SAND2019-7542C

Role of Classical Time Domain CEM Methods for Quantum Electromagnetics

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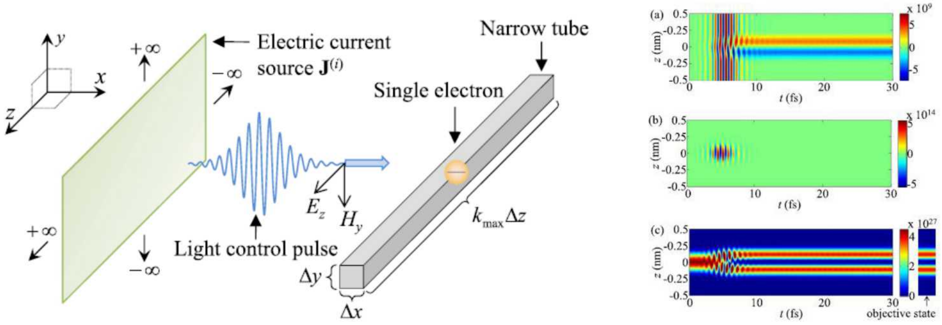
Quantum Physics & CEM

Semiclassical

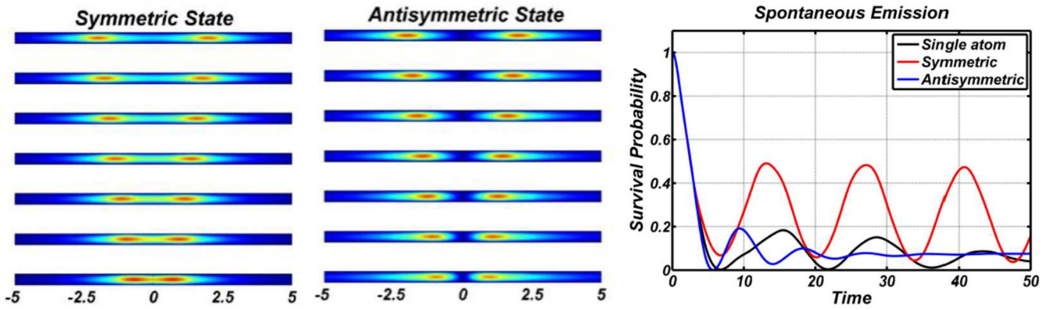
Maxwell-Schrödinger System



T. Takeuchi, DOI: 10.1103/PhysRevA.91.033401

Fully Quantized

Waveguide-QED



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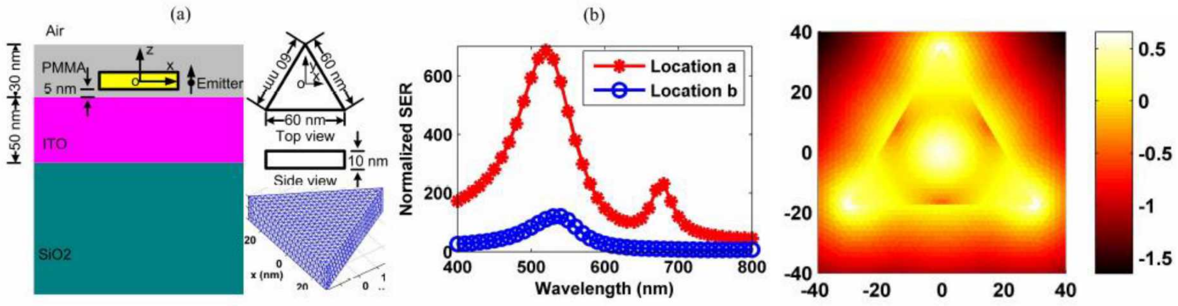
Requires Wider BW →

Nanoantenna SER



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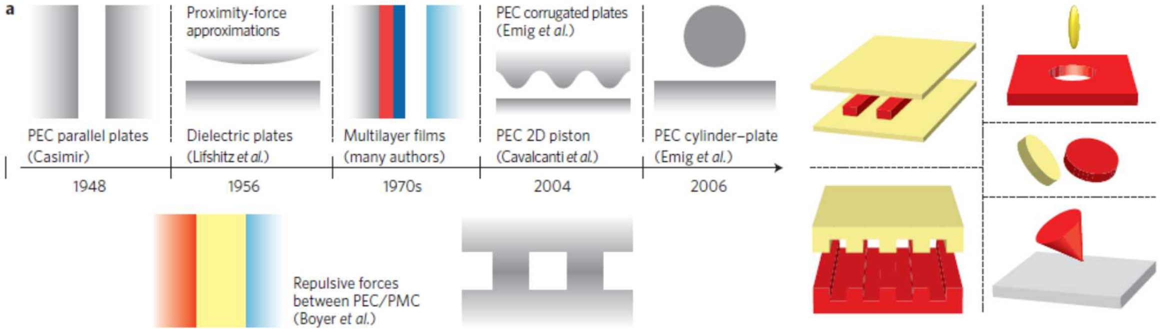
Casimir Force



