Quantum Electromagnetics: From Semi-Classical Framework to Full-Quantum Approach

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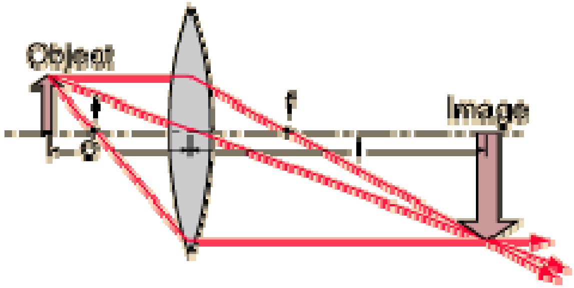
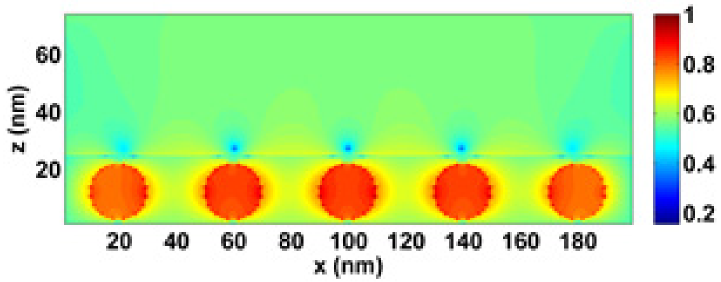
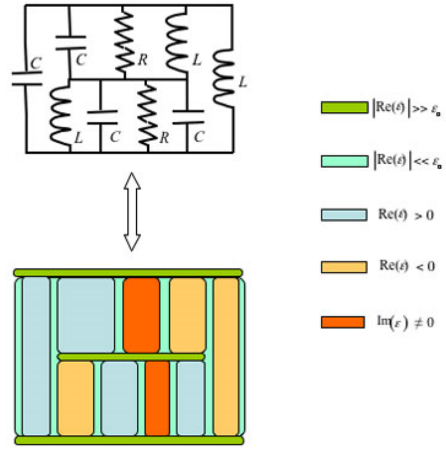
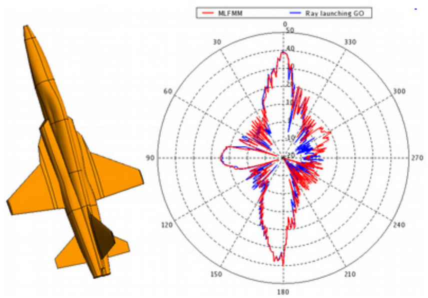
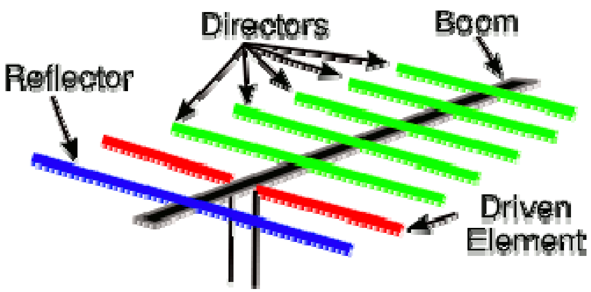
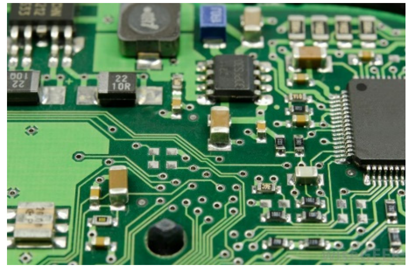












classical optics
ray physics
D>>λ

wave optics
wave physics
D~λ

nano-circuit
circuit physics
D<<λ

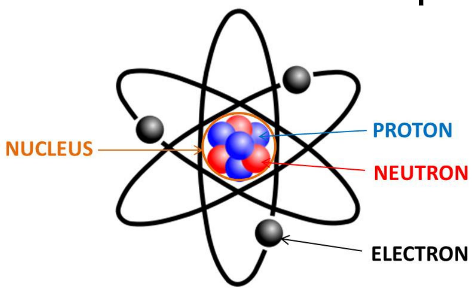
Quantum Regime—Semi-Classical versus Full-Quantum

strong field condition $\boxed{|\mathbf{E}| >> \frac{\sqrt{\hbar c}}{(c\Delta_t)^2}}$ electrostatic field $\Delta_t \to \infty$

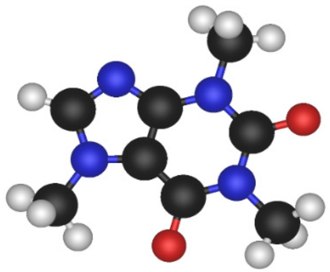
- At quantum regime, when the object size is tiny small (typically smaller than 10 nm) so that “homogenized” permittivity and permeability of Maxwell equation is invalid or meaningless.

- If the field intensity is strong or the number of photons is large, semi-classical Maxwell-Schrödinger system is required to describe the light-particle interaction, where Maxwell equation is still classical.

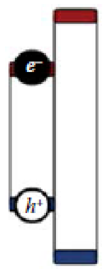
- If the field intensity is very weak and the number of photons is quite small (vacuum fluctuation, single photon source, etc), Maxwell equation should be quantized and classical Maxwell equation breaks down.

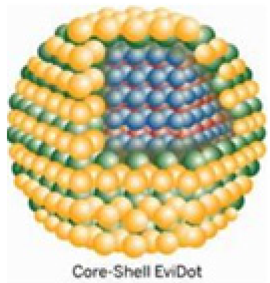


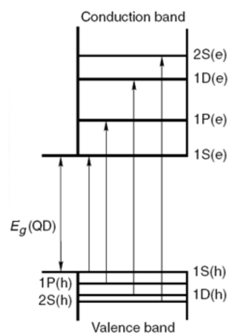
atoms



molecules



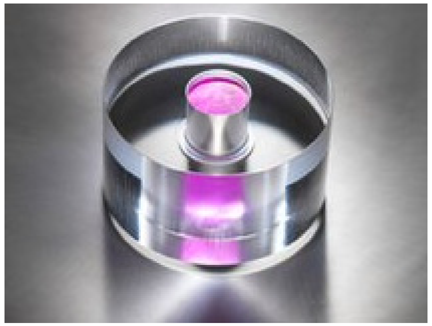


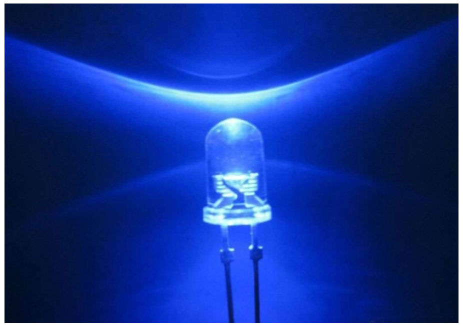


quantum dots

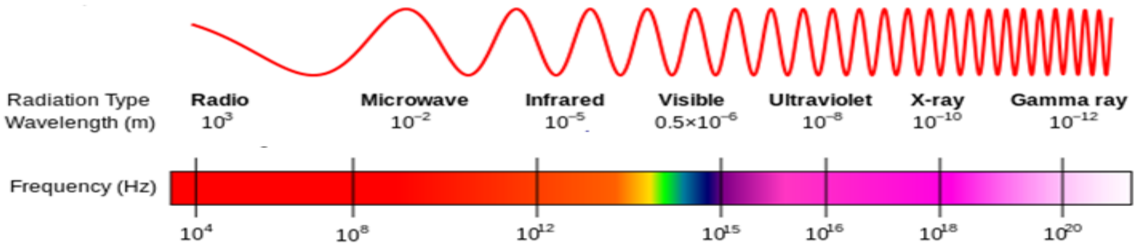
Why is Semi-Classical Framework Important?

The interaction between electromagnetic fields and particles (atoms and molecules) is responsible for emission and absorption processes of these particles. On one hand, the new sources of electromagnetic radiation have covered a broad spectral range from radio frequency to ultraviolet. On the other hand, after obtaining the information from radiation, the internal structure and dynamics of particles can be well understood and manipulated for generating new types of sources.



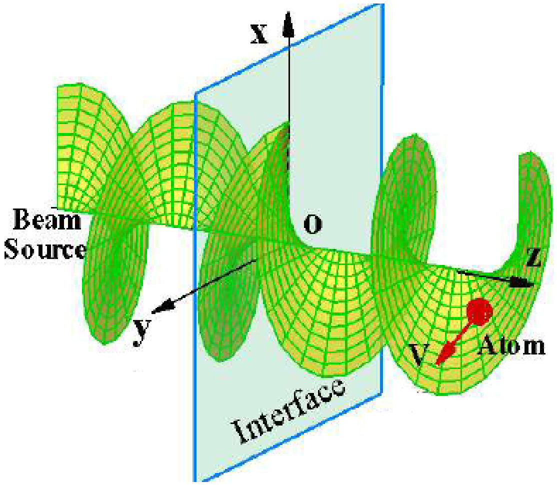



maser **laser** **light emitting diode** **synchrotron**



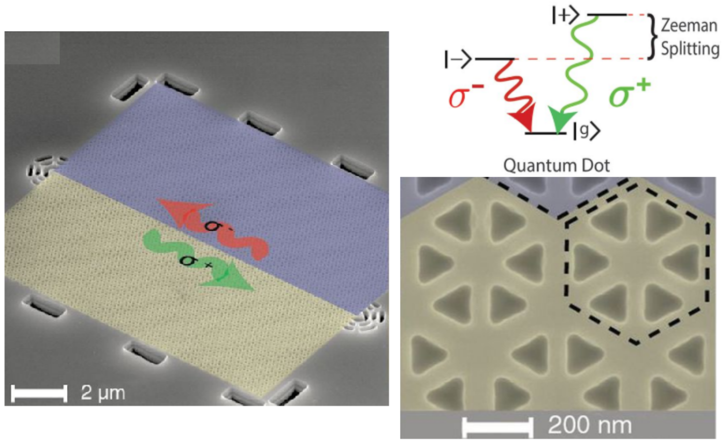
Why is Semi-Classical Framework Important? Cont.

EM-QM systems need to be rigorously modelled to break dipole approximation, rotating wave approximation, and no-back coupling approximation. Combining emerging light sources (structured light), material systems (2D materials), and EM structures (topological insulators) will result in extraordinary physical phenomena and novel operation scenarios for light-matter interaction at atomic level.



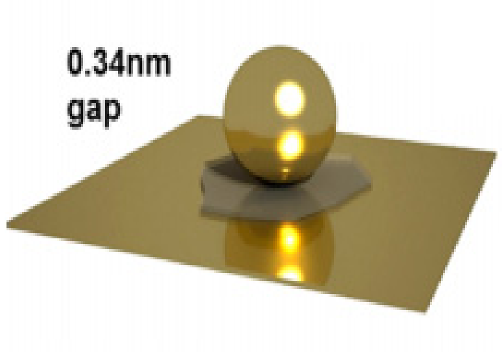
Laguerre-Gaussian beams

H. Luo, Physical Review A 80: 043810, 2009



Topological insulator

S. Barik, Science 359: 666-668, 2018



2D materials

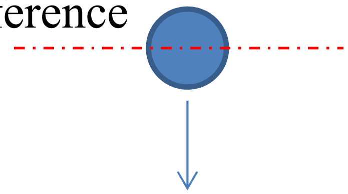
J. Mertens, Nano Letters 13: 5033−5038, 2013

Starting from a Simple Hamiltonian System

Consider a ball falling down to the ground, total energy of the system is given by

$$\boxed{H = \frac{\mathbf{p}\cdot\mathbf{p}}{2m} - m\mathbf{g}\cdot\mathbf{r}}$$

zero potential reference



$\mathbf{p}$ is the momentum and $\mathbf{r}$ is the coordinate. The first term is kinetic energy and the second term is potential energy. H is called Hamiltonian corresponds to the total energy of the system.

