

Efficient Solution of the Schrödinger-Poisson Equations in Semiconductor Device Simulations

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Abstract. This paper reviews the numerical issues arising in the simulation of electronic states in highly confined semiconductor structures like quantum dots. For these systems, the main challenge lies in the efficient and accurate solution of the self-consistent one-band and multi-band Schrödinger-Poisson equations. After a brief introduction of the physical background, we first demonstrate that unphysical solutions of the Schrödinger equation due to the presence of material boundaries can be avoided by combining a suitable ordering of the differential operators with a robust discretization method like box discretization. Next, we discuss algorithms for the efficient solution of the resulting sparse matrix problems even on small computers. Finally, we introduce a predictor-corrector-type approach for the stabilizing the outer iteration loop that is needed to obtain a self-consistent solution of both Schrödinger's and Poisson's equation.

1 Physical Background

1.1 Introduction

Due to the rapid progress in semiconductor technology, the dimensions of electronic devices are approaching the nanometer scale. At this scale, electronic properties will be increasingly dominated by quantum effects, until at some point these effects become essential for device operation. For instance, the electronic states in highly confined semiconductor structures like quantum dots are entirely controlled by quantum mechanical size quantization, which can be exploited for entirely new device designs like quantum well or quantum dot lasers. At the same time, the physical equations that describe these quantum systems are much too complex to be solved analytically and efficient numerical solution methods need to be used instead. For this reason, we review in this paper the numerical issues arising in the simulation of electronic states in confined quantum systems, with focus on the efficient solution of the self-consistent Schrödinger-Poisson equations.

1.2 The $k \cdot p$ (Schrödinger) Equations

Since these quantum structures are about one to two orders of magnitude larger than a single lattice constant (which is about 0.5 nm), atomistic models like

empirical tight binding theory or empirical pseudopotential methods are numerically not feasible and a continuum model with carefully tuned material parameters needs to be used. Such a continuum model is provided by the k-p-equations in the envelope function approximation [10, 5, 2].

In this model, we describe the electrons in the conduction band by an one-band k-p-equation which is called the effective-mass approximation. Here, the electron wave functions $\psi_n^e(\mathbf{x})$ obey the Schrödinger equation

$$E_n^e \psi_n^e(\mathbf{x}) = \hat{H}_{\text{eff}} \psi_n^e(\mathbf{x}) \quad (1)$$

with the effective mass Hamiltonian

$$\hat{H}_{\text{eff}} = \frac{1}{2} \hat{\mathbf{p}} \cdot \left(\frac{1}{m^*} \hat{\mathbf{p}} \right) + E_C(\hat{\mathbf{x}}) + \hat{V}_{\text{xc}}(\hat{\mathbf{x}}) \quad \hat{\mathbf{p}} = \frac{\hbar}{i} \nabla \quad (2)$$

where E_n^e is the energy of wave function $\psi_n^e(\mathbf{x})$, $E_C(\mathbf{x})$ the conduction band edge, and $V_{\text{xc}}(\mathbf{x})$ the exchange-correlation potential in the local density approximation. Finally, m^* is a 3×3 -tensor describing the effective electron mass in the semiconductor.

For holes in the valence bands, the effective-mass approximation is usually not accurate enough anymore, and a multi-band approach treating the three main valence bands simultaneously is needed. Since each of the three valence bands has two spin components, we need here the 6-band k-p-equation

$$E_n^h \psi_n^h(\mathbf{x}) = \hat{H}_{6 \times 6} \psi_n^h(\mathbf{x}) \quad (3)$$

where $\psi_n^h(\mathbf{x})$ is a 6-component hole wave function, and $\hat{H}_{6 \times 6}$ a Hermitian 6×6 -matrix operator

$$\hat{H}_{6 \times 6} = \begin{pmatrix} \hat{H}_{3 \times 3} & 0 \\ 0 & \hat{H}_{3 \times 3} \end{pmatrix} + \hat{H}_{\text{so}}^{6 \times 6} \quad (4)$$

