95680

LA-UR- 98-2613

Approved for public release; distribution is unlimited.

Title: High-Performance Computing of Electron Microstructures

Author(s): Alan Bishop, T-11

Bjorn Birnir, Bryan Galdrikian, Lihong Wang, University of California, Santa Barbara

Submitted to: DOE OFFICE OF SCIENTIFIC AND TECHNICAL INFORMATION (OSTI)

Los Alamos
NATIONAL LABORATORY

DISCLAIMER

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

High-Performance Computing of Electron Microstructures

Alan Bishop*
Los Alamos National Laboratory

Bjorn Birnir, Bryan Galdrikian and Lihong Wang
University of California, Santa Barbara

Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The project was a collaboration between the Quantum Institute at the University of California-Santa Barbara (UCSB) and the Condensed Matter and Statistical Physics Group at LANL. The project objective, which was successfully accomplished, was to model quantum properties of semiconductor nanostructures that were fabricated and measured at UCSB using dedicated molecular-beam epitaxy and free-electron laser facilities. A nonperturbative dynamic quantum theory was developed for systems driven by time-periodic external fields. For such systems, dynamic energy spectra of electrons and photons and their corresponding wave functions were obtained. The results are in good agreement with experimental investigations. The algorithms developed are ideally suited for massively parallel computing facilities and provide a fundamental advance in our ability to predict quantum-well properties and guide their engineering. This is a definite step forward in the development of nonlinear optical devices.

Background and Research Objectives

The University of California, Santa Barbara (UCSB) has a unique blend of resources for the fabrication and study of semiconductor nanostructures. The material science department can grow quantum wells of almost arbitrary shape using Molecular Beam Epitaxy (MBE), in which a single atomic layer of semiconductor crystal is deposited at a time. These wells are studied at the intense Free Electron Laser (FEL) facilities in the physics department. Researchers in the Quantum Institute at UCSB, linked in this project with theoretical groups interested in nanotechnology at the Los Alamos National Laboratory (LANL), used the LANL supercomputing facilities and made their techniques available to LANL. This resulted in many mutually beneficial interactions, where the

*Principal Investigator, e-mail: bishop_alan@lanl.gov

UCSB groups enjoyed the extensive Los Alamos expertise in many-body physics and numerical electronic structure methods, and in nonlinear material science, including classical and quantum chaos.

Importance to LANL's Science and Technology Base and National R&D Needs

The project was directly relevant to LANL programs in nanotechnology, semiconductor modeling and complexity in nonlinear systems. It was a paradigm for LANL's core competency in *Theory, Modeling and High-Performance Computing*. The project involved excellent complementary skills at UCSB and LANL and substantially benefited both institutions. A detailed understanding of new semiconductor devices based on this technology will enable engineers of the future to design devices which have nonlinear optical properties, such as strong harmonic generation, and use the intrinsic quantum nature of these devices to an advantage.

Scientific Approach and Accomplishments

Theoretical work consisted of a series of models of driven quantum wells, increasing in detail. We successfully modeled the electron-electron interactions within quantum wells. Assuming a carrier density in the well, we developed an explicitly time-dependent method for finding the self-consistent wavefunctions of the driven system, within the Hartree-Fock approximation. This allowed us to study nonlinear effects in quantum wells, such as harmonic generation, and drive amplitude-dependent depolarization effects. The effort represented the first serious attempt to extend density functional methods to nonlinear response in systems of interacting electrons.

We can at this stage compute the physical state of a laser-driven system of electrons and photons and make nonperturbative predictions for experiments. This is a nonperturbative dynamic quantum theory for systems driven by time-periodic potentials. For such systems, dynamic energy spectra of electrons and photons and their corresponding wave functions are obtained by taking a long-time average. We predicted: (1) the dynamic energy spectrum composed of subsets of sidebands; (2) a distribution of the wavefunction amplitudes for composite electron and photon systems; and (3) off-resonant and resonant processes. The predictions for experimental investigations turned out to be rather straightforward. Finally, we developed a theory of nonequilibrium transport in a double quantum dot system.

This project was responsible for the training of two postdoctoral fellows, both of whom have secured permanent positions in industrial research.

Publications

1. "Far-Infrared Second-Harmonic Generation in GaAs/AlGaAs Heterostructures: Perturbative and Nonperturbative Response," W. W. Bewley, C. L. Felix, J. J. Plombon, M. S. Sherwin, M. Sundaram, P. F. Hopkins and A. C. Gossard, to appear in Physical Review B.

2. "Nonlinear Multiphoton Resonances in Quantum Wells," B. Galdrikian, B. Birnir and M. Sherwin, Physics Letter A, July 31, 203, nr. 5-6, 319-332 (1995).

3. "Hartree-Fock Computation of Electrons in Quantum Wells," B. Birnir, V. Gudmundsson and K. Johnson, preprint (1997).

4. "Period doubling and strange attractors in quantum wells," B. Galdrikian and B. Birnir, Phys. Rev. Lett. 29, April 1996, 3308-3311.

5. "Theory of Quantized Dynamic Capacitance Charging Spectroscopy in Nanostructures", L. Wang, W. Z. Wang and A. R. Bishop, Phys. Rev. Lett. 74, 4710 (1995).

6. "Memory Function Approach to Interacting Quasiparticle Boson Systems", V. M. Kenkre, S. Raghavan, A. R. Bishop, M. Salkola, Phys. Rev. B 53, 5407 (1996).

7. "Nonequilibrium Transport and Population Inversion in Double Quantum Dot Systems", J. Zang, A. R. Bishop, J. Birman, L. Wang, Int. J. Mod. Phys. 11, 1463 (1997).

8. "Time-periodic quantum theory: interpretation of quasi-energies", L. Wang, B. Birnir and Y. Zhu, preprint (1997).

9. "The global attractor of the transverse Maxwell-Bloch equations," B. Birnir and J. Xin, preprint (1997).

10. "Coupled Spin-Boson Systems far from Equilibrium", M. Salkola, A. R. Bishop, V. M. Kenkre, S. Raghavan, Phys. Rev. B R54, 12645 (1996).

11. "A Finite Dimensional Attractor of the Moore-Greitzer PDE Model", B. Birnir and H. A. Hauksson, preprint (1997).