The time evolution of the system is uniquely defined by Hamilton's equations

$$\boxed{\begin{aligned} \frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{r}} \\ \frac{d\mathbf{r}}{dt} &= +\frac{\partial H}{\partial \mathbf{p}} \end{aligned}} \quad \begin{aligned} &\Leftrightarrow \quad \frac{d\mathbf{p}}{dt} = \mathbf{F} = m\mathbf{g} \\ &\Leftrightarrow \quad \frac{d\mathbf{r}}{dt} = \mathbf{v} = \frac{\mathbf{p}}{m} \end{aligned}$$

Hamiltonian System for Maxwell's Equations in Free Space

The total stored energy (Hamiltonian) of the electromagnetic system can be written as

$$H^{em} = \int \left[\frac{1}{2}\varepsilon_0 \mathbf{E}(\mathbf{r},t)\cdot\mathbf{E}(\mathbf{r},t) + \frac{1}{2}\mu_0 \mathbf{H}(\mathbf{r},t)\cdot\mathbf{H}(\mathbf{r},t) \right] dV = \int \frac{[-\varepsilon_0 \mathbf{E}(\mathbf{r},t)]^2}{2\varepsilon_0} + \frac{[\mu_0 \mathbf{H}(\mathbf{r},t)]^2}{2\mu_0} dV$$

$$\downarrow$$

$$H^{em} = \int \left[\frac{\mathbf{Y}(\mathbf{r},t)\cdot\mathbf{Y}(\mathbf{r},t)}{2\varepsilon_0} + \frac{\nabla\times\mathbf{A}(\mathbf{r},t)\cdot\nabla\times\mathbf{A}(\mathbf{r},t)}{2\mu_0} \right] dV$$

$$\boxed{\begin{aligned} \frac{\partial \mathbf{Y}}{\partial t} &= -\frac{\delta H^{em}}{\delta \mathbf{A}} \\ \frac{\partial \mathbf{A}}{\partial t} &= +\frac{\delta H^{em}}{\delta \mathbf{Y}} \end{aligned}}$$

coulomb gauge

$\nabla\cdot\mathbf{A} = 0$

$\Longrightarrow$

source-less

$\phi=0$

$$\frac{\partial \mathbf{Y}}{\partial t} = -\frac{\partial \mathbf{D}}{\partial t} = -\nabla\times\mathbf{H}(\mathbf{r},t) = -\frac{\nabla\times\nabla\times\mathbf{A}(\mathbf{r},t)}{\mu_0} = -\frac{\delta H^{em}}{\delta \mathbf{A}}$$

$$\frac{\partial \mathbf{A}}{\partial t} = -\mathbf{E}(\mathbf{r},t) = +\frac{\delta H^{em}}{\delta \mathbf{Y}}$$

Y is a generalized momentum and **A** is a generalized coordinate.

Hamiltonian Approach for Maxwell-Schrödinger System

Hamiltonian

$$H^s(\mathbf{A},\mathbf{Y},\psi,\psi^*) = H^{em}(\mathbf{A},\mathbf{Y}) + H^q(\psi,\psi^*,\mathbf{A})$$

$$H^{em}(\mathbf{A},\mathbf{Y}) = \int_v \left(\frac{1}{2\epsilon_0}|\mathbf{Y}|^2 + \frac{1}{2\mu_0}|\nabla\times\mathbf{A}|^2\right)d\mathbf{r}$$

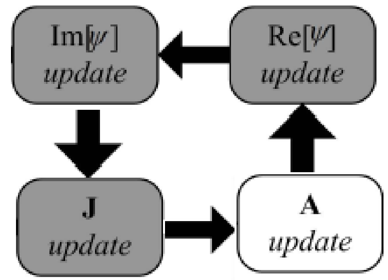
$$H^q(\psi,\psi^*,\mathbf{A}) = \int_v \left[\psi^*\frac{(\hat{\mathbf{p}}-q\mathbf{A})^2}{2m}\psi + \psi^* V\psi\right]d\mathbf{r}$$

Generalized coordinate and momentum

$$\mathbf{q} = (\mathbf{A},\psi_r) \qquad \mathbf{p} = (\mathbf{Y},\psi_i)$$

$$\frac{\partial\mathbf{p}}{\partial t} = -\frac{\partial H^s}{\partial\mathbf{q}}$$

$$\frac{\partial\mathbf{q}}{\partial t} = \frac{\partial H^s}{\partial\mathbf{p}}$$



Maxwell equation

$$\frac{\partial\mathbf{A}}{\partial t} = \frac{\partial H^s}{\partial\mathbf{Y}} = \frac{\mathbf{Y}}{\epsilon_0}$$

$$\frac{\partial\mathbf{Y}}{\partial t} = -\frac{\partial H^s}{\partial\mathbf{A}} = -\frac{\nabla\times\nabla\times\mathbf{A}}{\mu_0} + \mathbf{J}$$

Schrödinger equation

$$\frac{\partial\psi}{\partial t} = \frac{1}{i\hbar}\frac{\partial H^s}{\partial\psi^*} = \frac{1}{i\hbar}\left[\frac{(\hat{\mathbf{p}}-q\mathbf{A})^2}{2m} + V\right]\psi$$

$$\frac{\partial\psi^*}{\partial t} = \frac{-1}{i\hbar}\frac{\partial H^s}{\partial\psi} = -\frac{1}{i\hbar}\left[\frac{(\hat{\mathbf{p}}+q\mathbf{A})^2}{2m} + V\right]\psi^*$$

$$\mathbf{J} = \frac{q}{2m}\left[\psi^*(\hat{\mathbf{p}}-q\mathbf{A})\psi + \psi(-\hat{\mathbf{p}}-q\mathbf{A})\psi^*\right]$$

Quantum current

Computer Physics Communications, 215: 63-70, 2017.

Numerical Solution of Maxwell-Schrödinger Equation

Numerical difficulties in the self-consistent solution by the FDTD method

$$\lambda_q \ll \lambda_{em}$$

multiscale of electron and photon wavelengths

$$\psi(\mathbf{r},t) \sim \exp(-i\omega_g t),\ \exp(-i\omega_e t)$$

fast oscillation of wave function

$$\psi(\mathbf{r},t) \approx a(t)\exp(-i\omega_g t)\psi_g(\mathbf{r}) + b(t)\exp(-i\omega_e t)\psi_e(\mathbf{r})$$

reduced eigenstate expansion
(two-level atomic system)

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\frac{\partial H^s}{\partial \psi^*} = \frac{1}{i\hbar}\left[\frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m} + V\right]\psi$$

$$\left\langle \psi_g, \frac{\partial \psi}{\partial t}\right\rangle = \left\langle \psi_g, \frac{1}{i\hbar}\frac{\partial H^s}{\partial \psi^*}\right\rangle$$

$$\left\langle \psi_e, \frac{\partial \psi}{\partial t}\right\rangle = \left\langle \psi_e, \frac{1}{i\hbar}\frac{\partial H^s}{\partial \psi^*}\right\rangle$$

Galerkin strategy

similar to optical Bloch equation

$$i\hbar\frac{\partial a(t)}{\partial t} = -\frac{q\mathbf{A}}{m}\langle\psi_g|\hat{\mathbf{p}}|\psi_e\rangle b(t)e^{i(\omega_g-\omega_e)t} + \frac{q^2\mathbf{A}^2}{2m}a(t)$$

$$i\hbar\frac{\partial b(t)}{\partial t} = -\frac{q\mathbf{A}}{m}\langle\psi_e|\hat{\mathbf{p}}|\psi_g\rangle a(t)e^{i(\omega_e-\omega_g)t} + \frac{q^2\mathbf{A}^2}{2m}b(t)$$

$\Longleftrightarrow$

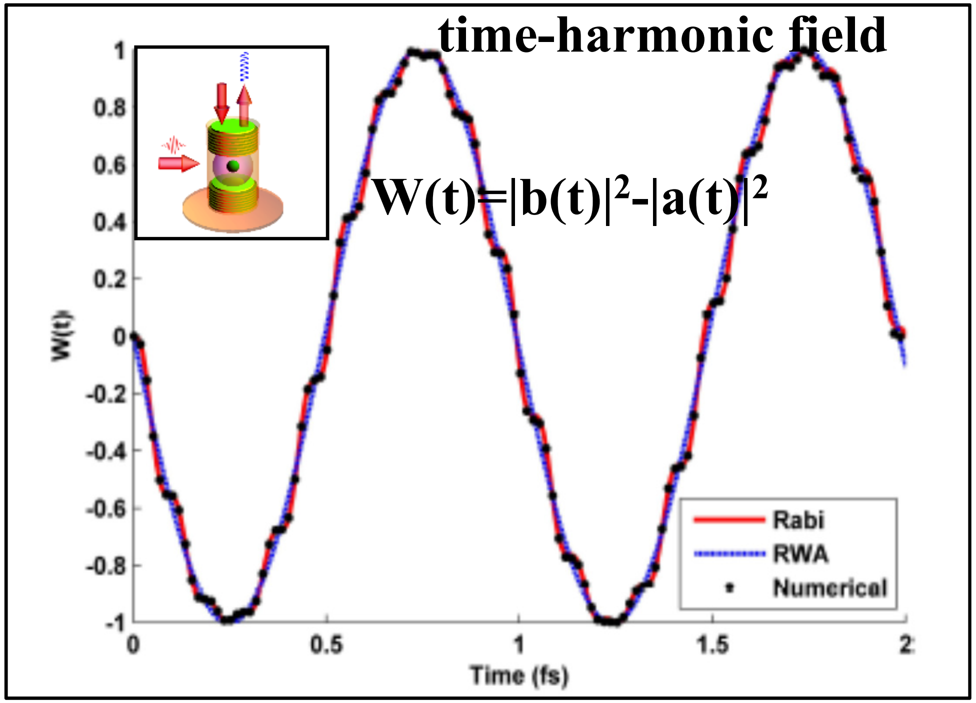
A-Y based Maxwell equation

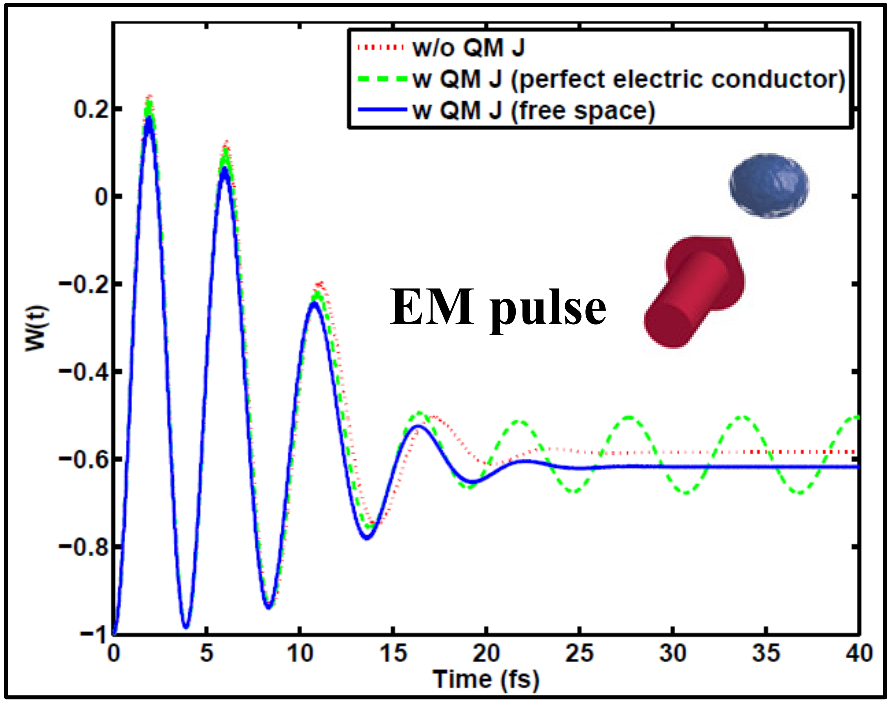
$$\frac{\partial \mathbf{A}}{\partial t} = \frac{\partial H^s}{\partial \mathbf{Y}} = \frac{\mathbf{Y}}{\epsilon_0}$$

$$\frac{\partial \mathbf{Y}}{\partial t} = -\frac{\partial H^s}{\partial \mathbf{A}} = -\frac{\nabla\times\nabla\times\mathbf{A}}{\mu_0} + \mathbf{J}$$

$$\langle \mathbf{J}\rangle = \frac{-q^2}{m}\mathbf{A}\left(|a|^2 + |b|^2\right) + \frac{q}{m}\left[a^*(t)b(t)e^{i(\omega_g-\omega_e)t}\langle\psi_g|\hat{\mathbf{p}}|\psi_e\rangle + b^*(t)a(t)e^{i(\omega_e-\omega_g)t}\langle\psi_e|\hat{\mathbf{p}}|\psi_g\rangle\right]$$

