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Role of Classical Time Domain CEM Methods for Quantum Electromagnetics

(Invited Paper)

Thomas E. Roth[†‡*] and Weng C. Chew[‡§]
[†]Sandia National Laboratories, Albuquerque, New Mexico, USA
[‡]Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA
Email: teroth2@illinois.edu
[§]School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana, USA
Email: wcchew@purdue.edu

***Abstract*—As quantum theory matures, quantum applications that significantly depend on electromagnetic effects are becoming increasingly of interest to engineers. We discuss a number of diverse computations that are needed in the engineering design of various devices leveraging these quantum effects. In each case, the broadband knowledge of the classical dyadic Green's function of the problem being analyzed plays an important role. As a result, many of these applications require the extremely broadband solution of classical electromagnetic scattering problems in complex geometries to evaluate components of the dyadic Green's functions. This suggests that classical time domain computational electromagnetics methods will play an important role in the future of quantum applications.**

I. Introduction

There are a number of emerging quantum physics applications where classical computational electromagnetics (CEM) methods can play an essential role in transitioning from the analysis of analytically solvable systems to problems of more practical interest [1]. We discuss different classes of computations that are of interest to practical engineering design; namely, spontaneous emission rate [2], (artificial) atom-photon dressed state dynamics [3], and Casimir force [4], [5].

Although relevant to a diverse set of applications, these computations are joined by their common need for the broadband computation of the classical dyadic Green's function (DGF) for an arbitrary, inhomogeneous medium. These computations also highlight that as the quantum model of the system becomes more complex, time domain CEM methods become increasingly attractive to complete the required analysis.

II. Spontaneous Emission Rate

The first, and simplest, computation to be discussed is the change in spontaneous emission rate (SER) of a quantum emitter (QE) due to its surrounding environment [2]. This is important for many quantum optics applications that rely on controlling the rate and direction of emitted EM fields.

A simple quantum model, based on Fermi's golden rule, relates the SER to the photon local density of states (LDOS), which is typically expressed through a summation of the eigenmodes of the EM environment [6]. Hence, the SER can be manipulated by changing the local EM environment to modify the photon LDOS near the QE, changing the probability of spontaneous emission.

However, directly computing a summation of eigenmodes for a complex EM environment is not computationally appealing. Recalling that the DGF can also be expanded as a summation of eigenmodes of the EM environment, it becomes apparent that a link should exist between the photon LDOS and DGF [6]. This is the case, and allows the SER to be

$$\gamma(\mathbf{r}_0, \omega_0) = \frac{2\omega_0^2}{\hbar\epsilon_0 c^2}\big\{\mathbf{d}\cdot \mathrm{Im}\big[\overline{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\big]\cdot\mathbf{d}\big\}, \qquad (1)$$

where $\mathbf{d}$ is the dipole moment of the QE, $\mathbf{r}_0$ is its location, and ω_0 is the angular frequency [2]. This is computationally appealing, since $\mathrm{Im}\big[\overline{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)\big]$ can be easily calculated through the solution of an appropriate classical EM scattering problem [2].

As mentioned previously, the simple quantum model here leads to only limited knowledge of the DGF being needed. As a result, time domain methods are mainly of interest for broadband or many excitation problems, similar to radar cross section analysis. However, as more detailed quantum models are needed time domain methods become more interesting, as will be seen shortly.

III. Dressed State Dynamics

The previous section discussed the semiclassical interaction of a QE with its EM environment. In the case where the EM field must also be quantized, a more detailed model is needed. This must be done, e.g., in quantum computing and information applications of circuit quantum electrodynamics (C-QED).

In many cases, the exact details of an artificial atom can be neglected, allowing for the quantum EM problem to be described by a Jaynes-Cummings model [3]. This model assumes the total Hamiltonian is given by the summation of simple atomic excitation and free field Hamiltonians, with additional terms to allow atom-field interactions. The coupling constants for the atom-field interactions are given in natural units ($\hbar = c = 1$) by

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

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where $\mathbf{E}_\mathrm{k}$ is the field eigenmode with eigenvalue ω_k [3].

