

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

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- 1. Quantum Regime
- 2. Semi-Classical Framework
- 3. Full Quantum Approach
- 4. Conclusion







 $D << \lambda$

 $D >> \lambda$

D~λ

 $|\operatorname{Re}(\ell)| << \epsilon_{e}$

 $\operatorname{Re}(\ell) > 0$

 $\operatorname{Re}(\varepsilon) < 0$

Quantum Regime—Semi-Classical versus Full-Quantum

strong field condition

$$|\mathbf{E}| \gg \frac{\sqrt{\hbar c}}{\left(c\Delta_t\right)^2}$$

- 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.





The symplectic schemes include a variety of different temporal discretization strategies designed to preserve the global symplectic structure of the phase space for a Hamiltonian system.

Hamiltonian equation
$$\dot{q} = \frac{\partial H}{\partial p}$$
 $\dot{p} = -\frac{\partial H}{\partial q}$





Symplectic Scheme of Maxwell Equation

Collaborators: Z.X. Huang and X.L. Wu from Anhui U



IEEE Transactions on Antennas and Propagation, 56(2): 493-500, 2008. Journal of Computational Physics, 225(1): 33-50, 2007. IEEE Microwave and Wireless Components Letters, 18(3): 149-151, 2008.

What We Will DO—Symplectic Scheme of Multiphysics System

Collaborators: Y.P. Chen (UESTC), Y.M. Wu (Fudan), L.J. Jiang (HKU), and W.C. Chew (UIUC)

HamiltonianGeneralized coordinate and momentum
$$H^s(\mathbf{A}, \mathbf{Y}, \psi, \psi^*) = H^{em}(\mathbf{A}, \mathbf{Y}) + H^q(\psi, \psi^*, \mathbf{A})$$
 $\mathbf{q} = (\mathbf{A}, \psi_r)$ $\mathbf{p} = (\mathbf{Y}, \psi_i)$ $H^{em}(\mathbf{A}, \mathbf{Y}) = \int_v \left(\frac{1}{2\epsilon_0}|\mathbf{Y}|^2 + \frac{1}{2\mu_0}|\nabla \times \mathbf{A}|^2\right) d\mathbf{r}$ $\frac{\partial \mathbf{p}}{\partial t} = -\frac{\partial H^s}{\partial \mathbf{q}}$ $\frac{\|\mathbf{m}_v\|}{\psi date}$ $H^q(\psi, \psi^*, \mathbf{A}) = \int_v \left[\psi^* \frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m}\psi + \psi^* V\psi\right] d\mathbf{r}$ $\frac{\partial \mathbf{q}}{\partial t} = \frac{\partial H^s}{\partial \mathbf{p}}$ $\frac{\partial \mathbf{H}^s}{\psi date}$ Maxwell equationSchrödinger equation

$$\frac{\partial \mathbf{A}}{\partial t} = \frac{\partial H^s}{\partial \mathbf{Y}} = \frac{\mathbf{Y}}{\epsilon_0}$$
$$\frac{\partial \Psi}{\partial t} = -\frac{\partial H^s}{\partial \mathbf{A}} = -\frac{\nabla \times \nabla \times \mathbf{A}}{\mu_0} + \mathbf{J}$$
$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \frac{\partial H^s}{\partial \psi^*} = \frac{1}{i\hbar} \left[\frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m} + V \right] \psi$$
$$\frac{\partial \psi^*}{\partial t} = \frac{-1}{i\hbar} \frac{\partial H^s}{\partial \psi} = -\frac{1}{i\hbar} \left[\frac{(\hat{\mathbf{p}} + q\mathbf{A})^2}{2m} + V \right] \psi^*$$