Numerical Results: Rabi Oscillation v.s. Radiative Decay





Rabi oscillation in a cavity

radiative decay in free space

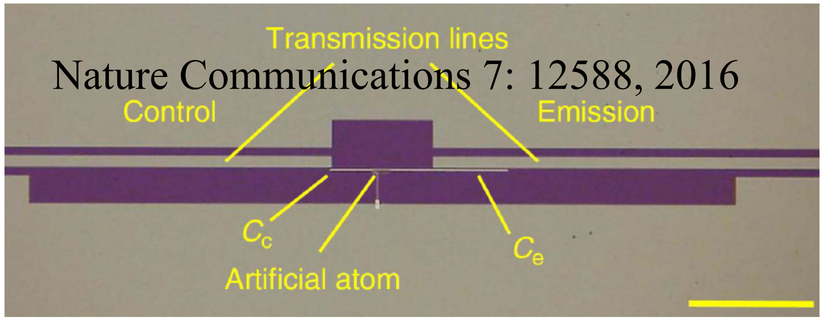
- ✓ Electromagnetic environments change dynamics of atomic transition.
- ✓ The self-consistent solution is required to capture radiative decay and shift.
- ✓ Semi-classical framework is not sufficient to capture spontaneous decay.

Full-Quantum Approach—Quantized Maxwell Equation

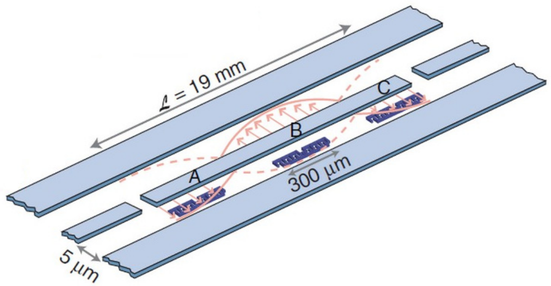
Nanofabrication techniques allow the construction of artificial atoms such as quantum dots that are microscopic in scale. In this case, semi-classical calculations do not suffice to support many of the emerging technologies, when the number of photons is limited, such as single photon devices/photodetectors.

Another interesting example is the circuit quantum electrodynamics at microwave frequencies where a superconducting quantum interference device based artificial atom is entangled with coplanar waveguide microwave resonators. For these situations, Maxwell equation should be quantized.

single photon source



circuit quantum electrodynamics

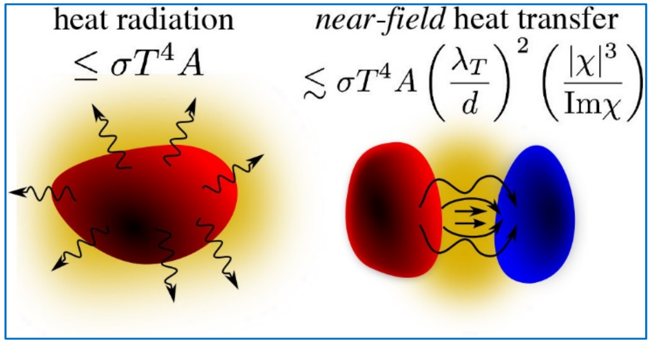


IEEE Journal on Multiscale and Multiphysics Computational Techniques, 1: 73-97, 2016.

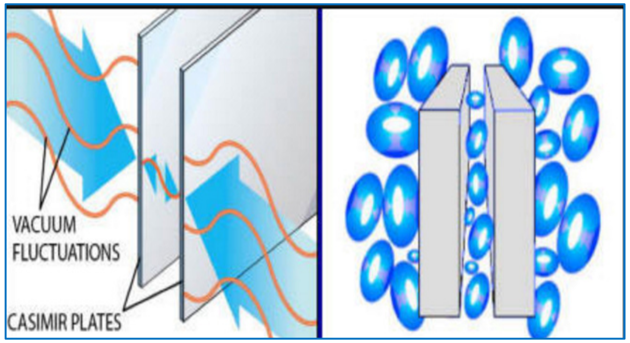
Why is Quantized Maxwell Equation Required? Cont.

Nano-fabrication also induces the quantum effects in heat transfer. While phonons require material media for heat transfer, photons can account for near-field heat transfer through vacuum where classical heat conduction equation and Kirchhoff law of thermal radiation are invalid.

Experiments confirmed that Casimir force is real, and entirely quantum: it can be only explained using quantum theory of electromagnetic field in its quantized form. Also, Casimir force cannot be explained by classic electromagnetics theory that assumes null electromagnetic field in vacuum.



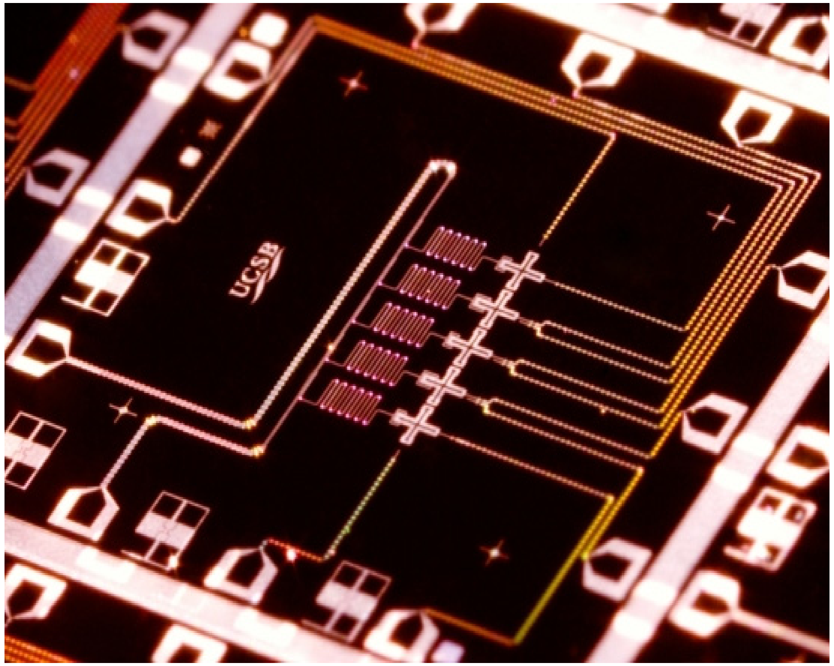
O. D. Miller, SPIE newsroom.
doi: 10.1117/2.1201610.006706



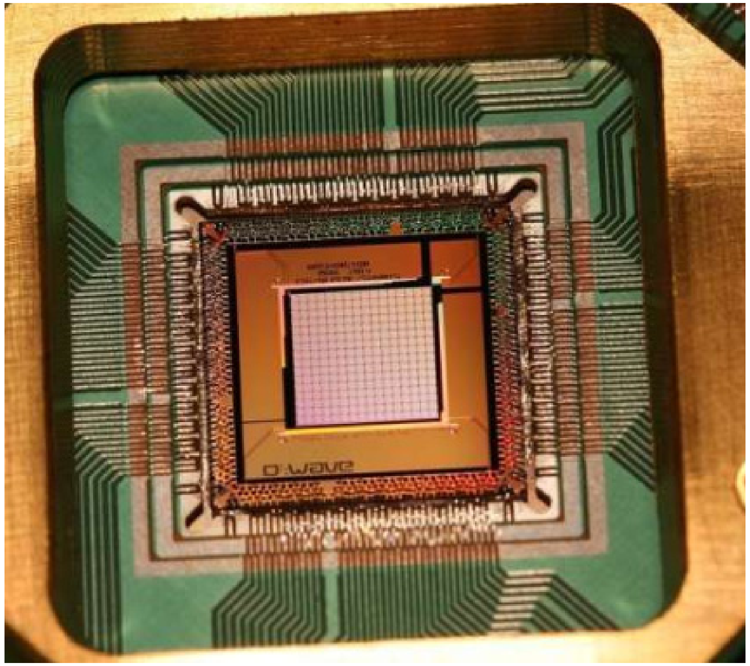
from wiki
https://en.wikipedia.org/wiki/Casimir_effect

Why is Quantized Maxwell Equation Required? Cont.

Quantum computer: Is it a reality or a science fiction?
No reliable solver for quantum electromagnetics!
(Quantum) electromagnetics is "engineering" (quantum) electrodynamics.



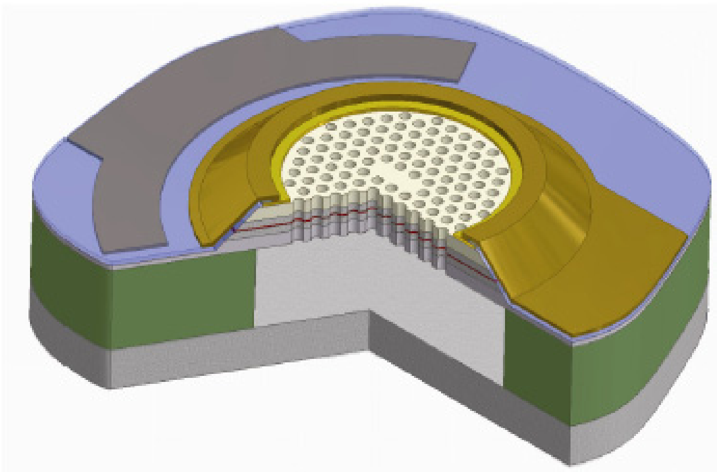
superconducting quantum circuits
R. Barends, Nature 508: 500-503, 2014

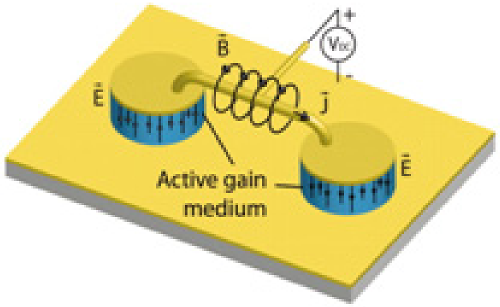


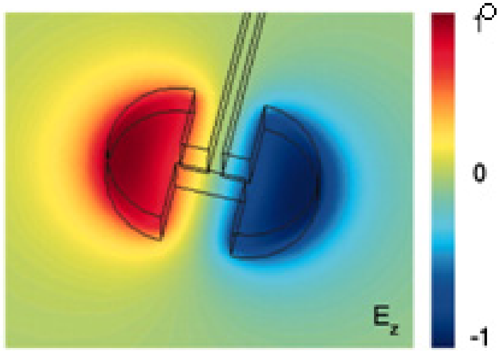
D-Wave's 1000+ qubit computer chip
under development (Google)

Starting from Spontaneous Emission (Decay)

Control of spontaneously emitted light lies at the heart of quantum electromagnetics. It is essential for diverse applications ranging from laser, light-emitting diode (LED), solar cell, and quantum computer.