Here, $\hat{H}_{\text{so}}^{6 \times 6}$ is a momentum independent complex matrix that describes the spin-orbit interaction, and $\hat{H}_{3 \times 3}$ a 3×3 -matrix that for a Zincblende crystal structure oriented along the coordinate axes has the form [9]

$$\begin{aligned} \left(\hat{H}_{3 \times 3} \right)_{ij} &= \left[E_V(\hat{\mathbf{x}}) + \hat{V}_{\text{xc}}(\hat{\mathbf{x}}) \right] \delta_{ij} + \frac{1}{2m_0} \hat{\mathbf{p}}^2 \delta_{ij} + \frac{N}{\hbar^2} \hat{p}_i \hat{p}_j \\ &+ \frac{L - N - M}{\hbar^2} \hat{p}_i^2 \delta_{ij} + \frac{M}{\hbar^2} \hat{\mathbf{p}}^2 \delta_{ij} \end{aligned} \quad (5)$$

where $E_V(\mathbf{x})$ is the valence band edge, m_0 the vacuum mass of the electron, and L , M , and N the Dresselhaus parameters for the semiconductor [5].

Since the focus of our simulations are closed systems, we use homogeneous Dirichlet conditions ($\psi \equiv 0$) for all resulting Schrödinger equations. But note that the energies and wave functions of bound states in a confining potential are only weakly affected by their boundary conditions, as long as the simulation region in which Schrödinger's equation is solved is large enough.

1.3 Carrier Densities and the Poisson Equation

In thermal equilibrium, the electron and hole densities $n(\mathbf{x})$ and $p(\mathbf{x})$ are calculated from the quantum states $\{E_n, \psi_n\}$ as [15]

$$n(\mathbf{x}) = 2 \sum_n |\psi_n^e(\mathbf{x})|^2 F\left(\frac{E_n^e - E_F}{k_B T}\right) \quad (6)$$

$$p(\mathbf{x}) = 2 \sum_n |\psi_n^h(\mathbf{x})|^2 F\left(\frac{E_F - E_n^h}{k_B T}\right) \quad (7)$$

where k_B is the Boltzmann constant, T the temperature of the system, and $F(E)$ a suitable distribution function. This $F(E)$ is in three dimensions equal to the Fermi function

$$F(E) = \frac{1}{1 + \exp(E)} \quad (8)$$

while in one and two dimensions $F(E)$ is proportional to the complete Fermi-Dirac integrals $\mathcal{F}_0(-E)$ and $\mathcal{F}_{-1/2}(-E)$. Furthermore, in addition to these carrier densities there may also be space charges

$$N_D^+(\mathbf{x}) = N_D^+[E_C(\hat{\mathbf{x}})] \quad N_A^-(\mathbf{x}) = N_A^-[E_V(\hat{\mathbf{x}})] \quad (9)$$

present due to doping with electron donors (N_D^+) and acceptors (N_A^-).

All these charge densities add up to a total charge

$$\rho(\mathbf{x}) = e [p(\mathbf{x}) - n(\mathbf{x}) + N_D^+(\mathbf{x}) - N_A^-(\mathbf{x})] \quad (10)$$

which then results through Poisson's equation

$$\nabla \cdot [\epsilon(\mathbf{x}) \nabla \phi(\mathbf{x})] = -\rho(\mathbf{x}) \quad (11)$$

into an electric potential $\phi(\mathbf{x})$ that warps the band edges E_C and E_V as

$$E_C(\mathbf{x}) \longrightarrow E_C[\phi](\mathbf{x}) = E_C(\mathbf{x}) - e\phi(\mathbf{x}) \quad (12)$$

$$E_V(\mathbf{x}) \longrightarrow E_V[\phi](\mathbf{x}) = E_V(\mathbf{x}) - e\phi(\mathbf{x}) \quad (13)$$

As consequence, the charge density ρ becomes potential dependent and the Poisson equation (11) nonlinear in ϕ

$$\nabla \cdot (\epsilon \nabla \phi) = -e (p - n + N_D^+[\phi] - N_A^-[\phi]) \quad (14)$$

Note that the carrier densities n and p depend here indirectly on ϕ , since the band edges $E_C[\phi]$ and $E_V[\phi]$ enter the Hamiltonian, which of course makes also all wave functions and energies potential dependent. As a consequence, the nonlinear Poisson equation (14) and the Schrödinger equations become a coupled system of differential equations for which we need to find a self-consistent solution.

