aligned}
\mathcal{H} &= \frac{1}{i\hbar}\pi_\psi(\vec{x},t)[(-\frac{\hbar^2}{2m})(\partial_\mu + \frac{iq}{\hbar}A_\mu)^2 + V(\vec{x},t)]\psi(\vec{x},t) \\
&+ [\frac{1}{2\varepsilon_0}\vec{\pi}^2(\vec{x},t) + \frac{1}{2\mu_0}\vec{B}^2(\vec{x},t)] \\
&+ (\vec{\nabla}.\pi(\vec{x},t) + q|\psi(\vec{x},t)|^2)\phi(\vec{x},t) \qquad (11)
\end{aligned}
$$

$\vec{\pi} = -\varepsilon_0 \vec{E}$ $\qquad$ $\pi_\psi = i\hbar\psi^\star$ Canonical momenta

Canonical procedure: (Dirac)

$$
[\hat{A}(\vec{x},t), \hat{\pi}(\vec{x'},t)] = \underbrace{i\hbar\{\vec{A}(\vec{x},t), \vec{\pi}(\vec{x'},t)\}}_{\text{Poisson brackets}}
$$

But QED is a constrained theory…

Canonical procedure: (Dirac)

$$[\hat{A}(\vec{x},t),\hat{\pi}(\vec{x'},t)] = i\hbar\{\vec{A}(\vec{x},t),\vec{\pi}(\vec{x'},t)\}$$

Poisson brackets have to take constraints into account:

- The Maxwell-Gauss equation $\vec{\nabla}.\vec{E}(\vec{x},t) = \frac{q}{\varepsilon_0}\psi^\star(\vec{x},t)\psi(\vec{x},t)$

+ Gauge constraint:

$$[\hat{A}(\vec{x},t),\hat{\pi}(\vec{x'},t)] = i\hbar\underbrace{\{\vec{A}(\vec{x},t),\vec{\pi}(\vec{x'},t)\}_D}_{\text{Dirac brackets}}$$

But QED is a constrained theory…

Canonical procedure: (Dirac)

$$[\hat{A}(\vec{x},t),\hat{\pi}(\vec{x'},t)] = i\hbar\underbrace{\{\vec{A}(\vec{x},t),\vec{\pi}(\vec{x'},t)\}_{\mathrm{D}}}_{\text{Dirac brackets}}$$

Dirac brackets take constraints into account:

- The Maxwell-Gauss equation
- Gauge constraint

Ex: Coulomb gauge: div A = 0

$$\Delta K(\vec{x},\vec{y}) = -\delta(\vec{x}-\vec{y})$$

$$[\hat{A}_i^{\perp}(\vec{x},t),\hat{\pi}^{\perp}(\vec{y},t)] = i\hbar\delta^{T}_{i,j}(\vec{x}-\vec{y})$$

$$[\hat{A}_i^{\perp}(\vec{x},t),\perp\pi^{\perp}(\vec{y},t)] = i\hbar\{\delta_{i,j}\delta(\vec{x}-\vec{y}) + \overbrace{\frac{\partial^2}{\partial x_i\partial y_j}}K(\vec{x},\vec{y})\}$$

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Commutators in the Poincaré gauge

The Poincaré gauge condition $\vec{r}.\vec{A} = 0$

Unpublished results

Commutators between physical fields are gauge invariant

$$\boxed{[\hat{E}_i(\vec{x},t),\hat{B}_j(\vec{y},t)] = \frac{i\hbar}{\varepsilon_0}\varepsilon_{i,j,k}\partial_{y_k}[\delta(\vec{x}-\vec{y})]}$$

Quantum Hamiltonian in the Poincaré gauge

Unpublished results

The scalar potential doesn’t appear explicitly
Appears in the Schrödinger equation with the help of the commutators!

Hamiltonian of the free electromagnetic field, no displacement field!

The original error of Power-Zienau-Woolley

$$i\hbar\dot{\hat{\psi}}(\vec{x},t) = -\frac{\hbar^2}{2m}[\vec{\nabla} + \frac{iq}{\hbar}\vec{x}\times\int_0^1 du u \hat{B}(u\vec{x},t)]^2\hat{\psi}(\vec{x},t) + [V(\vec{x},t) - q\vec{x}.\int_0^1 du \hat{E}(u\vec{x},t)]\hat{\psi}(\vec{x},t)$$

$$\mathbf{E}_{\mathrm{NEW}} = U\mathbf{E}_{\mathrm{OLD}}U^{+} = \mathbf{E}_{\mathrm{OLD}} + 4\pi\mathbf{P}^{\perp}$$

Not correct!!

They applied the unitary transformation to the electromagnetic field
Which doesn't not act to the wave-function!!

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The 2nd error of Power

Quantum electrodynamics with nonrelativistic sources. I. Transformation to the multipolar formalism for second-quantized electron and Maxwell interacting fields

PRA 28, 2649 (1983)

$$L_{\min}(\vec{a}^{\perp},\psi,\bar{\psi};\dot{\vec{a}}^{\perp},\dot{\psi},\dot{\bar{\psi}})=\int \mathscr{L}_{\min} dV$$

$$= -\int \bar{\psi}(\vec{q})\left[\frac{1}{2m}\left[-i\hbar\vec{\nabla}^{(q)}+\frac{e}{c}\vec{a}^{\perp}(\vec{q})\right]^2+V(\vec{q})+\frac{e^2}{2}\int\frac{\bar{\psi}(\vec{q}\,')\psi(\vec{q}\,')}{|\vec{q}-\vec{q}\,'|}d^3q'\right]\psi(\vec{q})d^3q$$

$$+\frac{i\hbar}{2}\int[\bar{\psi}(\vec{q})\dot{\psi}(\vec{q})-\dot{\bar{\psi}}(\vec{q})\psi(\vec{q})]d^3q+\frac{1}{8\pi}\int\{[\dot{\vec{a}}^{\perp}(\vec{r})/c]^2-[\mathrm{curl}\,\vec{a}(\vec{r})]^2\}d^3r\ .$$

The multipolar formalism is related to the above through a change of the generalized coordinates describing the system. Although the electromagnetic field coordinate $\vec{a}^{\perp}(\vec{r})$, the vector potential, is unchanged, the one describing the electron field is transformed according to

$$\psi(\vec{q})=e^{-iS(\vec{q})}\phi(\vec{q})\ , \qquad (2.9)$$

They do not transform the electromagnetic field in order to recover their result given by unitary transformation!!

LABORATOIRE CHARLES COULOMB MONTPELLIER

Conclusion

The Power-Zienau-Woolley hamiltonian doesn't derived from the minimal-coupling hamiltonian in the Coulomb gauge with the help of a gauge transformation

Quantum hamiltonian and commutation rules in the Poincaré gauge

At the quantum level, the gauge constraints are taken into account through the commutators.

Future work:

The modes decomposition in the multipolar gauge

Superradiance in the metamaterials geometry