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Emerging quantum applications require *classical* CEM tools for *increasingly* broadband analysis of multiscale, subwavelength, and lossy dielectrics

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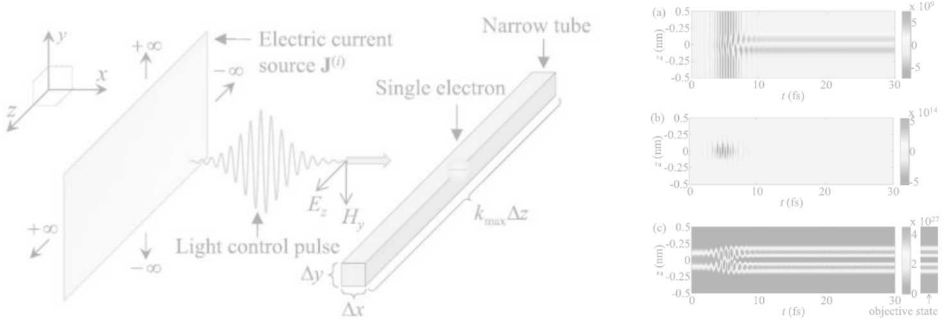

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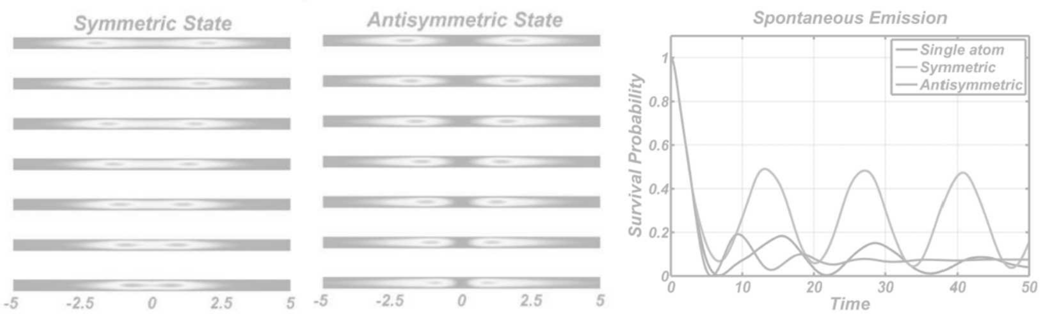

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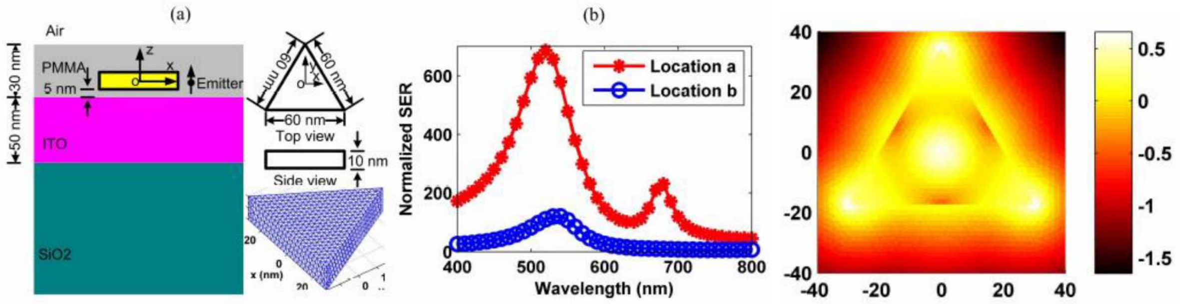

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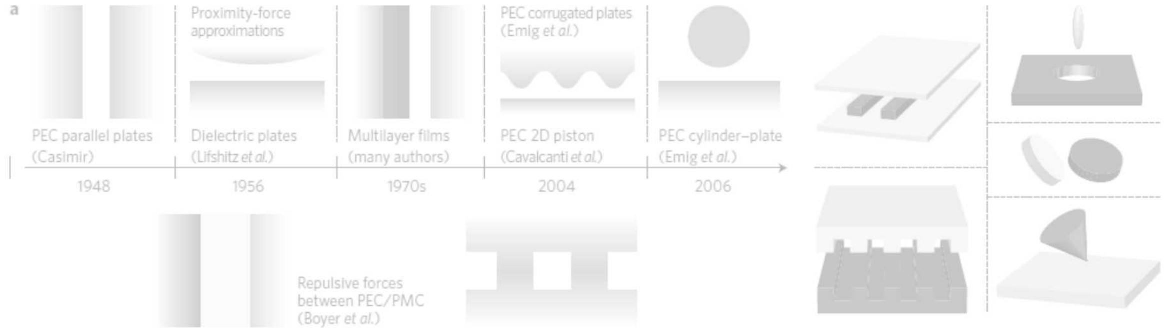