LED (photonic crystal cavity)

Purcell factor

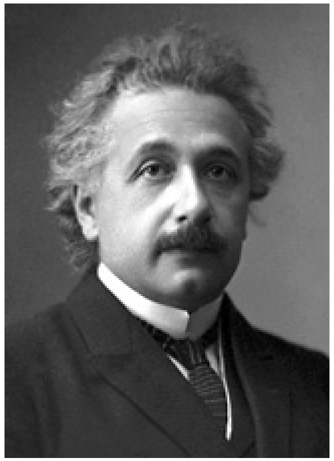
Laser (metallic microcavity)

M. Francardi, Applied Physics Letters 93: 143102, 2008.
C. Walther, Science 327: 1495-1497, 2010.

History of Spontaneous Emission (A Classical View)

Boltzmann statistics

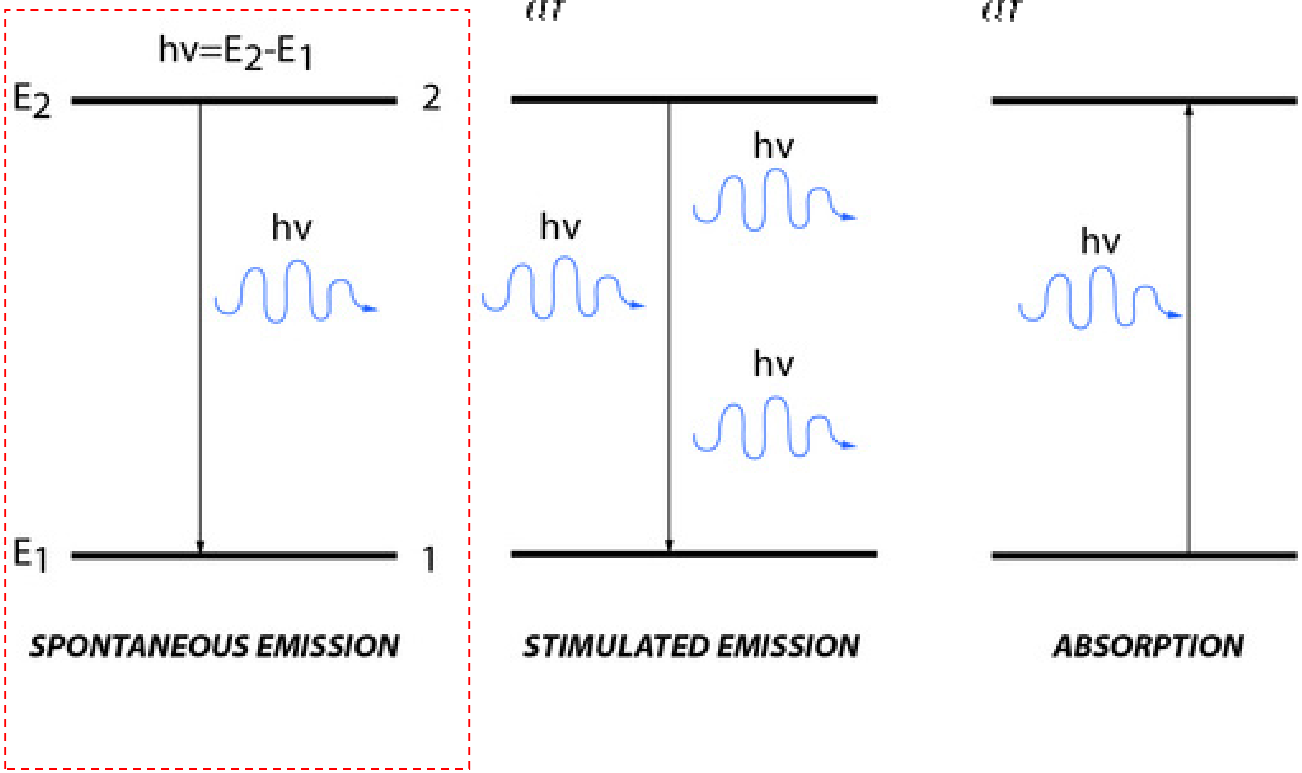
$$\frac{N_2}{N_1} = e^{\frac{-(E_2 - E_1)}{kT}}$$



$$\frac{dN_2}{dt} = -\boxed{A} N_2$$

Light-intensity dependent

$$\frac{dN_2}{dt} = -W_{21} N_2 \qquad \frac{dN_1}{dt} = -W_{12} N_1$$



spontaneous emission: an exited electron decays to the ground state and emits a photon

Quantization of Maxwell Equation by Mode Decomposition

$$\hat{H}\left(\hat{\mathbf{A}},\hat{\mathbf{Y}},\hat{\mathbf{p}}\right)=\hat{H}^{em}\left(\hat{\mathbf{A}},\hat{\mathbf{Y}}\right)+H_0^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right)+H_I^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right) \qquad \hat{H}\Psi(t)=i\hbar\frac{\partial\Psi(t)}{\partial t}$$

electromagnetic part | atomic part | interaction part

$$\hat{H}^{em}\left(\hat{\mathbf{A}},\hat{\mathbf{Y}}\right)=\int_\Omega\left(\frac{1}{2\epsilon_0}\left|\hat{\mathbf{Y}}\right|^2+\frac{1}{2\mu_0}\left|\nabla\times\hat{\mathbf{A}}\right|^2\right)d\mathbf{r} \qquad H_0^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right)=\frac{\hat{\mathbf{p}}^2}{2m}+V \qquad H_I^q\left(\hat{\mathbf{p}},\hat{\mathbf{A}}\right)\approx\frac{q\hat{\mathbf{p}}\cdot\hat{\mathbf{A}}}{m}$$

quantized field (wave-particle duality)

$$\hat{\mathbf{A}}=\sum_k\frac{\alpha_k}{\omega_k}\left(\mathbf{U}_k(\mathbf{r})\hat{a}_k+\mathbf{U}_k^*(\mathbf{r})\hat{a}_k^+\right),\ \alpha_k=\sqrt{\frac{\hbar\omega_k}{2\epsilon_0}}$$

$$\hat{H}^{em}=\sum_k\left(a_k^+a_k+\frac{1}{2}\right)\hbar\omega_k$$

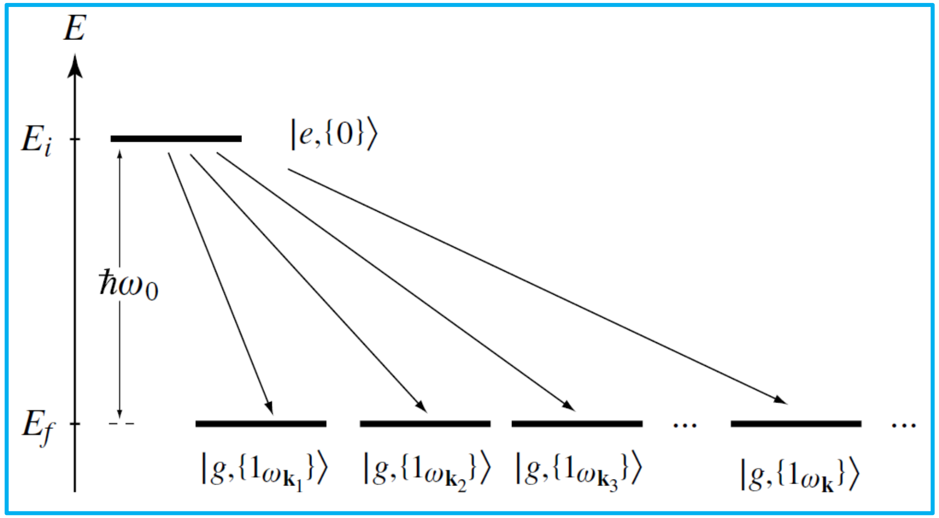
eigenmode (wave) — annihilation and creation operators (particle)

wave function expansion

$$\Psi(t)=a(t)|e,0>+\sum_k b_k(t)|g,1_k>$$

e: excited state, 0: no photon; g: ground state, 1: one photon

Quantum Electromagnetics Interpretation for Spontaneous Emission



$\boxed{\dfrac{d}{dt}|a(t)|^2}$ spontaneous decay rate

$$\gamma(\mathbf{r}_0,\omega_0)=\frac{\pi\omega_0}{\epsilon_0\hbar}\sum_k[\mathbf{p}\cdot(\mathbf{u}_\mathrm{k}\mathbf{u}_\mathrm{k}^*)\cdot\mathbf{p}]\delta(\omega_\mathrm{k}-\omega_0)$$

$$\gamma(\mathbf{r}_0,\omega_0)=\frac{2\omega_0^2}{\epsilon_0\hbar c^2}\langle\mathbf{p}\cdot\mathrm{Im}[\bar{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)]\cdot\mathbf{p}\rangle$$

eigenmode expansion

$$\mathrm{Im}\left[\bar{\mathbf{G}}(\mathbf{r},\mathbf{r}',\omega_0)\right]=\frac{\pi c^2}{2\omega_0}\sum_k\mathbf{u}_\mathbf{k}(\mathbf{r},\omega_k)\mathbf{u}_\mathbf{k}^*(\mathbf{r}',\omega_k)\delta\left(\omega_k-\omega_0\right)$$

photon local density of states (LDOS)

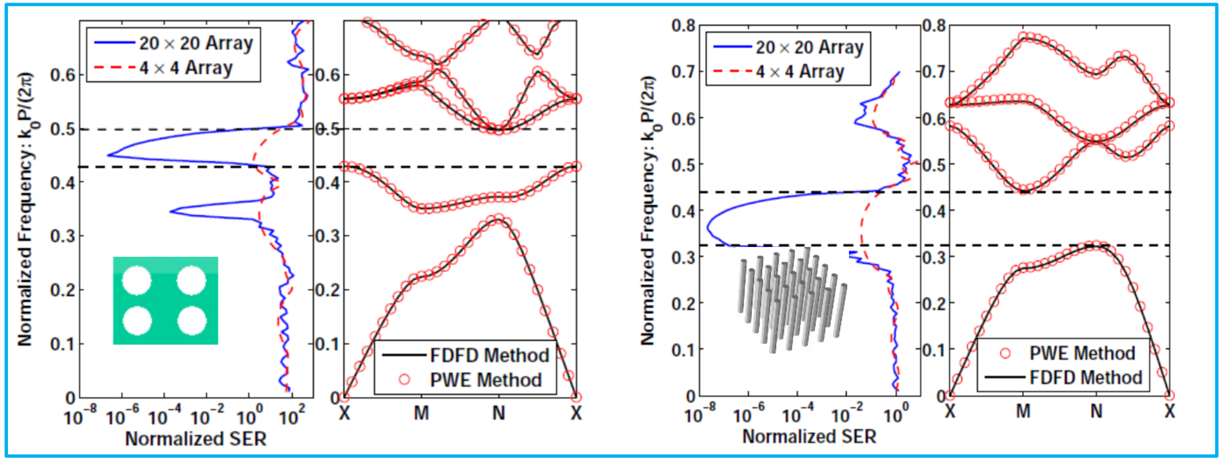
$$\begin{aligned}\rho(\mathbf{r}_0,\omega_0)&=\sum_\mathbf{k}|\mathbf{u}_\mathbf{k}|^2\delta(\omega_\mathbf{k}-\omega_0)\\&=\frac{2\omega_0}{\pi c^2}\mathrm{Im}\left\{\mathrm{Tr}\left[\bar{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\right]\right\}\end{aligned}$$