1.4 Operator Ordering and Symmetrization

An important issue we have ignored so far is that the material parameters in (2) and (5) are position dependent in heterostructures. This is a major problem since both Hamiltonians are strictly speaking only valid for a homogeneous semiconductor with slowly varying band edges $E_C(\mathbf{x})$ and $E_V(\mathbf{x})$. Some numerical experimentation now shows that even in the presence of material induced discontinuities in the band edges these Hamiltonians still deliver physically reasonable results. This empirical observation can also be partially justified using Burt's exact envelope function theory [3, 4].

Unfortunately, variations in m^* and L, M, N are much more problematic, since here we need also to define the operator ordering between these material parameters and the momentum operator $\hat{\mathbf{p}}$. While it is clear that any symmetrization procedure used must yield a Hermitian Hamiltonian

$$H(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = H(\hat{\mathbf{x}}, \hat{\mathbf{p}})^\dagger \quad (15)$$

this requirement is not sufficient for uniquely defining $H(\hat{\mathbf{x}}, \hat{\mathbf{p}})$. Furthermore, a poorly chosen $H(\hat{\mathbf{x}}, \hat{\mathbf{p}})$ will result in wave functions that become unphysical at material interfaces and lead to highly incorrect solutions [7].

For the effective mass approximation (2), we can use in analogy to Poisson's equation (11) the Hamiltonian [11]

$$H_{\text{eff}}(\hat{\mathbf{x}}, \hat{\mathbf{p}}) = \frac{1}{2}\hat{\mathbf{p}} \cdot \left[\frac{1}{m^*(\hat{\mathbf{x}})}\hat{\mathbf{p}} \right] + E_C(\hat{\mathbf{x}}) + \hat{V}_{\text{xc}}(\hat{\mathbf{x}}) \quad (16)$$

where compared to (2) we have just replaced the effective mass m^* by the operator $m^*(\hat{\mathbf{x}})$. This Hamiltonian is flux conserving and leads to wave functions that are continuous at material interfaces and smooth everywhere else. Since most alternative Hamiltonians do not share these properties [11], Hamiltonian (16) is widely used in quantum simulations.

For the 6-band k·p-Hamiltonian (4-5) finding a suitable symmetrization is more difficult since $\hat{H}_{6 \times 6}$ as 6×6 -matrix requires only

$$\left(\hat{H}_{6 \times 6}\right)_{ij}^\dagger = \left(\hat{H}_{6 \times 6}\right)_{ji} \quad (17)$$

in order to become Hermitian. Here, one can show that starting again from Burt's exact envelope function theory a suitable 6-band k·p-Hamiltonian $\hat{H}_{6 \times 6}(\hat{\mathbf{x}}, \hat{\mathbf{p}})$ can be constructed using the rather complicated operators [7, 8]

$$\begin{aligned} [H_{3 \times 3}(\hat{\mathbf{x}}, \hat{\mathbf{p}})]_{ij} = & \left[E_V(\hat{\mathbf{x}}) + \hat{V}_{\text{xc}}(\hat{\mathbf{x}}) \right] \delta_{ij} + \frac{1}{2m_0}\hat{\mathbf{p}}^2 \delta_{ij} + \hat{p}_i \frac{N(\hat{\mathbf{x}})}{\hbar^2} \hat{p}_j \\ & + \hat{p}_i \left[\frac{L(\hat{\mathbf{x}}) - N(\hat{\mathbf{x}}) - M(\hat{\mathbf{x}})}{\hbar^2} \right] \hat{p}_i \delta_{ij} + \hat{\mathbf{p}} \cdot \left[\frac{M(\hat{\mathbf{x}})}{\hbar^2} \hat{\mathbf{p}} \right] \delta_{ij} \\ & - \hat{p}_i \frac{M(\hat{\mathbf{x}})}{\hbar^2} \hat{p}_j + \hat{p}_j \frac{M(\hat{\mathbf{x}})}{\hbar^2} \hat{p}_i \end{aligned} \quad (18)$$