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Emerging quantum applications require *classical* CEM tools for *increasingly* broadband analysis of multiscale, subwavelength, and lossy dielectrics

Spontaneous Emission Rate Computations

- In the weak coupling regime, Fermi's Golden Rule gives spontaneous emission rate (SER) as

$$\gamma = \frac{2\pi}{\hbar^2} \sum_f |\langle f|\hat{H}_I|i\rangle|^2 \delta(\omega_i - \omega_f).$$

- Using the dipole approximation for the interaction Hamiltonian, this becomes a sum over field modes as

$$\gamma = \frac{\pi\omega_0}{\hbar\epsilon_0} \sum_{\mathrm{k}} \left[\mathbf{d} \cdot (\mathbf{u}_{\mathrm{k}}\mathbf{u}_{\mathrm{k}}^*) \cdot \mathbf{d}\right] \delta(\omega_{\mathrm{k}} - \omega_0).$$

- Recalling that the Dyadic Green's function (DGF) can be expanded in field modes as

$$\overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega) = \sum_{\mathrm{k}} c^2 \frac{\mathbf{u}_{\mathrm{k}}(\mathbf{r}, \omega_{\mathrm{k}})\mathbf{u}_{\mathrm{k}}^*(\mathbf{r}', \omega_{\mathrm{k}})}{\omega_{\mathrm{k}}^2 - \omega^2},$$

and using standard mathematical identities we have that

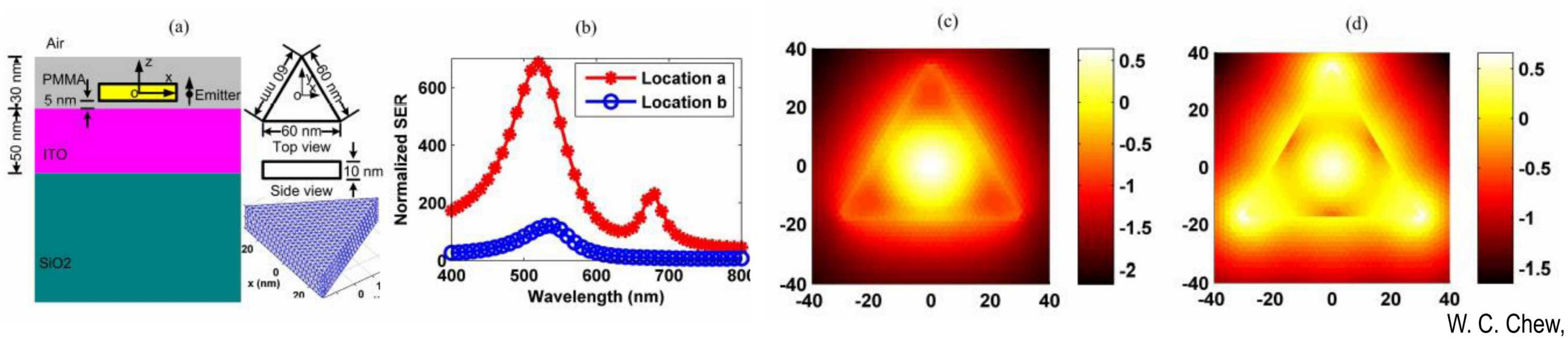
$$\mathrm{Im}\left\{\overline{\mathbf{G}}(\mathbf{r}, \mathbf{r}, \omega)\right\} = \frac{\pi c^2}{2\omega} \sum_{\mathrm{k}} \mathbf{u}_{\mathrm{k}}(\mathbf{r}, \omega_{\mathrm{k}})\mathbf{u}_{\mathrm{k}}^*(\mathbf{r}, \omega_{\mathrm{k}})\delta(\omega - \omega_{\mathrm{k}}).$$

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

Spontaneous Emission Rate Computations

$$\frac{\gamma(\mathbf{r}_0,\omega_0)}{\gamma_0(\mathbf{r}_0,\omega_0)}=\frac{\hat{\mathrm{d}}\cdot\mathrm{Im}\left[\overline{\mathbf{G}}_0(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\right]\cdot\hat{\mathrm{d}}}{\hat{\mathrm{d}}\cdot\mathrm{Im}\left[\overline{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\right]\cdot\hat{\mathrm{d}}}$$