Purcell factor

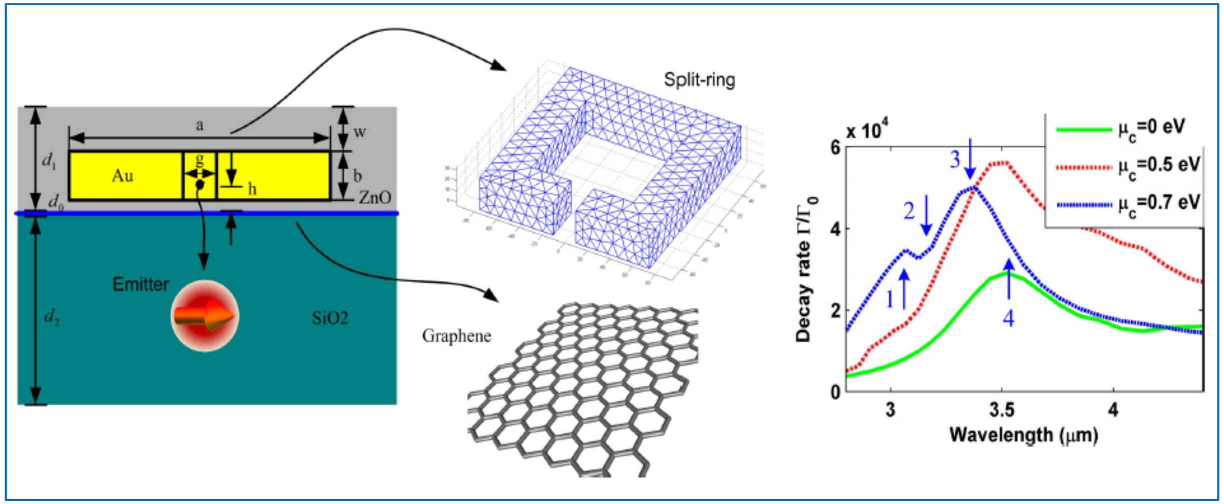
$$\frac{\gamma}{\gamma_0}=\frac{\rho(\mathbf{r}_0,\omega_0)}{\rho_0(\mathbf{r}_0,\omega_0)}=\frac{\mathrm{Im}\left\{\mathrm{Tr}\left[\bar{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\right]\right\}}{\mathrm{Im}\left\{\mathrm{Tr}\left[\bar{\mathbf{G}}_0(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\right]\right\}}$$

Spontaneous Emission by Computational Electromagnetics (CEM) Method

Physical Review A, 83(4): 043824, 2011.
Optics Express, 23(3): 2798-2807, 2015.



Finite-difference method is adopted to find Green's function in inhomogeneous environment.



PMCHWT formula and multilayer Green's functions are adopted to find Green's function in inhomogeneous environment.

Computational quantum electromagnetics (CQEM) is future of CEM !

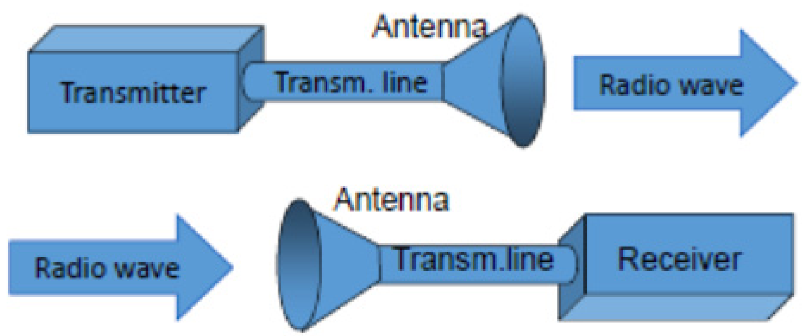
Why is Quantum Electromagnetics Important to Optical Antenna?

<u>Radio</u>

Transmitter:
current (voltage) source

Receiver:
electrical load

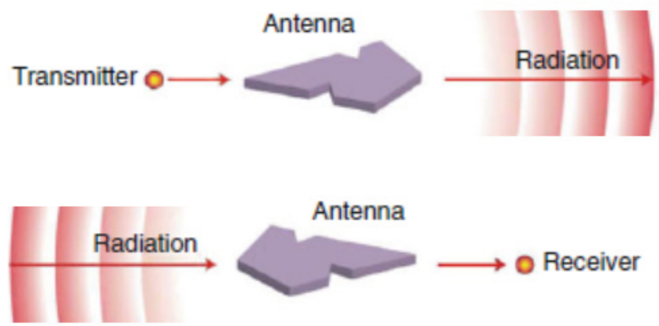
Resonant Transducer (PEC):
half-wavelength limit
scaling law



<u>Optical</u>

Transmitter/Receiver:
quantum dots
atoms
molecules
ions

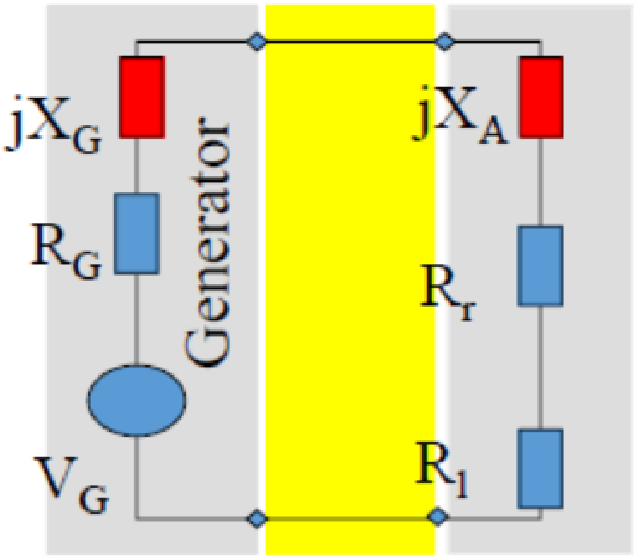
Resonant Transducer (Silver, Gold):
break half-wavelength limit
break scaling law



Transmitter and receiver in optical antennas are quantum emitters!

Input Impedance v.s. Local Density of States (1)

impedance matching for radio antennas



Maximum Power Condition

$$R_A = R_r + R_l = R_G,\ X_A = -X_G$$

$$P_G = P_A = \frac{V_G^2}{4R_G},\ P_r = P_A \frac{R_r}{(R_r + R_l)}$$

complex conjugate matching

The transmitter with the transmission line is represented by an (Thevenin) equivalent generator (with V_G, R_G and X_G)

The antenna is represented by its **input impedance** (which is frequency-dependent and is influenced by objects nearby) as seen from the generator

jX_A represents energy stored in electric (E_e) and magnetic (E_m) near-field components; if $|E_e| = |E_m|$ then $X_A = 0$ (antenna resonance)

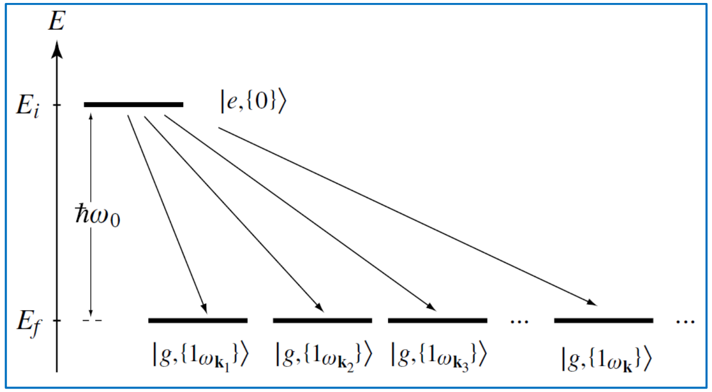
R_r represents energy radiated into space (far-field components)

R_l represents energy lost, i.e. transformed into heat in the antenna structure

Input Impedance v.s. Local Density of States (2)

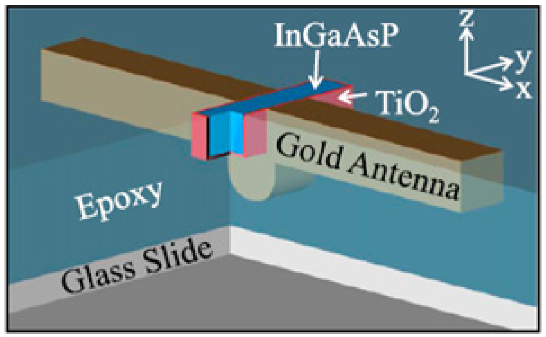
local density of states for <u>optical antennas</u>

The LDOS counts the number of EM modes at the emitter point. Each EM mode can be taken as a decay channel. The more decay channels there are, the easier it is for an excited atom to emit photons via returning to its ground state.

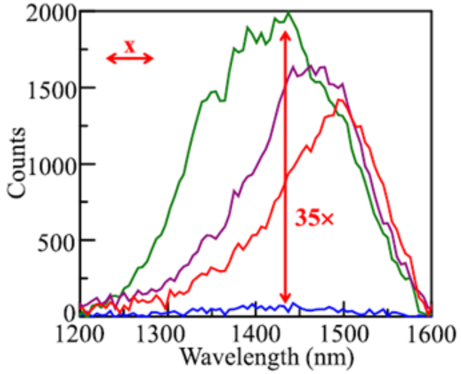


In isotropic, inhomogeneous, and nonmagnetic medium, LDOS is represented by the dyadic Green's function in inhomogeneous environment

$$\rho(\mathbf{r}_0,\omega_0)=\frac{2\omega_0}{\pi c^2}\mathrm{Tr}\left\{\Im\mathrm{m}\left[\overline{\mathbf{G}}^{c}(\mathbf{r}_0,\mathbf{r}_0;\omega_0)\right]\right\}$$



PNAS, 112(6): 1704, 2015



Optical antennas significantly boost LDOS due to localized near-field enhancement by plasmonic effects.

blue: without antenna; others: with antenna of different arm lengths

Field-Matter Hamiltonian in Dispersive Media

In dispersive and lossy media, eigenmodes are not orthogonal with each other. The completeness of eigenmodes is questionable. Thus, quantization of Maxwell equation with the mode decomposition is not proper. Here, we start from a field-matter Hamiltonian and the dispersive media is modeled by classical Lorenz model.

field-matter Hamiltonian

$$H = \int dx^4 \frac{1}{2}\left[\underbrace{\mathbf{E}^2 + \mathbf{H}^2}_{\text{field}} + \underbrace{\beta \mathbf{V}^2 + f\mathbf{P}^2}_{\text{matter}}\right] \quad \beta = 1/\omega_p^2,\ f = \omega_0^2/\omega_p^2$$

A-Phi-P-V Hamiltonian

$$H = \int d\mathrm{r}\,\frac{1}{2}\Big[(\mathbf{\Pi}_{AP} + \mathbf{P})^2 + (\nabla \times \mathbf{A})^2 + (\nabla \cdot \mathbf{A})^2 - \Pi_\Phi^2 - (\nabla\Phi)^2 + \mathbf{\Pi}_P^2/\beta + f\mathbf{P}^2 + 2\mathbf{P}\cdot\nabla\Phi\Big]$$

quantized Hamiltonian

$$\hat{H} = \int d\mathrm{r}\,\frac{1}{2}\Big[\left(\hat{\mathbf{\Pi}}_{AP} + \hat{\mathbf{P}}\right)^2 + \left(\nabla \times \hat{\mathbf{A}}\right)^2 + \left(\nabla \cdot \hat{\mathbf{A}}\right)^2 - \hat{\Pi}_\Phi^2 - \left(\nabla\hat{\Phi}\right)^2 + \hat{\mathbf{\Pi}}_P^2/\beta + f\hat{\mathbf{P}}^2 + 2\hat{\mathbf{P}}\cdot\nabla\hat{\Phi}\Big]$$

IEEE Journal on Multiscale and Multiphysics Computational Techniques
Dissipative Quantum Electromagnetics, DOI: 10.1109/JMMCT.2018.2881691.