where the two last terms vanish in a bulk semiconductor. The resulting Hamiltonian $H_{6 \times 6}(\hat{\mathbf{x}}, \hat{\mathbf{p}})$ is again flux conserving and yields wave functions that are continuous at material interfaces and smooth everywhere else.

2 Numerical Issues

2.1 Discretization

Both the Poisson equation and the Schrödinger equations are discretized using box integration on a nonuniform tensor product grid. Such a grid can be seen as the tensor product of D nonuniform one-dimensional grids $\{x_i\}$ along each coordinate axis, where D is the dimension of the simulation domain. Such tensor grids have the advantage that no complicate meshing algorithm is required, and the discretization can be easily and efficiently implemented. In our implementation, the user provides the desired density of grid lines at selected locations along the coordinate axes. The resulting tensor product grid is then calculated by interpolating these line densities.

For the box integration finite difference method [14–page 184], we cover the simulation domain with N non-overlapping rectangular boxes, where each box is centered on a grid node. We then integrate our differential equations over each box volume Ω to obtain an integral equation which can then be discretized. For instance, the Poisson equation (14) becomes after integration over Ω

$$\int_{\partial\Omega} \mathbf{n}(\mathbf{x}) \cdot [\epsilon(\mathbf{x}) \nabla \phi(\mathbf{x})] = - \int_{\Omega} \rho(\mathbf{x}) \quad (19)$$

which after discretization then yields the familiar three, five, or seven-point stencils for ϕ .

Compared to standard finite differences, box integration has the advantage that discontinuities in a material parameter A are naturally taken into account for second order differential operators $\hat{\partial}_i A(\hat{\mathbf{x}}) \hat{\partial}_j$, since this method is in first order flux conservative due to the Gauss theorem. This makes box integration a natural choice for discretizing the Poisson equation (14) and the Schrödinger equations resulting from (16) and (18).

After the discretization, all operators $\hat{\partial}_i A(\hat{\mathbf{x}}) \hat{\partial}_j$ in these equations become banded sparse matrices. Such matrices can be easily stored and manipulated using banded storage schemes that store only the non-zero diagonals. In specific, the Schrödinger equation belonging to the Hamiltonians (16) or (18) becomes after discretization a generalized symmetric matrix eigenvalue problem of the form

$$H\psi_n = E_n D\psi_n \quad D_{ij} = \delta_{ij} \text{Vol}(\Omega_i) \quad (20)$$

with D being a diagonal matrix containing the volumes of the box regions Ω_i on the main diagonal. Similarly, the Poisson equation (14) as a boundary value problem yields a linear system, if we ignore the dependence of the charge density $\rho(\phi)$ on the potential ϕ for now.

2.2 Solving the Nonlinear Poisson Equation

At this point, solving each of the two differential equations offers its own set of challenges. For solving the nonlinear Poisson equation (14)

$$f(\phi) \equiv \nabla \cdot (\epsilon \nabla \phi) + \rho(\phi) = 0 \quad (21)$$

we can immediately use Newton-Raphson iteration with inexact line search as

$$\tilde{\phi}_k(\lambda) \equiv \phi_k - \lambda [(D_\phi f)(\phi_k)]^{-1} \cdot f(\phi_k) \quad (22)$$

$$\phi_{k+1} \equiv \tilde{\phi}_k(\lambda) \quad \text{with} \quad \left\| f(\tilde{\phi}_k(\lambda)) \right\| \equiv \min \quad \lambda = 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \dots \quad (23)$$

in order to find a solution of the nonlinear problem (experience shows that local minima in $\|f(\phi)\|$ or multiple solutions do not occur for nanostructures).