- ***Summary:***
  - DGF is computed through *classical* near-field scattering problems.
  - SER found through the correspondence between DGF and photon local density of states.
  - Normalized SER (Purcell factor) characterizes impact that inhomogeneous environment has on spontaneous emission.
  - *Time domain methods of interest as bandwidth being analyzed increases.*



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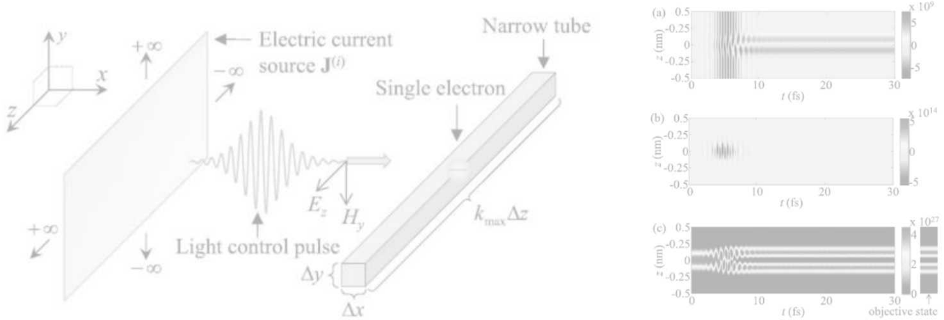

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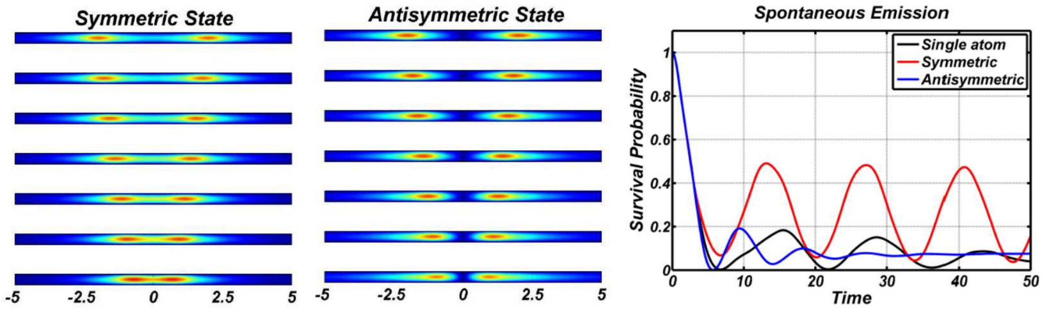

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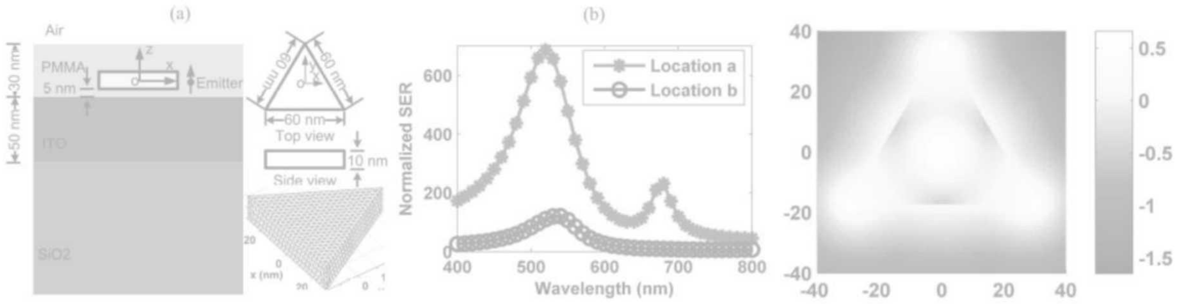
Nanoantenna SER



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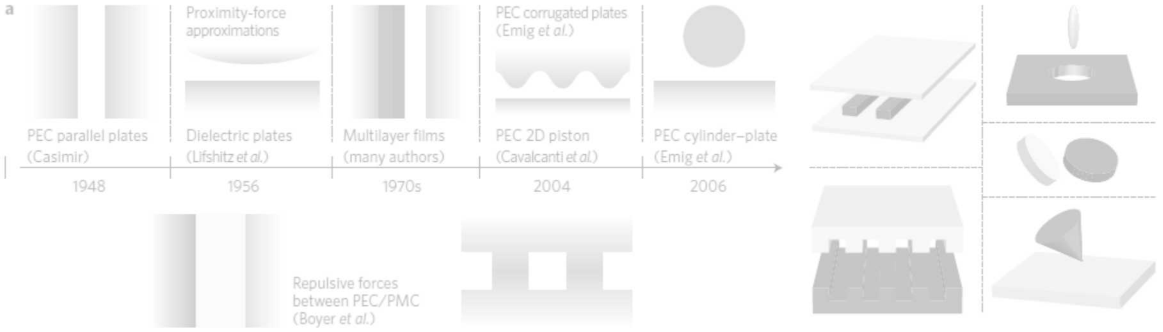

