On the Numerics of 3D Kohn-Sham System

Kurt Hoke

Weierstrass Institute for
Applied Analysis and Stochastics

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Mathematical Models for Transport in Macroscopic and Mesoscopic Systems, Feb. 2008

Outline

1. Physical System
   - The Kohn-Sham System
2. Analytical Results
   - Existence and Uniqueness of Solutions
3. Numerics
   - The Kerkhoven Scheme
   - Results

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The System

Poisson equation:

$$-\nabla \cdot (\epsilon \nabla \varphi) = q \left(N_A - N_D + \sum e_\xi u_\xi \right) \quad \text{on } \Omega + \text{mixed b.c.}$$

Schrödinger equation:

$$\left[-\frac{\hbar^2}{2} \nabla (m_\xi^{-1} \nabla) + V_\xi \right] \psi_{l,\xi} = \mathcal{E}_{l,\xi} \psi_{l,\xi} \quad \text{on } \Omega + \text{hom. Dirichl. b.c.}$$

with carrier density $\mathbf{u} = (u_1, \ldots, u_\sigma)$, $\sigma \in \mathbb{N}$

$$u_\xi(x) = \sum_{l=1}^{\infty} N_{l,\xi}(V_\xi) |\psi_{l,\xi}(V_\xi)(x)|^2$$

and effective potential

$$V_\xi(\mathbf{u}) = -e_\xi \triangle E_\xi + V_{xc,\xi}(\mathbf{u}) + e_\xi q \varphi(\mathbf{u})$$

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quasi Fermi-Level and Fermi-Function

- occupation factor $N_{l,\xi}(V_\xi)$ given by

$$N_{l,\xi}(V_\xi) = f_\xi(\mathcal{E}_{l,\xi}(V_\xi) - \mathcal{E}_{F,\xi}(V_\xi))$$

- f_ξ a distribution function, i.e. Fermi's function (3D)

$$f(s) = \frac{1}{1 + e^{s/k_B T}}$$

- and quasi Fermi-level $\mathcal{E}_{F,\xi}(V_{eff,\xi})$ defined

$$\int_\Omega u_\xi(V_{eff,\xi}(x))dx = \sum_{l=1}^{\infty} N_{l,\xi}(V_{eff,\xi}) = N_\xi$$

N_ξ being the fixed total number of ξ-type carriers.

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The Particle Density Operator

Definition

Define the carrier density operator corresponding to f and m by

$$\mathcal{N}(V)(x) = \sum_{l=1}^{\infty} f(\mathcal{E}_l(V) - \mathcal{E}_F(V))|\psi_l(V)(x)|^2 \,, \quad V \in L^2(\Omega) \; x \in \Omega \,.$$

- $\mathcal{E}_l(V)$ and $\psi_l(V)$ are EV and L^2-normalized EF of H_V
- $\mathcal{E}_F(V)$ defined by

$$\int \mathcal{N}(\mathcal{V})dx = \sum f(\mathcal{E}_l(V) - \mathcal{E}_F(V)) = N \,.$$

- eigenvlue asymptotics of H_V and properties of f ensure well-definedness of $\mathcal{E}_F$
  $\rightarrow$ right-hand side series absolutely converges

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Solution of the Kohn-Sham System

Definition

Suppose

$$N_A - N_D \in W_\Gamma^{-1,2}(\Omega)\,, \quad \triangle E_\xi \in L^2(\Omega)\,,\ \xi \in \{1,\dots,\sigma\}\,.$$

Let $\epsilon, m_1,\dots,m_\sigma$, $f_1,\dots,f_\sigma$ be from $L_\infty(\Omega,\mathcal{B}(\mathbb{R}^3,\mathbb{R}^3))$ and φ_Γ given. Define the external potentials V_ξ and the effective doping D by

$$D = q(N_A - N_D) - \tilde{\varphi}_\Gamma\,, \quad V_\xi = e_\xi q \varphi_\Gamma - e\xi \triangle E_\xi\,,\ \xi \in \{1,\dots,\sigma\}\,.$$

$(V, u_1,\dots,u_\sigma) \in W_\Gamma^{1,2} \times (L^2(\Omega)^\sigma)$ is a solution of the Kohn-Sham system, if

$$\begin{aligned} AV &= D + q\sum_\xi e_\xi u_\xi\,, \\ u_\xi &= \mathcal{N}_\xi(V_\xi + V_{xc,\xi}(\mathbf{u}) + e_\xi q V)\,. \end{aligned}$$

Existence and Uniqueness of Solution without V_{xc}

Monotonicity and Lipschitz continuity of the Operator A yield the result:

Theorem

The Schrödinger-Poisson system without exchange-correlation potential has the unique solution

$$(\underline{V}, \mathcal{N}_1(V_1 + \underline{V}), \ldots, \mathcal{N}_\sigma(V_\sigma + \underline{V}))\,.$$