We also note that, except for the extra diagonal term $D_\phi \rho$, the Jacobian matrix in (22)

$$(D_\phi f)(\phi) = \hat{\nabla} \cdot (\epsilon \hat{\nabla}) + (D_\phi \rho)(\phi) \quad (24)$$

is identical to the Poisson operator $\hat{\nabla} \cdot (\epsilon \hat{\nabla})$. Since $\hat{\nabla} \cdot (\epsilon \hat{\nabla})$ is positive definite and $D_\phi \rho$ is positive for all physical $\rho(\phi)$, the Jacobian $D_\phi f$ must be positive definite as well. Therefore, we can employ the preconditioned conjugate gradient method [12–chapter 6] for solving the linear system in (22). As preconditioner we use here the very fast fill-in free Dupont-Kendall-Rachford method [6] in order to achieve rapid convergence of the conjugate gradient iteration.

2.3 Solving the Schrödinger Equations

Solving the matrix eigenvalue systems resulting from the discretization of the Schrödinger equations is computationally much more demanding. Especially the 6-band k-p-Hamiltonian (18) results here into extremely large sparse matrices that prohibit the use of standard diagonalization routines. Luckily enough, all distribution functions $F(E)$ that are used in calculating the electron and hole densities (6) and (7) fall off exponentially as

$$F(E) \propto \exp(-E), \quad E \gg 0. \quad (25)$$

For this reason, only relatively few quantum states at the lower end of the energy spectrum are needed to calculate the densities, which allows us to use highly efficient iterative eigenvalue methods like the Lanczos or Arnoldi iteration [12].

One software package that implements such iteration methods for both real and complex matrices is ARPACK [1]. In the authors' experience, ARPACK appears quite reliable and moderately fast for the matrices that occur in the simulation of quantum structures. However, ARPACK is still not fast enough for the huge system matrices that arise in three-dimensional quantum simulations and an additional preconditioner is needed.

Such a preconditioner can be easily obtained by utilizing the Chebyshev polynomials $T_n(x)$ for a spectral transformation. Here we use that if the Hermitian matrix \hat{H} has the spectrum $\{E_n\}$, the matrix $T(\hat{H})$ must have the spectrum $\{T(E_n)\}$. Since the polynomials $T_n(x)$ increase very rapidly for $|x| > 1$, we can use these $T_n(x)$ to make the desired eigenvalues at the lower end of the spectrum very large, which accelerates the convergence of the Arnoldi iteration in ARPACK tremendously.

As a quick test for this preconditioned ARPACK code, we solve the eigenvalue problem for test matrices obtained by discretizing an one-band problem (16). For these matrices, we get for a 3 GHz PC and 15-th order Chebyshev polynomials as solution times

grid size	# states	CPU time
$50 \times 50 \times 50$	30	17 s
$50 \times 50 \times 50$	200	357 s
$100 \times 100 \times 100$	30	269 s

This test shows that memory exhaustion now surpasses excessive CPU time as the main concern for quantum simulations.

2.4 Solution of the Coupled System

As the last step, we need to tackle the self-consistent solution of the coupled nonlinear Poisson and Schrödinger equations. Here, a simple iteration does not converge due to the strong coupling between the equations. Similarly, under-relaxation stabilizes the outer iteration only very poorly, and we still observe strong charge oscillations from one iteration step to the next that interfere with convergence [13].