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

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

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

$$\begin{split} \psi(\mathbf{r},t) &\approx a(t) \exp(-i\omega_g t) \psi_g(\mathbf{r}) + b(t) \exp(-i\omega_e t) \psi_e(\mathbf{r}) \\ \\ \frac{\partial \psi}{\partial t} &= \frac{1}{i\hbar} \frac{\partial H^s}{\partial \psi^*} = \frac{1}{i\hbar} \left[\frac{(\hat{\mathbf{p}} - q\mathbf{A})^2}{2m} + V \right] \psi \\ \begin{pmatrix} \psi_g, \frac{\partial \psi}{\partial t} \end{pmatrix} &= \left\langle \psi_g, \frac{1}{i\hbar} \frac{\partial H^s}{\partial \psi^*} \right\rangle \\ \left\langle \psi_e, \frac{\partial \psi}{\partial t} \right\rangle &= \left\langle \psi_e, \frac{1}{i\hbar} \frac{\partial H^s}{\partial \psi^*} \right\rangle \end{split}$$

fast oscillation of wave function

reduced eigenstate expansion (two-level atomic system)

Galerkin strategy

similar to optical Bloch equation

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

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

$$A-Y \text{ based Maxwell equation}$$

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

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

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

Numerical Results: Rabi Oscillation versus Radiative Decay



Rabi oscillation in a cavity

radiative decay in free space

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

Why Quantized Maxwell equation?

Collaborators: W.C. Chew, A.Y. Liu, and C. Salazar-Lazaro from UIUC

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 Quantized Maxwell equation? 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.









$$\hat{H}\left(\hat{\mathbf{A}}, \hat{\mathbf{Y}}, \hat{\mathbf{p}}\right) = \hat{H}^{em}\left(\hat{\mathbf{A}}, \hat{\mathbf{Y}}\right) + H_0^q\left(\hat{\mathbf{p}}, \hat{\mathbf{A}}\right) + H_I^q\left(\hat{\mathbf{p}}, \hat{\mathbf{A}}\right) \qquad \hat{H}\Psi(t) = i\hbar\frac{\partial\Psi(t)}{\partial t}$$
electromagnetic part atomic part interaction part
$$\hat{H}^{em}\left(\hat{\mathbf{A}}, \hat{\mathbf{Y}}\right) = \int_{\Omega} \left(\frac{1}{2\epsilon_0} \left|\hat{\mathbf{Y}}\right|^2 + \frac{1}{2\mu_0} \left|\nabla \times \hat{\mathbf{A}}\right|^2\right) d\mathbf{r} \quad H_0^q\left(\hat{\mathbf{p}}, \hat{\mathbf{A}}\right) = \frac{\hat{\mathbf{p}}^2}{2m} + V \quad H_I^q\left(\hat{\mathbf{p}}, \hat{\mathbf{A}}\right) \approx \frac{q\hat{\mathbf{p}} \cdot \hat{\mathbf{A}}}{m}$$
quantized field
(wave-particle duality)
$$\hat{\mathbf{A}} = \sum_k \frac{\alpha_k}{\omega_k} \left(\mathbf{U}_k(\mathbf{r})\hat{a}_k + \mathbf{U}_k^*(\mathbf{r})\hat{a}_k^+\right), \quad \alpha_k = \sqrt{\frac{\hbar\omega_k}{2\epsilon_0}}$$
eigenmode annihilation and creation operators
(wave) (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

Spontaneous Emission by Classical CEM Methods

Collaborators: Y.P. Chen (UESTC), L.J. Jiang (HKU), and J. Hu (UESTC)



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

Optics Express, 23(3): 2798-2807, 2015.

