Quantum Wells,wires and dots (QWWAD): development of an open-source simulation suite for semi-conductor nanostructures

VALAVANIS, A, COOPER, J D, GRIER, A and HARRISON, Paul
<http://orcid.org/0000-0001-6117-0896>

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Quantum wells, wires and dots (QWWAD): development of an open-source simulation suite for semiconductor nanostructures

A. Valavanis,[a,1] J. D. Cooper,[1] A. Grier,[1] and P. Harrison,[2]

[1]School of Electronic and Electrical Engineering, University of Leeds, Leeds, LS2 9JT, UK

[2]Materials and Engineering Research Institute, Sheffield Hallam University, S1 1WB, UK

[a)]Email: a.valavanis@leeds.ac.uk

A number of robust software tools are available for simulating semiconductor nanostructures, including purpose-made products such as Nextnano [1] and generic finite-element solvers such as COMSOL Multiphysics [2]. Although the existing tools are highly regarded, the majority of available software is supplied under a proprietary license, meaning that its source code cannot be studied, modified or redistributed freely by its users. As such, there is currently a lack of free software for students wishing to learn the mathematical and computational techniques that underpin modern nanoscale semiconductor physics.

We present a non-commercial, free-and-open-source project, *Quantum Wells, Wires and Dots* (QWWAD) [3], which is released under the GNU General Public License 3.0 [4]. This software accompanies the forthcoming 4th edition of the eponymous textbook [5], and includes analytical and numerical solvers for the Schrödinger and Poisson equations, subband populations, tunnelling and scattering phenomena, diffuse structures, impurity and exciton states, and effective-mass and pseudopotential models of quantum wires and dots.

In this paper, we explain our design methodology and software engineering approach, and give an overview of the calculations that are included in the simulation suite. In particular, we focus on the adoption of automated testing, which ensures the reliability of the underlying calculations in the software, and on the provision of a large number of computational examples, enabling the use of the software as an educational tool. Fig. 1 shows exemplar plots of the data generated by these example scripts. Finally, we discuss the development of an application programming interface (API), enabling the functionality in QWWAD to be adopted easily into other free software tools.

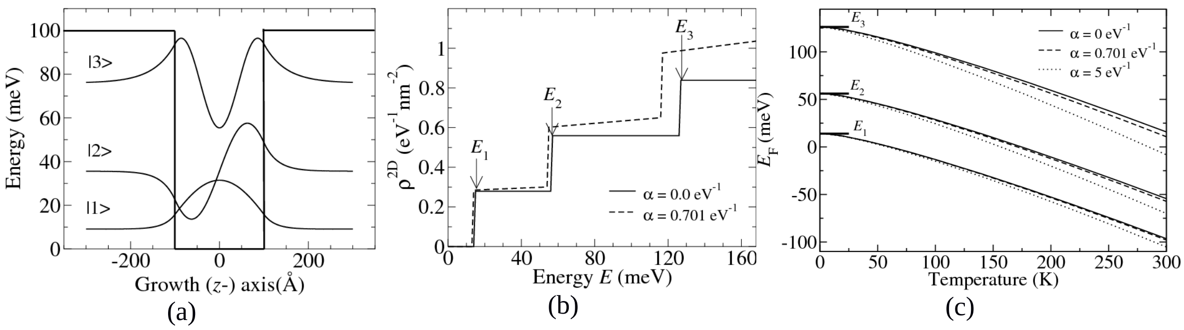

Fig. 1: Sample plots of the output data from the QWWAD educational example scripts. (a) The first three eigenstates in a finite GaAs quantum well. (b) Density of states in 200-Å GaAs infinite well assuming parabolic dispersion (solid lines) and nonparabolic dispersion (dashed lines). (c) Effect of carrier temperature on quasi-Fermi levels in an infinite quantum well, with a range of nonparabolicity factors.

References

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[5] P. Harrison and A. Valavanis, *Quantum Wells, Wires and Dots*, 4th Ed. Wiley, Chichester, (in preparation).