Quantization in Dispersive Media

quantized motion equations

$$\left[\hat{\Pi}_{AP}(\mathbf{r},t),\hat{H}\right]=-i\hbar\frac{\delta\hat{H}}{\delta\hat{\mathbf{A}}(\mathbf{r},t)}=i\hbar\dot{\hat{\Pi}}_{AP}(\mathbf{r},t)$$

$$\left[\hat{\mathbf{A}}(\mathbf{r},t),\hat{H}\right]=i\hbar\frac{\delta\hat{H}}{\delta\hat{\Pi}_{AP}(\mathbf{r},t)}=i\hbar\dot{\hat{\mathbf{A}}}(\mathbf{r},t)$$

$$\left[\hat{\Pi}_{\Phi}(\mathbf{r},t),\hat{H}\right]=i\hbar\frac{\delta\hat{H}}{\delta\hat{\Phi}(\mathbf{r},t)}=i\hbar\dot{\hat{\Pi}}_{\Phi}(\mathbf{r},t)$$

$$\left[\hat{\Phi}(\mathbf{r},t),\hat{H}\right]=-i\hbar\frac{\delta\hat{H}}{\delta\hat{\Pi}_{\Phi}(\mathbf{r},t)}=i\hbar\dot{\hat{\Phi}}(\mathbf{r},t)$$

$$\left[\hat{\Pi}_{P}(\mathbf{r},t),\hat{H}\right]=-i\hbar\frac{\delta\hat{H}}{\delta\hat{\mathbf{P}}(\mathbf{r},t)}=i\hbar\dot{\hat{\Pi}}_{P}(\mathbf{r},t)$$

$$\left[\hat{\mathbf{P}}(\mathbf{r},t),\hat{H}\right]=i\hbar\frac{\delta\hat{H}}{\delta\hat{\Pi}_{P}(\mathbf{r},t)}=i\hbar\dot{\hat{\mathbf{P}}}(\mathbf{r},t)$$

quantized Maxwell equation

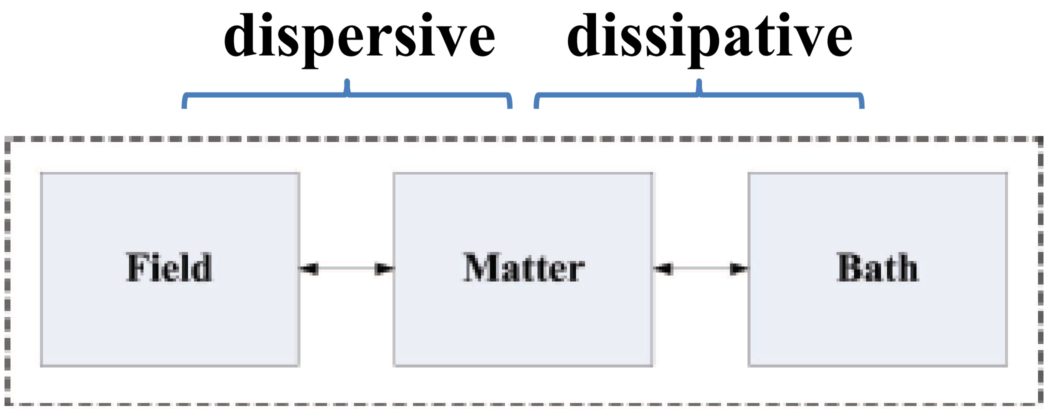
$$\ddot{\hat{\mathbf{P}}}(\mathbf{r},t)+\omega_0^2\hat{\mathbf{P}}(\mathbf{r},t)=\omega_p^2\hat{\mathbf{E}}(\mathbf{r},t)$$

$$\dot{\hat{\mathbf{H}}}(\mathbf{r},t)=-\nabla\times\dot{\hat{\mathbf{E}}}(\mathbf{r},t)$$

$$\dot{\hat{\mathbf{E}}}(\mathbf{r},t)=\nabla\times\dot{\hat{\mathbf{H}}}(\mathbf{r},t)-\hat{\mathbf{V}}(\mathbf{r},t)$$

$$\dot{\hat{\mathbf{P}}}(\mathbf{r},t)=\hat{\mathbf{V}}(\mathbf{r},t)$$

Matter-Bath Coupled System



The matter-bath model can be understood that the matter system expressed by a single quantum harmonic oscillator (QHO) is coupled to the noise bath system, which is expressed by infinite number of QHOs. The matter-bath Hamiltonian still satisfies the energy conversion property

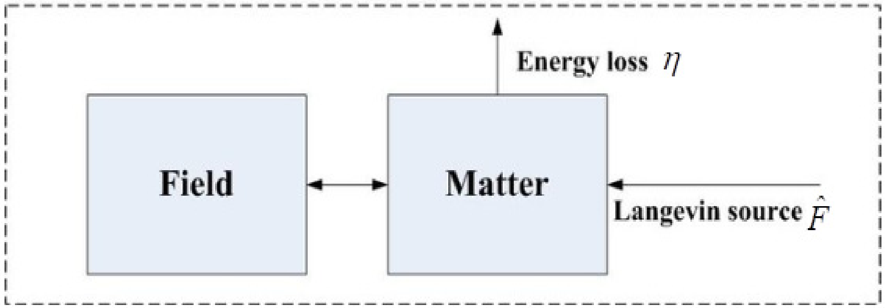
$$\hat{H}_{PB} = \frac{1}{2}\hbar\omega_0\left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right) + \sum_j \frac{1}{2}\hbar\omega_j\left(\hat{b}_j\hat{b}_j^\dagger + \hat{b}_j^\dagger\hat{b}_j\right)$$

matter **bath**

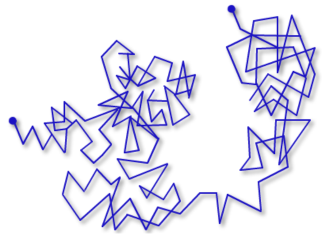
$$+\sum_j \hbar\frac{\alpha_j^\zeta + \alpha_j^\pi}{\sqrt{2}}\left(\hat{a}\hat{b}_j^\dagger + \hat{a}^\dagger\hat{b}_j\right)$$
$$+\sum_j \hbar\frac{\alpha_j^\zeta - \alpha_j^\pi}{\sqrt{2}}\left(\hat{a}\hat{b}_j + \hat{a}^\dagger\hat{b}_j^\dagger\right)$$

interaction

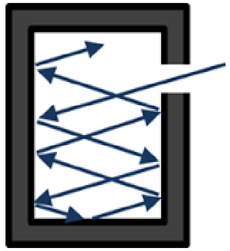
Introduction of Loss in Quantization Procedure



Brownian motion



Blackbody radiation



Motion equation of matter-bath system (quantized coupled mode equations)

$$\dot{\hat{a}} = -i\left(\omega_0 \hat{a} + \sum_j \tilde{\gamma}_j \hat{b}_j\right)$$

$$\dot{\hat{b}}_j = -i\left(\omega_j \hat{b}_j + \tilde{\gamma}_j \hat{a}\right)$$

$\Rightarrow$

Motion equation of matter system in ensemble average sense

$$\dot{\hat{a}} = -i\omega_0 \hat{a} - \eta \hat{a} + \hat{F}(t)$$

$$\langle [\hat{F}(t), \hat{F}^\dagger(t')] \rangle = 2\eta\delta(t - t')$$

When the matter (single QHO) is coupled to bath (many QHOs like white noise), it loses energy to the bath (related to $\boldsymbol{\eta}$). Simultaneously, the bath pumps energy back to the matter (related to $\boldsymbol{F}$). By energy conservation, at thermal equilibrium, the loss and gain energy, should be equal to each other in the ensemble average sense.

Connection to Fluctuation-Dissipation Theorem

Maxwell equation in time-domain

$$\dot{\hat{\mathbf{H}}} = -\nabla \times \hat{\mathbf{E}}$$

$$\dot{\hat{\mathbf{E}}} = \nabla \times \hat{\mathbf{H}} - \dot{\hat{\mathbf{P}}}$$

$$\dot{\hat{\mathbf{\Pi}}} = -\omega_0 \hat{\mathbf{P}} - \eta \hat{\mathbf{\Pi}} + \hat{\mathbf{F}}_I + \frac{\omega_p^2}{\omega_0} \hat{\mathbf{E}}$$

$$\dot{\hat{\mathbf{P}}} = \omega_0 \hat{\mathbf{\Pi}} - \eta \hat{\mathbf{P}} + \hat{\mathbf{F}}_R$$

$$\left\langle \left[\hat{\mathbf{F}}_R, \hat{\mathbf{F}}_I \right] \right\rangle = i2\eta \frac{\omega_p^2 \hbar}{\omega_0} \delta(t - t') \hat{\bar{\mathbf{I}}}$$

Wave equation in frequency domain

$$\nabla \times \nabla \times \hat{\mathbf{E}}(\mathbf{r}, \omega) - \omega^2 \epsilon(\mathbf{r}, \omega) \hat{\mathbf{E}}(\mathbf{r}, \omega) = i\omega \hat{\mathbf{j}}_n(\mathbf{r}, \omega)$$

$$\hat{\mathbf{j}}_n(\mathbf{r}, \omega) = \frac{-i\omega\omega_0 \hat{\mathbf{F}}_I(\mathbf{r}) - i\omega \left[\eta(\mathbf{r}) - i\omega \right] \hat{\mathbf{F}}_R(\mathbf{r})}{\left[\eta(\mathbf{r}) - i\omega \right]^2 + \omega_0^2}$$

$$\epsilon(\mathbf{r}, \omega) = 1 + \frac{\omega_p^2}{\left[\eta(\mathbf{r}) - i\omega \right]^2 + \omega_0^2}$$

$$\langle [\hat{\mathbf{F}}_R(\omega), \hat{\mathbf{F}}_I^\dagger(\omega')] \rangle = \frac{i\eta}{\pi} \frac{\omega_p^2 \hbar}{\omega_0} \delta(\omega - \omega')$$

$$\left\langle \left[\hat{\mathbf{j}}_n(\mathbf{r}, \omega), \hat{\mathbf{j}}_n^\dagger(\mathbf{r}, \omega') \right] \right\rangle = \frac{\hbar\omega}{\pi} \sigma(\mathbf{r}, \omega) \delta(\omega - \omega')$$