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Emerging quantum applications require *classical* CEM tools for *increasingly* broadband analysis of multiscale, subwavelength, and lossy dielectrics

Waveguide Quantum Electrodynamics Computations

- Exact details of (artificial) atoms can often be neglected so that Jaynes-Cummings model can describe the atom-photon interaction. The resulting Hamiltonian is

$$\hat{H} = \underbrace{\omega_e \hat{b}^\dagger \hat{b}}_{\text{Boson Atom}} + \sum_{\mathrm{k}} \underbrace{\omega_{\mathrm{k}} \hat{a}_{\mathrm{k}}^\dagger \hat{a}_{\mathrm{k}}}_{\text{Field}} + \sum_{\mathrm{k}} \underbrace{\left[g_{\mathrm{k}} \hat{b}^\dagger \hat{a}_{\mathrm{k}} + g_{\mathrm{k}}^* \hat{a}_{\mathrm{k}}^\dagger \hat{b} \right]}_{\text{RWA dipole interaction}},$$

where

$$g_{\mathrm{k}} = \sqrt{\frac{\omega_{\mathrm{k}}}{2\epsilon}} \mathbf{E}_{\mathrm{k}}(\mathbf{r}_0) \cdot \mathbf{d}.$$

- Dynamics of this system can be solved through a generalized Fano diagonalization of the Hamiltonian as

$$\hat{H} = \sum_{\nu} \omega_\nu \hat{c}_\nu^\dagger \hat{c}_\nu,$$

where the *dressed state operators* satisfy the commutation relation

$$\left[\hat{c}_\nu, \hat{c}_{\nu'}^\dagger\right] = \delta_{\nu,\nu'}.$$

- Time evolution of dressed state operators can be easily found as

$$\left[\hat{c}_\nu, \hat{H}\right] = \omega_\nu \hat{c}_\nu.$$

Waveguide Quantum Electrodynamics Computations

- Dressed states are solved for by representing them as a linear combination of the original operators, given by

$$\hat{c}_\nu = A(\nu)\hat{b} + \sum_{\mathrm{k}} F(\nu,\mathrm{k})\hat{a}_{\mathrm{k}}, \quad \hat{c}_\nu^\dagger = A^*(\nu)\hat{b}^\dagger + \sum_{\mathrm{k}} F^*(\nu,\mathrm{k})\hat{a}_{\mathrm{k}}^\dagger.$$

- Plugging this representation into the commutator and time evolution equations results in a system of equations to solve

$$A(\nu)[\omega_\nu - \omega_e] = \sum_{\mathrm{k}} F(\nu,\mathrm{k}) g_{\mathrm{k}}^*,$$

$$A(\nu) g_{\mathrm{k}} = F(\nu,\mathrm{k})[\omega_\nu - \omega_{\mathrm{k}}],$$

$$A(\nu)A^*(\nu') + \sum_{\mathrm{k}} F(\nu,\mathrm{k})F^*(\nu',\mathrm{k}) = \delta_{\nu,\nu'}.$$

- Partially solving for a discrete EM spectrum (cavity case) results in

$$\omega_\nu = \omega_e + \sum_{\mathrm{k}} \frac{\omega_{\mathrm{k}}}{2\epsilon} \frac{\mathbf{d}\cdot\left[\mathbf{E}_{\mathrm{k}}(\mathbf{r_0})\mathbf{E}_{\mathrm{k}}^*(\mathbf{r_0})\right]\cdot\mathbf{d}}{\omega_\nu - \omega_{\mathrm{k}}}$$

Waveguide Quantum Electrodynamics Computations

- When EM spectrum has a continuum (e.g., waveguide case), the solution becomes

$$Z(\omega_\nu) = \frac{1}{\Gamma(\omega_\nu)}\left[\omega_\nu - \omega_e - \Delta(\omega_\nu)\right] \qquad |A(\omega_\nu)|^2 = \frac{\Gamma(\omega_\nu)}{\left[\pi\Gamma(\omega_\nu)\right]^2 + \left[\omega_\nu - \omega_e - \Delta(\omega_\nu)\right]^2}$$