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What We Will DO—Quantization in Dispersive and Lossy Media

Collaborators: A.Y. Liu and W.C. Chew from UIUC

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

field-matter Hamiltonian	$H = \int dx^4 \frac{1}{2} \begin{bmatrix} \mathbf{E}^2 + \mathbf{H}^2 + \beta \mathbf{V}^2 + f \mathbf{P}^2 \end{bmatrix} \beta = 1/\omega_p^2, \ f = \omega_0^2/\omega_p^2$ field matter
A-Phi-P-V Hamiltonian	$\begin{aligned} H &= \int d\mathbf{r} \frac{1}{2} \left[\left(\mathbf{\Pi}_{AP} + \mathbf{P} \right)^2 + \left(\nabla \times \mathbf{A} \right)^2 + \left(\nabla \cdot \mathbf{A} \right)^2 \right. \\ &- \left. \Pi_{\Phi}^2 - \left(\nabla \Phi \right)^2 + \left. \Pi_P^2 / \beta + f \mathbf{P}^2 + 2 \mathbf{P} \cdot \nabla \Phi \right] \end{aligned}$
quantized Hamiltonian	$\begin{split} \hat{H} &= \int d\mathbf{r} \frac{1}{2} \left[\left(\hat{\Pi}_{AP} + \hat{\mathbf{P}} \right)^2 + \left(\nabla \times \hat{\mathbf{A}} \right)^2 + \left(\nabla \cdot \hat{\mathbf{A}} \right)^2 \right. \\ &\left \hat{\Pi}_{\Phi}^2 - \left(\nabla \hat{\Phi} \right)^2 + \hat{\Pi}_P^2 / \beta + f \hat{\mathbf{P}}^2 + 2 \hat{\mathbf{P}} \cdot \nabla \hat{\Phi} \right] \end{split}$

Dissipative Quantum Electromagnetics: A Novel Approach, arXiv:1704.02448



quantized motion equations

$$\begin{split} \left[\hat{\Pi}_{AP}(\mathbf{r},t),\hat{H}\right] &= -i\hbar\frac{\delta\hat{H}}{\delta\hat{\Lambda}(\mathbf{r},t)} = i\hbar\dot{\hat{\Pi}}_{AP}(\mathbf{r},t)\\ \left[\hat{\Lambda}(\mathbf{r},t),\hat{H}\right] &= i\hbar\frac{\delta\hat{H}}{\delta\hat{\Pi}_{AP}(\mathbf{r},t)} = i\hbar\dot{\hat{\Lambda}}(\mathbf{r},t)\\ \left[\hat{\Pi}_{\Phi}(\mathbf{r},t),\hat{H}\right] &= i\hbar\frac{\delta\hat{H}}{\delta\hat{\Phi}(\mathbf{r},t)} = i\hbar\dot{\hat{\Pi}}_{\Phi}(\mathbf{r},t)\\ \left[\hat{\Phi}(\mathbf{r},t),\hat{H}\right] &= -i\hbar\frac{\delta\hat{H}}{\delta\hat{\Pi}_{\Phi}(\mathbf{r},t)} = i\hbar\dot{\hat{\Phi}}(\mathbf{r},t)\\ \left[\hat{\Pi}_{P}(\mathbf{r},t),\hat{H}\right] &= -i\hbar\frac{\delta\hat{H}}{\delta\hat{P}(\mathbf{r},t)} = i\hbar\dot{\hat{\Pi}}_{P}(\mathbf{r},t)\\ \left[\hat{P}(\mathbf{r},t),\hat{H}\right] &= i\hbar\frac{\delta\hat{H}}{\delta\hat{\Pi}_{P}(\mathbf{r},t)} = i\hbar\dot{\hat{P}}(\mathbf{r},t) \end{split}$$

quantized Maxwell equation

$$\begin{split} \ddot{\hat{\mathbf{P}}}(\mathbf{r},t) &+ \omega_0^2 \hat{\mathbf{P}}(\mathbf{r},t) = \omega_p^2 \hat{\mathbf{E}}(\mathbf{r},t) \\ \dot{\hat{\mathbf{H}}}(\mathbf{r},t) &= -\nabla \times \dot{\hat{\mathbf{E}}}(\mathbf{r},t) \\ \dot{\hat{\mathbf{E}}}(\mathbf{r},t) &= \nabla \times \dot{\hat{\mathbf{H}}}(\mathbf{r},t) - \hat{\mathbf{V}}(\mathbf{r},t) \\ \dot{\hat{\mathbf{P}}}(\mathbf{r},t) &= \hat{\mathbf{V}}(\mathbf{r},t) \end{split}$$