This situation can be much improved by partially decoupling both partial differential equations using a predictor-corrector-type approach. In order to do this, we replace the exact carrier densities $n(\mathbf{x})$ and $p(\mathbf{x})$ from (6) and (7) by the ϕ -dependent predictors [13]

$$\tilde{n}[\phi](\mathbf{x}) = 2 \sum_n |\psi_n^e(\mathbf{x})|^2 F \left(\frac{E_n^e - E_F + e[\phi(\mathbf{x}) - \phi_{\text{prev}}(\mathbf{x})]}{k_B T} \right) \quad (26)$$

$$\tilde{p}[\phi](\mathbf{x}) = 2 \sum_n |\psi_n^h(\mathbf{x})|^2 F \left(\frac{E_F - E_n^h - e[\phi(\mathbf{x}) - \phi_{\text{prev}}(\mathbf{x})]}{k_B T} \right) \quad (27)$$

where ϕ_{prev} is the electrostatic potential from the previous outer iteration step. These predictors for the quantum densities n and p are then used in the nonlinear Poisson equation

$$\nabla \cdot (\epsilon \nabla \phi) = -e (\tilde{p}[\phi] - \tilde{n}[\phi] + N_D^+[\phi] - N_A^-[\phi]) \quad (28)$$

in order to determine the new potential $\phi(\mathbf{x})$. Using this $\phi(\mathbf{x})$ we update the band edges $E_C(\mathbf{x})$ and $E_V(\mathbf{x})$ in the Hamiltonians (16) and (18), and solve the respective Schrödinger equations for a new set of energies and wave functions.

Obviously, once the iteration has converged we have $\phi = \phi_{\text{prev}}$ and therefore with $n = \tilde{n}[\phi]$ and $p = \tilde{p}[\phi]$ also the correct densities. The numerical experiment then shows [13] that this approach leads to rapid convergence with the residuals in the quantum densities n and p decreasing by about one order of magnitude. No further steps are necessary to ensure convergence [13].

References

1. ARPACK libraries and related publications <http://www.caam.rice.edu/software/ARPACK/>.
2. Bastard, G.: Superlattice band structure in the envelope-function approximation. *Phys. Rev. B* **24** (1981) 5693–5697
3. Burt, M.G.: The justification for applying the effective-mass approximation to semiconductors. *J. Phys.: Condens. Matter* **4** (1992) 6651–6690
4. Burt, M.G.: Fundamentals of envelope function theory for electronic states and photonic modes in nanostructures. *J. Phys.: Condens. Matter* **11** (1999) R53–R83
5. Dresselhaus, G., Kip, A.F., Kittel, C.: Cyclotron Resonance of Electrons and Holes in Silicon and Germanium Crystals. *Phys. Rev.* **98** (1955) 368–384
6. Dupont, T., Kendall, R.P., Rachford, H.H.: An approximate factorization procedure for solving self-adjoint elliptic difference equations. *SIAM J. Numerical Analysis* **5** (1968) 559–573
7. Foreman, B.A.: Effective-mass Hamiltonian and boundary conditions for the valence bands of semiconductor microstructures. *Phys. Rev. B* **48** (1993) 4964–4967
8. Foreman, B.A.: Elimination of spurious solutions from eight-band k-p theory. *Phys. Rev. B.* **56** (1997) R12748–12751
9. Kane, E.O.: The k-p method. In: *Semiconductors and Semimetals: III–V compounds*, vol. 1, ed by R.K. Willardson, A.C. Beer (Academic Press, New York 1966) 75–100
10. Luttinger, J.M., Kohn, W.: Motion of Electrons and Holes in Perturbed Periodic Fields. *Phys. Rev.* **97** (1955) 869–883
11. Morrow, R.A., Brownstein, K.R.: Model effective-mass Hamiltonians for abrupt heterojunctions and the associated wave-function-matching conditions. *Phys. Rev. B* **30** (1984) 678–680
12. Trefethen, L.N., Bau III, D.: *Numerical Linear Algebra* (SIAM Society for Industrial & Applied Mathematics, Philadelphia 1997)
13. Trellakis, A., Galick, A. T., Pacelli, A., Ravaioli, U.: Iteration scheme for the solution of the two-dimensional Schrödinger-Poisson equations in quantum structures. *J. Applied Phys.* **81** (1997) 7880–7884
14. Varga, R. S.: *Matrix Iterative Analysis* (Prentice-Hall, Englewood Cliffs 1962)
15. Yu, P.Y., Cardona, M.: *Fundamentals of Semiconductors* (Springer, Berlin Heidelberg New York 1996)