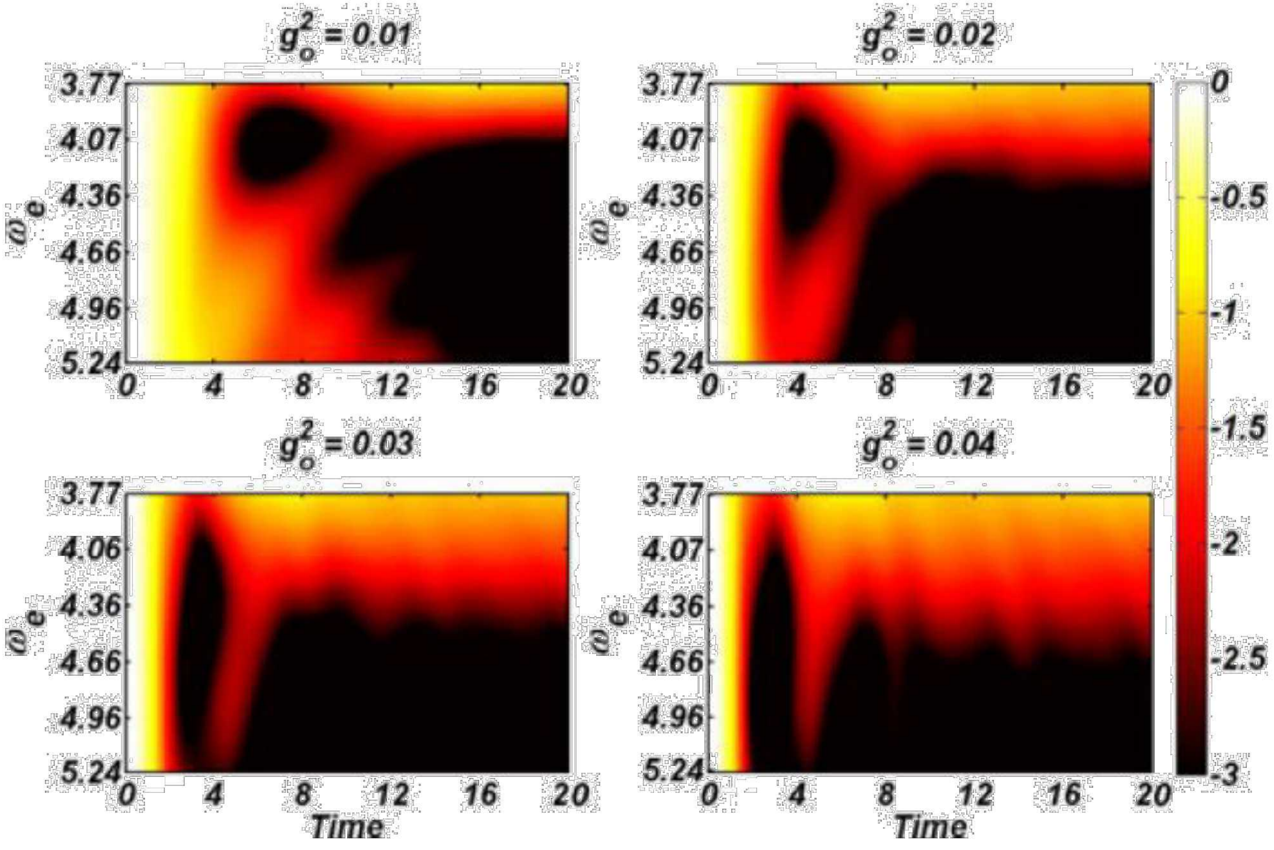
where the decay rate and radiative shift are given by

$$\Gamma(\omega_\nu) = \frac{k^2}{\epsilon\pi}\left\{\mathbf{d}\cdot\mathrm{Im}\left[\overline{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_\nu)\right]\cdot\mathbf{d}\right\}, \quad \Delta(\omega_\nu) = \mathrm{P.V.}\int_0^\infty \frac{\Gamma(\omega)}{\omega_\nu - \omega}d\omega.$$

- ***Summary:***
  - Dressed state dynamics are solved once the decay rate and radiative shift have been determined.
  - Decay rate is related to the *classical* DGF due to its correspondence with photon local density of states.
  - Radiative shift is found through the Hilbert transform of decay rate.
  - *Broadband time domain methods can solve near-field scattering problems so that the Hilbert transform can be evaluated.*