Fluctuation-dissipation theorem

Comparisons between Our Approach and Welsch's Approach

polariton Hamiltonian

$$\hat{H} = \int d^3\mathbf{r} \int_0^\infty d\omega\ \hbar\omega \hat{\mathbf{f}}^\dagger(\mathbf{r},\omega)\cdot\hat{\mathbf{f}}(\mathbf{r},\omega)$$

commutation relation

$$[\hat{f}_i(\mathbf{r},\omega), \hat{f}_j^\dagger(\mathbf{r}',\omega')] = \delta_{ij}\delta(\mathbf{r}-\mathbf{r}')\delta(\omega-\omega')$$

postulated noise current operator

$$\hat{\underline{\mathbf{j}}}_{\mathrm{n}}(\mathbf{r},\omega) = \frac{\omega}{c^2}\sqrt{\frac{\hbar}{\pi\epsilon_0}\epsilon_{\mathrm{I}}(\omega)}\hat{\mathbf{f}}(\mathbf{r},\omega)$$

Welsch

$$\xrightarrow{\text{derivation}}$$

$$\xleftarrow[\text{proof}]{}$$

preservation of canonical field commutation

$$[\hat{A}_i(\mathbf{r}), \hat{E}_j(\mathbf{r}')] = -\frac{i\hbar}{\epsilon_0}\delta_{ij}^{\perp}(\mathbf{r}-\mathbf{r}')$$

Phys. Rev. A 51(4): 3246, 1995; Phys. Rev. A 53(3): 1818, 1996; Phys. Rev. A 57(5): 3931, 1998.

$$\sigma/(\omega\varepsilon_0) = \varepsilon_{\mathrm{I}}$$

energy conservation of matter-bath system

$$\xrightarrow{\text{derivation}}$$

$$\left\langle \left[\hat{\mathbf{j}}_n(\mathbf{r},\omega), \hat{\mathbf{j}}_n^\dagger(\mathbf{r},\omega')\right] \right\rangle = \frac{\hbar\omega}{\pi}\sigma(\mathbf{r},\omega)\delta(\omega-\omega')$$

Conclusion

1. Quantum electromagnetics is fundamentally important to emerging quantum communication, computer, and information.

2. When field intensity is strong, the classical Maxwell equation can be coupled to Schrödinger equation to model the semi-classical quantum electromagnetic problems.

3. When field intensity is weak, equivalently, the photon number is limited, the Maxwell equation should be quantized and then coupled to Schrödinger equation to model the full quantum electromagnetics problems.

4. For lossless media or loss can be ignored, the Maxwell equation can be quantized by mode decomposition approach. For lossy and dispersive media, the Maxwell equation should be quantized by introducing the Langevin source.

5. In future, we will explore applications of the semi-classical quantum electromagnetics and also develop the numerical solution to the full quantum electromagnetics problems in inhomogeneous, lossy, and dispersive media.

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Future Works — Gauge Problems

Coulomb gauge

$$\nabla\cdot\epsilon\mathbf{A}=0$$

$$-\nabla\cdot(\epsilon\nabla\phi)=\rho,\ \ \rho(\mathbf{r},t)=q(n_p(\mathbf{r},t)+n_q(\mathbf{r},t))$$

$$\nabla\times\nabla\times\mathbf{A}+\mu_0\epsilon\frac{\partial^2\mathbf{A}}{\partial t^2}=\mu_0(\mathbf{J}_p^t+\mathbf{J}_q^t)$$

Lorenz gauge

$$\epsilon^{-1}\nabla\cdot\epsilon\mathbf{A}=-\epsilon\mu_0\partial\phi/\partial t$$

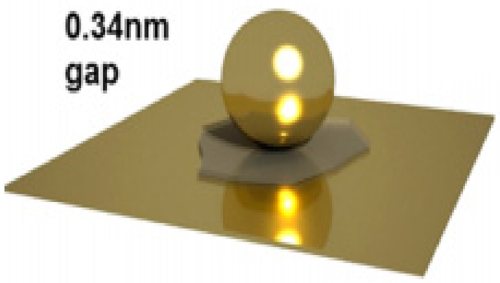
$$\nabla\cdot\epsilon\nabla\phi-\epsilon^2\mu_0\frac{\partial^2\phi}{\partial t^2}=-\rho$$

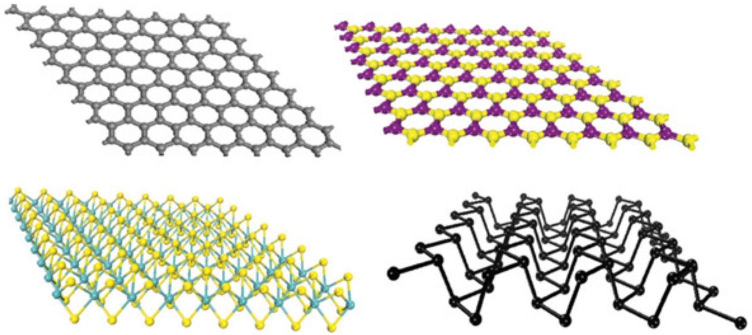
$$\nabla\times\nabla\times\mathbf{A}+\mu_0\epsilon\frac{\partial^2\mathbf{A}}{\partial t^2}-\epsilon\nabla\epsilon^{-2}\nabla\cdot\epsilon\mathbf{A}=\mu_0(\mathbf{J}_p+\mathbf{J}_q)$$

simple gauge $\nabla\cdot\mathbf{A}=-\epsilon_0\mu_0\partial\phi/\partial t$

1. Complexity of solving Poisson equation is large.
2. Second-order time derivatives will introduce more memory.
3. Generalized Lorenz gauge will face material discontinuities.
4. Does Gauge invariant still hold in inhomogeneous media?

Future Works — Real Material Systems





EM response
from 2D materials

Vector Potential Equations

$$-\frac{1}{c}\frac{\partial}{\partial t}\vec{\nabla}\vec{A} = 4\pi e\,(n_{\text{ion}} - n)$$

$$\frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} - \nabla^2 \vec{A} + \vec{\nabla}(\vec{\nabla}\cdot\vec{A}) = -\frac{4\pi e}{c}\vec{j}$$

$$\Updownarrow$$

$$i\hbar\frac{\partial}{\partial t}\psi_{i,\mathbf{R}}(\vec{r},t) = \left\{\frac{1}{2m}\left[-i\hbar\nabla_{\vec{r}} + \frac{e}{c}\vec{A}_{\mathbf{R}}(t)\right]^2 - e\phi_{\mathbf{R}}(\vec{r},t) + \frac{\delta E_{xc}}{\delta n}\right\}\psi_{i,\mathbf{R}}(\vec{r},t)$$

$$n_{\mathbf{R}}(\vec{r},t) = \sum_i |\psi_{i,\mathbf{R}}(\vec{r},t)|^2$$

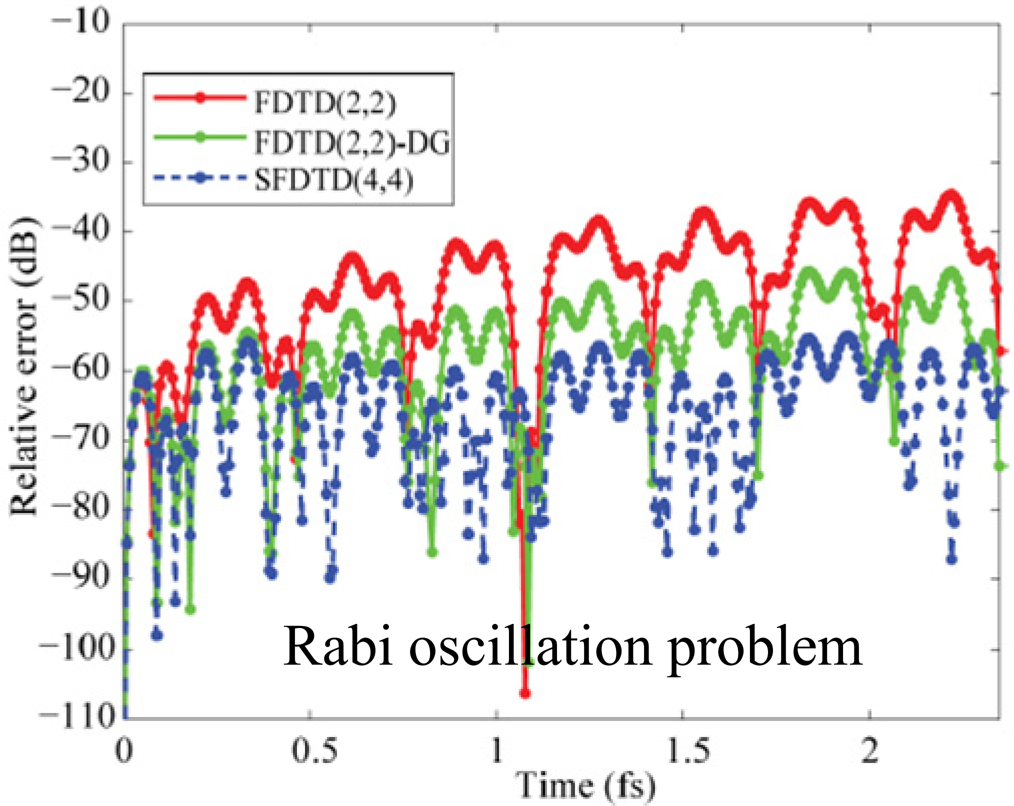
$$\vec{j}_{\mathbf{R}}(\vec{r},t) = \frac{1}{2m}\sum_i \left\{\psi^*_{i,\mathbf{R}}(\vec{r},t)\left[-i\hbar\vec{\nabla}_{\vec{r}} + \frac{e}{c}\vec{A}_{\mathbf{R}}(t)\right]\psi_{i,\mathbf{R}}(\vec{r},t) - \psi_{i,\mathbf{R}}(\vec{r},t)\left[i\hbar\vec{\nabla}_{\vec{r}} + \frac{e}{c}\vec{A}_{\mathbf{R}}(t)\right]\psi^*_{i,\mathbf{R}}(\vec{r},t)\right\}$$

Time-Dependent Density Functional Theory

Future Works — Reliable Solvers (Unpublished Results)

1. Does perfectly matched layer (PML) perform well for A-Phi equations?
2. Is FDTD accurate or stable enough for the semi-classical framework?

High-order symplectic scheme



Error increases by FDTD even with dense grids (DG) !

