Development of electronic device simulations for educational purposes

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Abstract A comprehensive set of semiconductor device simulation tools, written in Java, is being developed for instructional use. These interactive programs can be launched from an electronic textbook or from lecture presentation material. At present these tools demonstrate introductory quantum mechanics, several aspects of semiconductor physics, and both zero-current and drift-diffusion device simulations in one dimension. Development of two-dimensional simulations is in progress.

Keywords Java · Thomas–Fermi · Hartree · Drift-diffusion

1 Introduction

Students studying electron device theory need to visualize the workings of devices in a way that can only be addressed by device simulation. But professional-level simulators are not particularly accessible in an instructional context. Thus device calculations intended for instruction have simply implemented the quasi-analytic approximations traditionally found in the textbooks [1, 2].

To change this situation, I have undertaken the development of a comprehensive set of interactive device simulation tools written in Java. They are designed to be launched directly from an electronic textbook on active device theory. Because this work is only intended for electronic distribution, publication cost is not an issue, and the material is presented at all appropriate levels of sophistication: undergraduate, graduate, and professional. One particular goal is to develop and present a new synthesis of active electron device theory which emphasizes the common mechanisms of rather than the detailed differences between bipolar and field-effect transistors (and even vacuum tubes).

The scope of the work includes background material consisting of introductory quantum mechanics, solid-state theory applicable to semiconductors and related materials, and quantum treatment of irreversible systems. Equilibrium properties and non-equilibrium transport in semiconductors, and the properties of surfaces and interfaces provide the basis for understanding active device mechanisms. Active devices are primarily treated by fully-functional simulations that are unconstrained by the preconceptions of quasi-analytic models.

2 Introductory quantum mechanics

The thrust of this work is to demonstrate the power of numerical solution procedures, as opposed to simple numerical evaluation of expressions obtained by analytic manipulation. The vast majority of solutions are obtained by either a variation of Gaussian elimination on linear systems, or Newton-Raphson solution of nonlinear systems (or the combination of both methods).

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The tool developed to introduce the Schrödinger equation provides a good example of the present approach. A potential is described by a piecewise-analytic specification and the resulting domain is discretized subject to open boundary conditions [3]. When the user selects an energy and direction of incidence by dragging a cursor, the wavefunction is evaluated by solving the inhomogeneous open-system problem and displayed as in Fig. 1. Animating these wavefunctions (multiplying by $e^{-iEt/\hbar}$) leads to an understanding of the distinction between traveling and standing waves.
The same machinery can be used to evaluate and display the retarded Green’s function:

\[ \hat{G}(z, z', E) = \left[ E - \hat{H} + i\epsilon \right]^{-1}(z, z'). \]  

\( G \) is plotted versus \( z \) as illustrated in Fig. 2. The location of the impulse \( z' \) is set by dragging the horizontal cursor and the energy is selected by the vertical cursor. The ability to vary these quantities interactively provides a means to explore the behavior of the very complicated object \( \hat{G} \). Because the density of states can be obtained from the imaginary part of \( \hat{G}(z, z) \), it can be easily evaluated and displayed in a grayscale plot as in Fig. 3.

3 Semiconductor device simulations

A work on device theory of course requires device simulation tools, and these tools depend upon an extensive library of semiconductor physics code and material data. By exposing these capabilities to the user via an interactive interface, we can help a student to develop an intuitive understanding of the more difficult aspects of these subjects. A good example of this is the determination of the charge-neutral Fermi level as shown in Fig. 4. Finding the Fermi level requires the solution of an extremely nonlinear equation. The interactive interface graphically displays the components of this equation and permits the user to adjust the semiconductor material, dopant types and concentrations, and the temperature. The code itself evaluates the Fermi level by Newton–Raphson iterations.

In the present context a “device simulation” means that Poisson’s equation is solved self-consistently with some model of the mobile charge carrier distribution. At present, two main types of simulations have been implemented: zero-current and drift-diffusion models. Zero-current models are just the electrostatic screening models of solid-state physics,