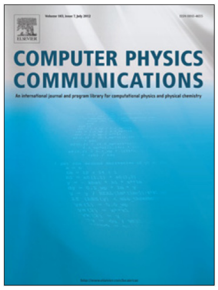
Accepted Manuscript



A unified Hamiltonian solution to Maxwell–Schrödinger equations for modeling electromagnetic field-particle interaction

Yongpin P. Chen, Wei E.I. Sha, Lijun Jiang, Min Meng, Yu Mao Wu, Weng Cho Chew

PII: S0010-4655(17)30048-6
DOI: http://dx.doi.org/10.1016/j.cpc.2017.02.006
Reference: COMPHY 6154

To appear in: *Computer Physics Communications*

Received date : 2 April 2015
Revised date : 14 November 2016
Accepted date : 10 February 2017

Please cite this article as: Y.P. Chen, et al., A unified Hamiltonian solution to Maxwell–Schrödinger equations for modeling electromagnetic field-particle interaction, *Computer Physics Communications* (2017), http://dx.doi.org/10.1016/j.cpc.2017.02.006

A Unified Hamiltonian Solution to Maxwell-Schrödinger Equations for Modeling Electromagnetic Field-Particle Interaction

Yongpin P. Chen[a], Wei E. I. Sha[b,*], Lijun Jiang[b,*], Min Meng[a], Yu Mao Wu[c], and Weng Cho Chew[d,b]

[a] *School of Electronic Engineering, University of Electronic Science and Technology of China, Chengdu, 611731, China*

[b] *Department of Electrical and Electronic Engineering, The University of Hong Kong, Hong Kong, China*

[c] *School of Information Science and Technology, Fudan University, Shanghai, 200433, China*

[d] *Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801 USA*

Abstract

A novel unified Hamiltonian approach is proposed to solve Maxwell-Schrödinger equation for modeling the interaction between classical electromagnetic (EM) fields and particles. Based on the Hamiltonian of electromagnetics and quantum mechanics, a unified Maxwell-Schrödinger system is derived by the variational principle. The coupled system is well-posed and symplectic, which ensures energy conserving property during the time evolution. However, due to the disparity of wavelengths of EM waves and that of electron waves, a numerical implementation of the finite-difference time-domain (FDTD) method to the multiscale coupled system is extremely challenging. To overcome this difficulty, a reduced eigenmode expansion technique is first applied to represent the wave function of the particle. Then, a set of ordinary differential equations (ODEs) governing the time evolution of the slowly-varying expansion coefficients are derived to replace the original Schrödinger equation. Finally, Maxwell's equations represented by the vector potential with a Coulomb

*wsha@eee.hku.hk(W. E. I. Sha); jianglj@hku.hk(L. Jiang)