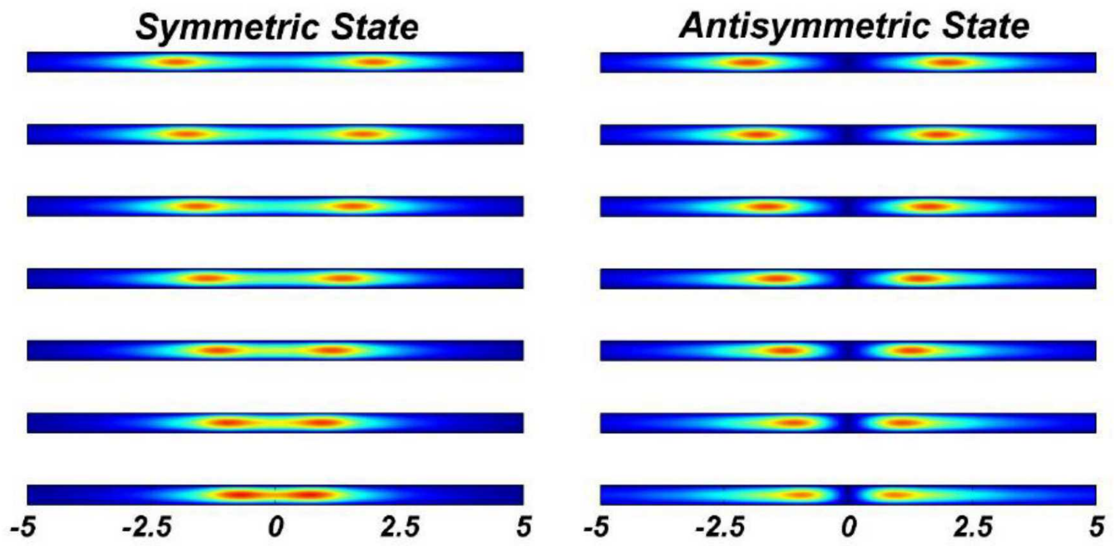
Waveguide Quantum Electrodynamics Computations

Atom Survival Probability



W. C. Chew, DOI: 10.1109/JMMCT.2017.2698341

Multi-Atom Bound States



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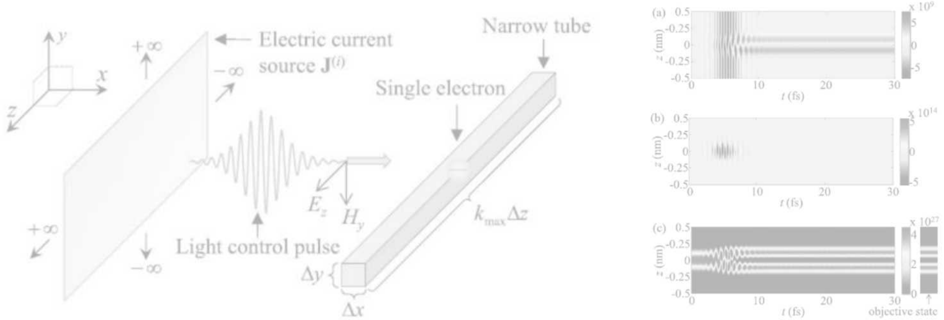

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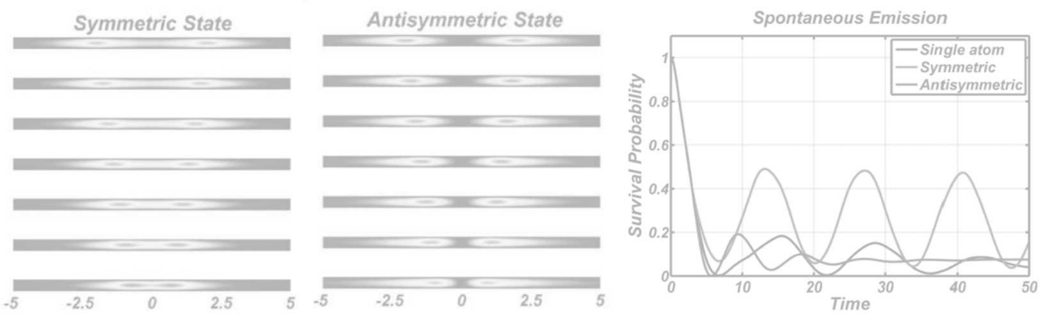

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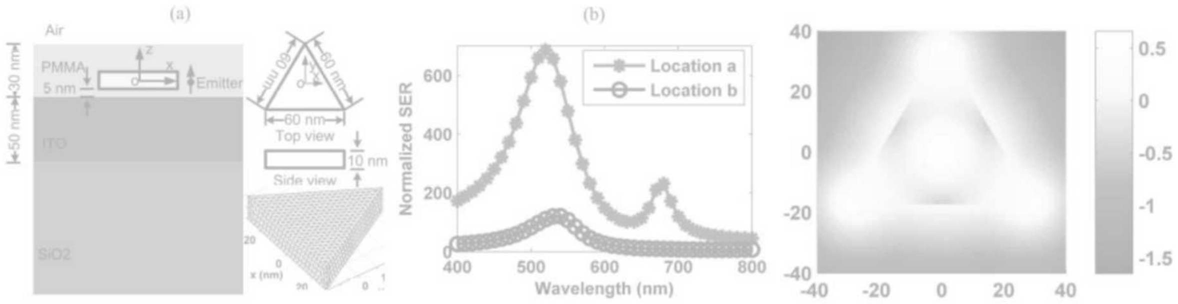