One approach to solve this atom-photon interaction is to perform a generalized Fano diagonalization of the Hamiltonian [3]. This amounts to finding new creation and annihilation operators that correspond to *dressed* states. These dressed states are linear combinations of the original atom and photon operators, representing real excitations that are part atom and part field (also called polaritons in some contexts).

Solving for their dynamics (and the dynamics of the original operators) relies on computing the radiative shift (Δ) and decay rate (Γ). The decay rate is given by

$$\Gamma(\omega) = \sum_{\mathrm{k}} \rho_\mathrm{k}(\omega)|g_\mathrm{k}(\omega)|^2, \tag{3}$$

where ρ_k is the density of states for the kth field mode [3]. This is in fact the LDOS "measured" by the atom's dipole moment, and can be related to the DGF as

$$\Gamma(\omega) = \frac{k^2}{\epsilon\pi}\{\mathbf{d}\cdot \mathrm{Im}[\overline{\mathbf{G}}(\mathbf{r}_0,\mathbf{r}_0,\omega_0)]\cdot \mathbf{d}\}. \tag{4}$$

Computing Δ is then possible, since it is simply the Hilbert transform of Γ [3]. However, evaluating this transform requires very broadband knowledge of the DGF, found by solving classical EM scattering problems. As a result, time domain methods that can efficiently analyze extremely broadband pulses are of significant interest to C-QED applications.

IV. Casimir Force

The Casimir force is an attractive or repulsive force between charge-neutral bodies due to quantum vacuum fluctuations of the EM field [4], [5]. This becomes a dominant force for small object separations, and so can be important in micro/nano-electromechanical systems.

There exist multiple ways to formulate and compute this force, however, we will only focus on the Maxwell stress tensor approach. The Maxwell stress tensor captures the interactions between EM forces and mechanical momentum, so it should not be surprising that it can play a central role in the computation of Casimir force. In particular, the Casimir force in the ith direction on a body enclosed by a surface S is

$$F_i = \int_0^\infty d\omega \oiint_S \sum_j \langle T_{ij}(\mathbf{r},\omega)\rangle dS_j, \tag{5}$$

where $\langle T_{ij}(\mathbf{r},\omega)\rangle$ is the mean Maxwell stress tensor [5]. This mean stress tensor is given in terms of correlation functions of the field operators, i.e., $\langle \mathbf{E}_i(\mathbf{r},\omega),\mathbf{E}_j(\mathbf{r},\omega)\rangle$ and $\langle \mathbf{H}_i(\mathbf{r},\omega),\mathbf{H}_j(\mathbf{r},\omega)\rangle$. These can be related to correlation functions of appropriately defined vector potentials, $\mathbf{A}_i^\mathrm{E}$ and $\mathbf{A}_i^\mathrm{H}$, for the electric and magnetic fields, respectively. The correlation functions of vector potentials can be related to the DGF through the fluctuation-dissipation theorem as

$$\langle \mathbf{A}_i^{\mathrm{E/H}}(\mathbf{r},\omega),\mathbf{A}_j^{\mathrm{E/H}}(\mathbf{r}',\omega)\rangle = -\frac{\hbar}{\pi}\mathrm{Im}[G_{ij}^{\mathrm{E/H}}(\mathbf{r},\mathbf{r}',\omega)], \tag{6}$$

where $G_{ij}^{\mathrm{E/H}}$ is the ij-component of the DGF [5]. Similar to the previous cases, these components of the DGF can be computed through appropriately defined classical EM scattering problems.

From this discussion, it is clear that computing the Casimir force on a body is not a trivial task. It involves solving a number of classical EM scattering problems for differently oriented sources placed at points along the enclosing surface S. As was the case for solving dressed state dynamics, these computations must cover an extremely broad frequency range. As a result, time domain simulations are again of interest for these applications. Indeed, the Casimir force computation discussed here can actually be computed directly in the time domain, rather than evaluating the spectral integral in (5) [5].

V. Conclusion

This work discussed three types of computations important for emerging applications that leverage quantum effects. In each case, it was shown that knowledge of the *classical* DGF could be leveraged to analyze systems of practical interest. Further, as the quantum model needed to describe the physics became more complicated, it became clear that extremely broadband knowledge of the DGF was needed. As a result, classical time domain CEM methods that can analyze complicated geometries and materials are expected to play an important role in the future for these applications.

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