# Path Integral Simulations of Charged Multiexcitons in InGaAs/GaAs Quantum Dots

M. Harowitz* and J. Shumway*

*Dept. of Physics and Astronomy, Arizona State University, Tempe, AZ 85287

**Abstract.** We give an introduction and brief overview of our path integral simulation technique for quantum dots. We have studied the effects of spectators on photoluminescence spectra in an applied electric field. The path integral simulations also allow us to directly simulate the charge profile of the exciton in an electric field, with full treatment of correlation and spectators. The dipole moment is negative (electron-over-hole) in all cases, even for a dot with uniform composition.

## INTRODUCTION

Self assembled InGaAs/GaAs dots are small, optically active structures that can confine electrons and holes. When several electrons and holes occupy the dot, these particles interact with coulomb forces. At a mean-field level, one observes coulomb contributions to charging energies in capacitance-voltage measurements. Single dot spectroscopy reveals more subtle effects of few-body interactions, and a full determination of exchange and correlation energies are needed to explain "spectator shifts" in multi-exciton spectra [1].

In this paper we use path-integral quantum Monte Carlo to investigate the photoluminescence (PL) spectra of an exciton as a function of applied electric field in the presence of spectators. The electric-field dependence of exciton PL spectra has been used to determine the intrinsic dipole moment of an exciton in a dot [2, 3]. This dipole gives a clue to the relative locations of electron and hole, which is important for designing prototype devices with dots coupled to neighboring dots, wells, or wires. Spectator electrons and holes modify the spatial distribution of the electron and hole densities, which leads to noticeable changes in the electric-field dependence of the PL spectra.

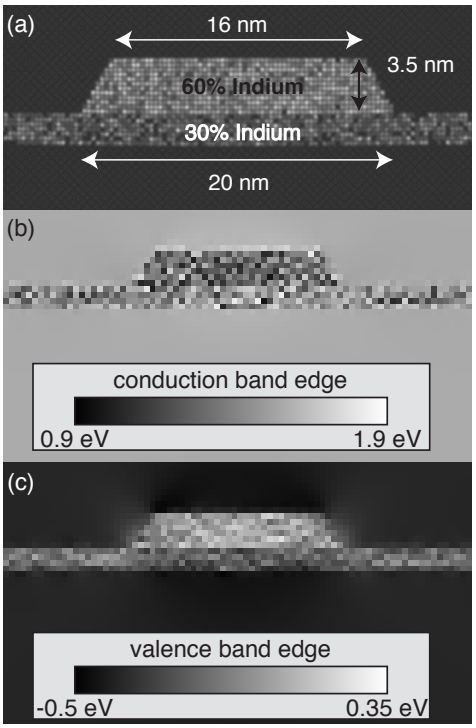


**FIGURE 1.** Our dot model: (a) composition profile, showing the truncated-conical dot, wetting layer, and random alloy material, (b) strain-modified conduction band confining potential, and (c) strain-modified valence-band confining potential.

## METHOD

*Choice of model.* Our detailed atomistic model of a dot, previously studied in Ref. [4], is shown in Fig. 1(a). We relax the atomic positions with a valence force field potential, and extract an effective mass model using the local composition and strain profile. The effective electron and hole potentials, Fig. 1(b) and 1(c), are stored on a grid, where each grid point has the averaged data from about eight atoms. Currently, our path integral simulations are restricted to single band effective mass models, but we are actively working on a formalism to dynamically include spin and band degrees of freedom. The large strain in the dot and wetting layer breaks valence

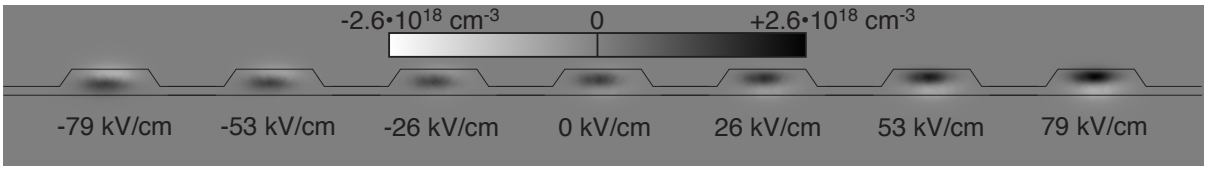


**FIGURE 2.** Net charge density profile of an exciton for different electric fields applied in the growth direction.

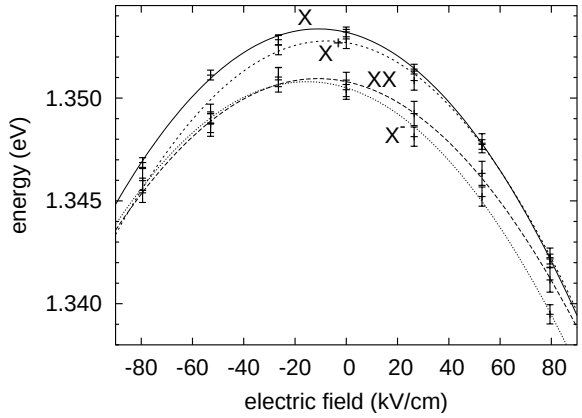


**FIGURE 3.** Energy of PL emission for an exciton ($X$), charged trion ($X^+$ and $X^-$) and biexciton ($XX$) as a function of applied electric field in the growth direction.

band degeneracy, so that approximating the hole states as heavy-hole only is reasonable. Models with multiple bands are better at predicting single particle properties, but in this study we are willing to trade accuracy of single particle properties in order to accurately describe the coulomb correlation. Comparison with Ref. [4] shows our absolute exciton energies may be off by about 0.1 eV, but our results for relative energies and spectator effects should be much better [5].

*Path Integral Technique.* A quantum system in thermal equilibrium is described by a thermal density matrix, $\hat{\rho} = e^{-\beta \hat{H}}$. The expectation value of an operator is given by a trace, $\langle \hat{\mathcal{O}} \rangle = Z^{-1} \operatorname{Tr} \hat{\mathcal{O}} \hat{\rho}$, where $Z = \operatorname{Tr} \hat{\rho}$. As a computational alternative to the Schrödinger equation, physical properties may be sampled directly from the path integral representation of the thermal density matrix,

$$\rho(R, R'; \beta) = \int \mathscr{D}R(t) e^{-S_E[R(t)]}, \qquad (1)$$

where $R$ refers to all $3N$ coordinates of the particles and $S_E[R(t)]$ is the Euclidean action [6]. The symbol $\int \mathscr{D}R(t)$ indicates a sum over all paths $R(t)$ starting at $R(0) = R'$ and ending at $R(\beta) = R$. Using Metropolis Monte Carlo, we sample the path integral and collect data on the energy, charge density, and dipole moments of an exciton, biexciton, and charged trions [7].

## RESULTS AND CONCLUSIONS

We show the charge density profile of an exciton, as a function of the applied field in Fig. 2. The non-linear stark effect for emission from an exciton with spectators is shown in Fig. 3 . We note that even with uniform composition, the dot has an inverted (electron-over-hole) dipole at zero applied field. The dipole moments and polarizability of the exciton is noticeably affected by carriers, and we note that the ordering of PL lines can change with application of an external field. Current work is underway to study different composition profiles and check against multi-band models. We are also extending these techniques to systems with many electrons and holes, such as dots coupled to quantum wells.

## ACKNOWLEDGMENTS

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