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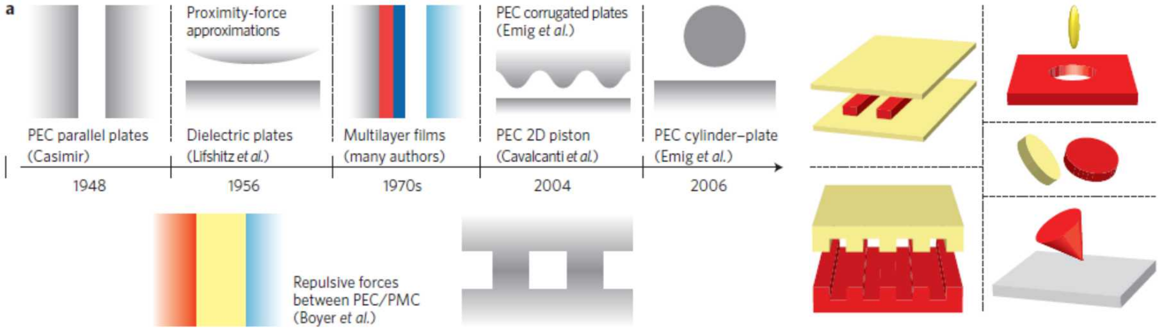

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Casimir Force Computations

- Casimir force on a body is given by an integral of the mean EM stress tensor over any closed surface surrounding the body,

$$F_i = \int_0^\infty d\omega \oiint_S \sum_j \langle T_{ij}(\mathbf{r},\omega)\rangle dS_j.$$

- Mean EM stress tensor is expressed through correlation functions of the field operators as

$$\langle T_{ij}(\mathbf{r},\omega)\rangle = \mu(\mathbf{r},\omega)\left[\langle H_i(\mathbf{r},\omega), H_j(\mathbf{r},\omega)\rangle - \frac{1}{2}\delta_{ij}\sum_k \langle H_k(\mathbf{r},\omega), H_k(\mathbf{r},\omega)\rangle\right]$$
$$+\epsilon(\mathbf{r},\omega)\left[\langle E_i(\mathbf{r},\omega), E_j(\mathbf{r},\omega)\rangle - \frac{1}{2}\delta_{ij}\sum_k \langle E_k(\mathbf{r},\omega), E_k(\mathbf{r},\omega)\rangle\right].$$

- For symmetry in the numerical method, electric and magnetic vector potentials are introduced that are related to the fields as

$$E_i(\mathbf{r},\omega) = -i\omega A_i^E(\mathbf{r},\omega), \qquad H_i(\mathbf{r},\omega) = -i\omega A_i^H(\mathbf{r},\omega).$$

Casimir Force Computations

- Fluctuation-dissipation theorem is applied to relate correlation functions of the vector potentials to the DGF as

$$\langle A_i^{E/H}(\mathbf{r},\omega), A_j^{E/H}(\mathbf{r}',\omega)\rangle = -\frac{\hbar}{\pi}\mathrm{Im}\big[G_{ij}^{E/H}(\mathbf{r},\mathbf{r}',\omega)\big].$$

- Direct evaluation of force integral is computationally inefficient due to the oscillatory integrand over frequency.
- Physical problem can be mapped to a new problem whose integrand decays rapidly – a simple equivalent problem is a medium with frequency-independent conductivity
- ***Summary:***
  - Casimir force is expressed in terms of mean EM stress tensor.
  - Fluctuation-dissipation theorem reduces the computation of an *entirely quantum* force to evaluation of a sequence of *entirely classical* near-field scattering problems.
  - *Casimir force can be efficiently evaluated directly in time domain by solving sequence of near-field scattering problems in a lossy medium*

Conclusion

- *Classical DGF* plays a central role in many *quantum EM* computations.
- Semiclassical computations tend to require knowledge of DGF over a limited bandwidth.
- Fully quantized computations require knowledge of DGF over increasingly wide bandwidths.
- Time domain CEM methods can play a central role in the future of these computations if they are:
  - Stable,
  - Efficient,
  - And applicable to subwavelength or multiscale systems

Future Work

- Advanced time domain methods can be applied to these and other quantum applications of interest to engineers
- Key quantum applications can continue to be (re)formulated in a way that the DGF is central to the calculation

Acknowledgments

This work was supported by the following sources: the Tuition Assistance Program at Sandia National Laboratories, AF Sub RRI PO0539, NSF ECCS 169195, and the Distinguished Professorship Grant at Purdue University.

This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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