Guoda Xie

Ming Fang

Zhixiang Huang

Future Works — Numerical Solution of Full-Quantum Approach

How to solve the full-quantum approach rigorously under interaction picture?

$$i\hbar \frac{\partial \Psi_I(t)}{\partial t} = \hat{\mathbf{V}}_I(t)\Psi_I(t)$$

$$|\Psi_S(0)\rangle = |g\rangle|0\rangle$$

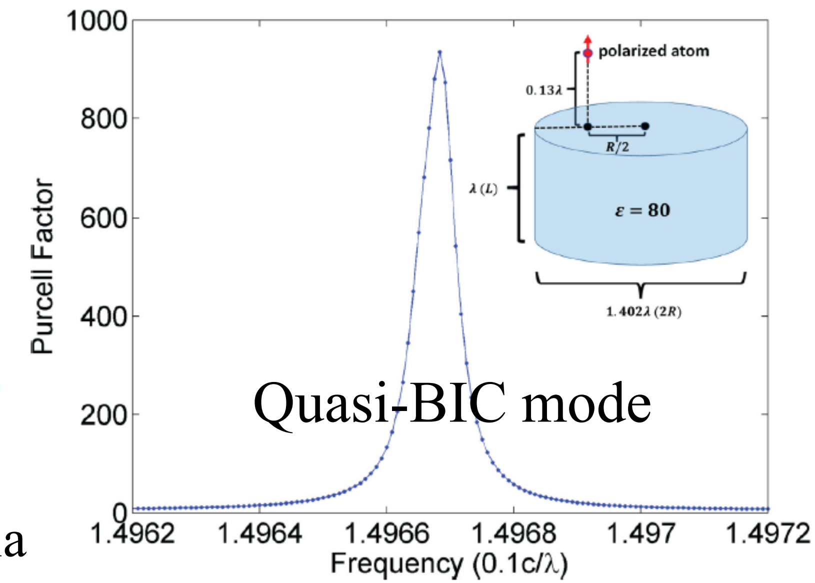
$$\longrightarrow \quad \boxed{\Psi_I(t) = \exp\left(\frac{1}{i\hbar}\int_0^t \hat{\mathbf{V}}_I(t)dt\right)|\Psi_S(0)\rangle}$$

Now, we only solve it perturbatively for spontaneous emission problem

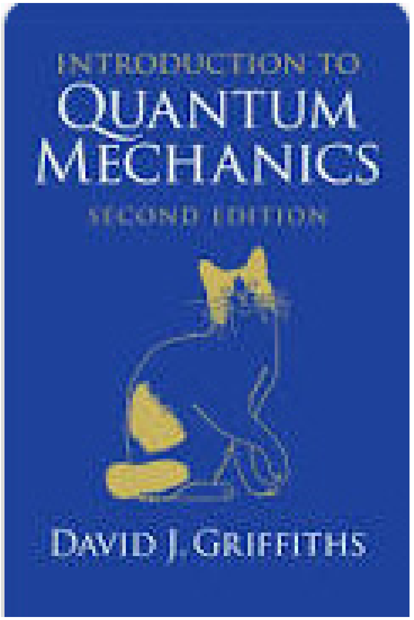
$$\gamma = \frac{d\langle\hat{\sigma}_e\rangle}{dt} = \frac{2\pi|\mu_{eg}|^2}{\hbar^2}\langle 0|\hat{\mathbf{E}}_S^+(\omega_{eg})\hat{\mathbf{E}}_S^-(\omega_{eg})|0\rangle$$

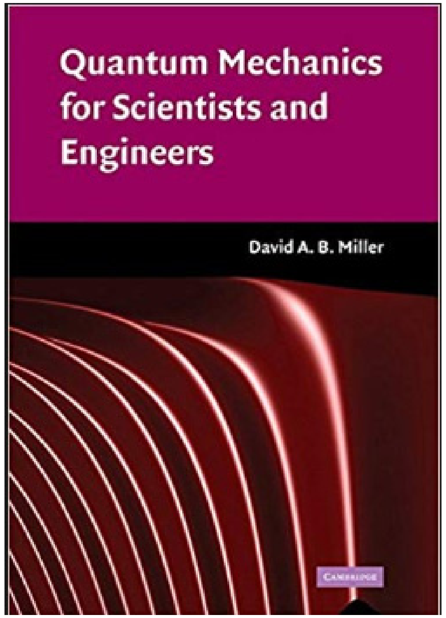
$$\langle 0|\hat{\mathbf{E}}_S^+(\mathbf{r}_0,\omega_{eg})\hat{\mathbf{E}}_S^-(\mathbf{r}_0,\omega_{eg})|0\rangle = \frac{\hbar\omega_{eg}^2}{\pi c^2\epsilon_0}[\bar{n}(\omega_{eg},T)+1]\Im\overline{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_{eg})$$

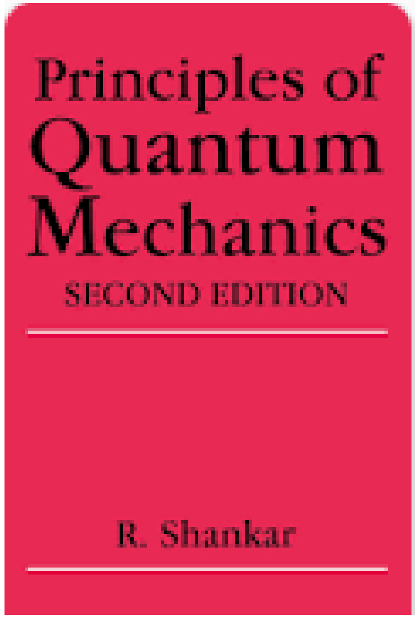
dyadic Green's function in inhomogeneous media

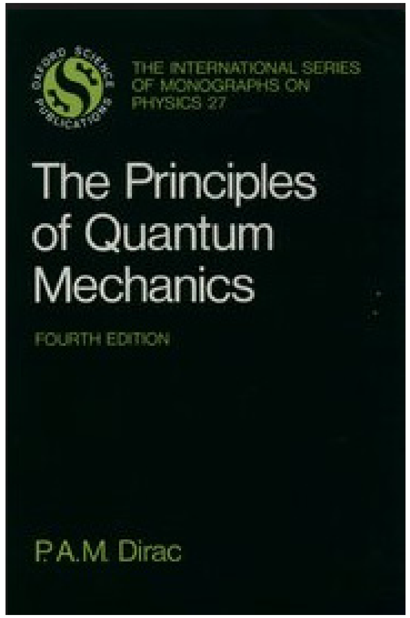


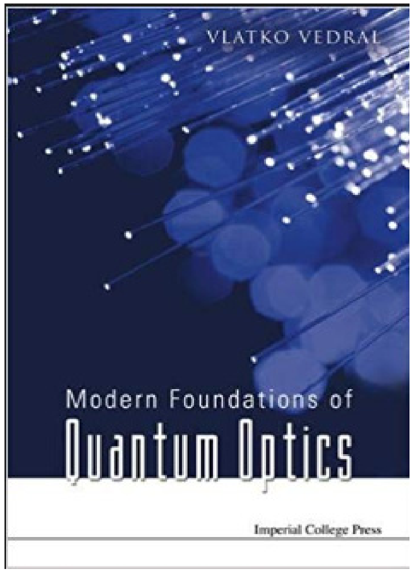
Books for Beginners in Field of Quantum Electromagnetics

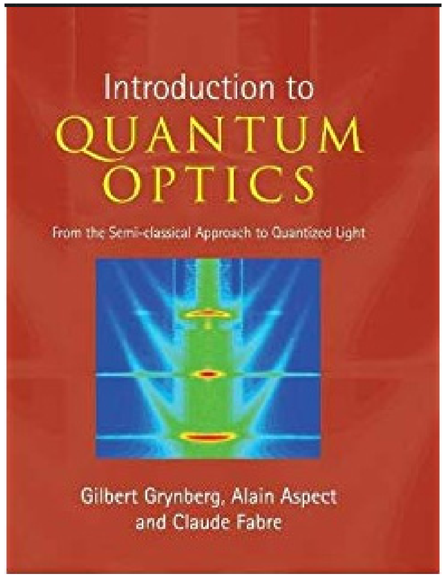


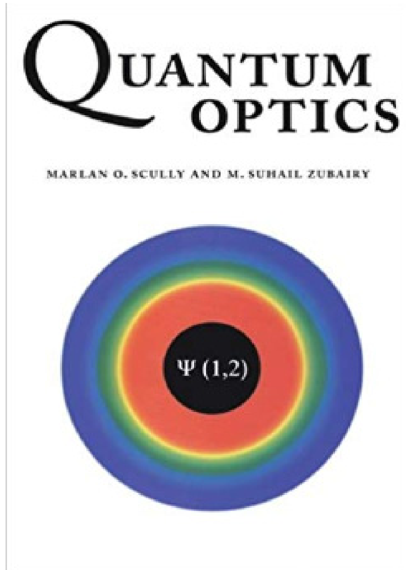


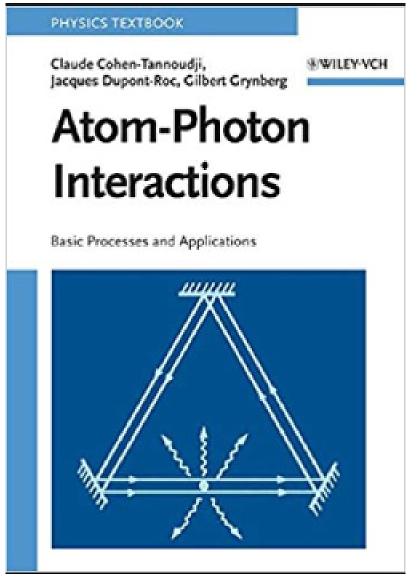




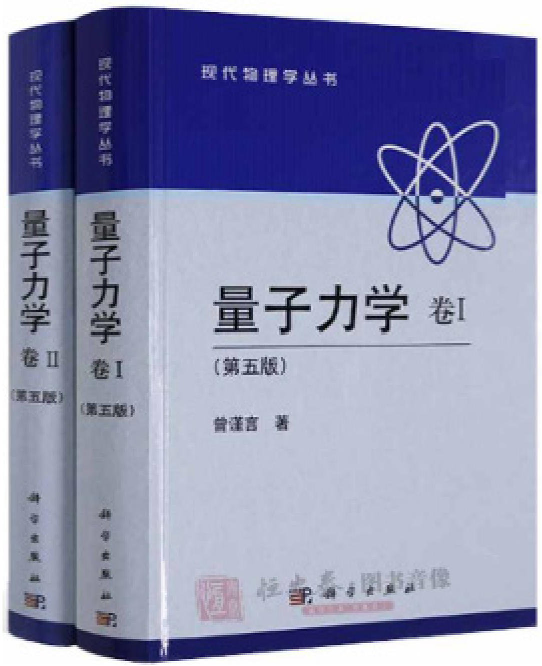


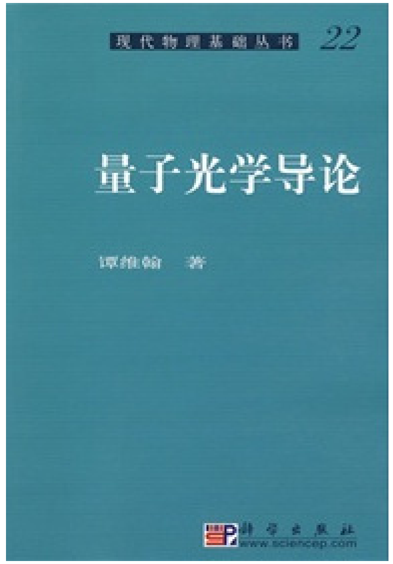






Books for Beginners in Field of Quantum Electromagnetics (Chinese)





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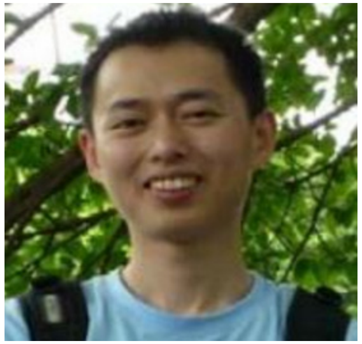
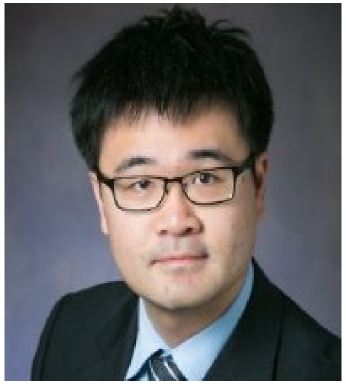


Yongpin Chen
(UESTC)

Carlos S.-Lazaro
(UIUC)



Michael Qiao
(Lumentum)

Yumao Wu
(FUDAN)

Jun Hu
(UESTC)

THANKS FOR YOUR ATTENTION!