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

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

interaction

Introduction of Loss in Quantization Procedure



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

$$\dot{\hat{a}} = -i\left(\omega_0\hat{a} + \sum_j \tilde{\gamma}_j\hat{b}_j\right) \qquad \qquad \dot{\hat{a}} = -i\left(\omega_j\hat{b}_j + \tilde{\gamma}_j\hat{a}\right) \qquad \qquad \dot{\hat{b}}_j = -i\left(\omega_j\hat{b}_j + \tilde{\gamma}_j\hat{a}\right) \qquad \qquad \langle [\hat{F}(a_j)] \rangle$$

Motion equation of matter system in ensemble average sense

Blackbody radiation

$$\dot{\hat{a}} = -i\omega_0\hat{a} - \eta\hat{a} + \hat{F}(t)$$
$$\langle [\hat{F}(t), \hat{F}^{\dagger}(t')] \rangle = 2\eta\delta(t - t')$$

When the matter (single QHO) is coupled to bath (many QHOs like white noise), it loses energy to the bath (related to η). Simultaneously, the bath pumps energy back to the matter (related to 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 Wave equation in frequency domain $\nabla \times \nabla \times \hat{\mathbf{E}}(\mathbf{r},\omega) - \omega^2 \epsilon(\mathbf{r},\omega) \hat{\mathbf{E}}(\mathbf{r},\omega) = i\omega \hat{\mathbf{j}}_n(\mathbf{r},\omega)$ $\dot{\hat{\mathbf{H}}}\,=-\nabla\times\hat{\mathbf{E}}$ $\mathbf{\hat{H}} = -\mathbf{\nabla} \times \mathbf{\hat{E}}$ $\dot{\hat{\mathbf{E}}} = \nabla \times \hat{\mathbf{H}} - \dot{\hat{\mathbf{P}}}$ $\dot{\hat{\mathbf{I}}} = -\omega_0 \hat{\mathbf{P}} - \eta \hat{\mathbf{\Pi}} + \hat{\mathbf{F}}_I + \frac{\omega_p^2}{\omega_0} \hat{\mathbf{E}}$ $\dot{\hat{\mathbf{P}}} = \omega_0 \hat{\mathbf{\Pi}} - \eta \hat{\mathbf{P}} + \hat{\mathbf{F}}_R$ $\hat{\mathbf{j}}_n(\mathbf{r},\omega) = \frac{-i\omega\omega_0\hat{\mathbf{F}}_I(\mathbf{r}) - i\omega\left[\eta(\mathbf{r}) - i\omega\right]\hat{\mathbf{F}}_R(\mathbf{r})}{\left[\eta(\mathbf{r}) - i\omega\right]^2 + \omega_n^2}$ $\epsilon(\mathbf{r},\omega) = 1 + \frac{\omega_p^2}{[n(\mathbf{r}) - i\omega]^2 + \omega^2}$ $\left\langle \begin{bmatrix} \hat{\mathbf{F}}_{R}, \hat{\mathbf{F}}_{I} \end{bmatrix} \right\rangle = i2\eta \frac{\omega_{p}^{2}\hbar}{\omega_{0}} \delta(t-t') \hat{\mathbf{I}} \qquad \left\langle \begin{bmatrix} \hat{\mathbf{F}}_{R}(\omega), \hat{\mathbf{F}}_{I}^{\dagger}(\omega') \end{bmatrix} \right\rangle = \frac{i\eta}{\pi} \frac{\omega_{p}^{2}\hbar}{\omega_{0}} \delta(\omega-\omega')$

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

Fluctuation-dissipation theorem



- 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 electromagnetic 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 electromagnetic problems in inhomogeneous, lossy, and dispersive media.













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THANKS FOR YOUR ATTENTION!