- the operator assigning the solution $\underline{V}$ to $\mathbf{V} = (V_1, \ldots, V_\sigma)$ is

$$\mathcal{L} : (L^2(\Omega))^\sigma \mapsto W_\Gamma^{1,2}(\Omega)\,, \quad \mathcal{L}(\mathbf{V}) = \underline{V}$$

- $\mathcal{L}$ is boundedly Lipschitz continuous

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Existence of Solution to the Kohn-Sham System

Definition (Fixed Point Mapping)

Let $\mathbf{V} = (V_1, \dots, V_\sigma) \in (L^2(\Omega))^\sigma$ be a given tupel of external potentials and $N_1 \dots, N_\sigma$ the fixed number of carriers. Define

$$L^1_N = \{\mathbf{u} = (u_1, \dots, u_\sigma) : u_\xi \geq 0, \int u_\xi(x)dx = N_\xi\}$$

and $\Phi : L^1_N \mapsto L^1_N$ as

$$\Phi_\xi(\mathbf{u}) =$$

$$\mathcal{N}_\xi \left(V_\xi + V_{xc,\xi}(\mathbf{u}) + e_\xi q \mathcal{L}(V_1 + V_{xc,1}(\mathbf{u}), \dots, V_\sigma + V_{xc,\sigma}(\mathbf{u}))\right)$$

Theorem (Existence of Fixed Point)

If $V_{xc,\xi}$ is for any $\xi \in \{1, \dots, \sigma\}$ a bounded and continuous mapping from $(L^1(\Omega))^\sigma$ into $L^2(\Omega)$, then the mapping Φ has a fixed point.

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Theorem (Equivalence of Solutions)

$\mathbf{u} = (u_1, \ldots, u_\sigma)$ is a fixed point of Φ if and only if

$$(V, u_1, \ldots, u_\sigma) = \left(A^{-1}\left(D + q\sum e_\xi u_\xi\right), u_1, \ldots, u_\sigma\right)$$

is a solution of the Kohn-Sham system.

$\Rightarrow$ the Kohn-Sham system always admits a solution.

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The Mapping $T(\eta) \mapsto \overline{\eta}$

- $\eta = (\eta_1, \dots, \eta_\sigma)$
- $u = e^\eta - \delta \,, \quad \delta > 0$ constant
- solve Poisson's equation for potential $\varphi(u, N_A - N_D)$
- obtain $V_\xi(u) = -e_\xi \triangle E_\xi + V_{xc,\xi}(u) + e_\xi q \varphi$
- solve EVP for Schrödinger's equation

$$[-(\hbar^2/2)\nabla \cdot (1/m_\xi \nabla) + V_{eff,\xi}]\psi_{l,\xi} = \mathcal{E}_{l,\xi}\psi_{l,\xi}$$

- compute carrier densities

$$\overline{u}_\xi(x) = \sum_l N_{l,\xi} |\psi_{l,\xi}(x)|^2$$

- $\overline{\eta} = log(\overline{u} + \delta)$

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Properties of $T(\eta)$

- Solution of Kohn-Sham system is a fixed point of $T(\eta)$
- $\delta = 10^{-14}$ added to avoid singularity of logarithm at zero
- additional smoothness of logarithm improves convergence
- pure iteration scheme may or may not converge
- stabilization and acceleration needed

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Heuristic Motivation via Gummel's Method

- Gummel's method
  $\longrightarrow$ originally for the drift-diffusion model
- Kerkhoven analyzed qualitative behavior
  $\longrightarrow$ converges while sufficiently far away from solution
  $\longrightarrow$ slows down when approaching to the solution
- opposite to Newton's method
- this behavior is due to the ellipticity of the involved equations
  $\longrightarrow$ true for the quantum-mechanical system as well

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Stabilization and Acceleration of $T(\eta)$

Stabilization:

- pure appliance of $T(\eta)$ causes convergence instabilities
- stabilize through adaptive underrelaxation
  $\rightarrow$ fixed point iteration $T(\eta) = \eta$
- until 'close' to the solution

Acceleration:

- accelerate convergence by employing Newton's method
  $\rightarrow$ root-finding problem $T(\eta) - \eta = 0$
- Jacobian-free version based on GMRES
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Adaptive Underrelaxation

- initialize: $\omega = 1$, choose η_0, set $\eta_{-1} = 0$ and $\eta_{-2} = \eta_0$
- Iterate on i: if

$$\frac{\|T(\eta_i) - \eta_i\|}{\|T(\eta_{i-1}) - \eta_{i-1}\|} > \frac{\|T(\eta_{i-1}) - \eta_{i-1}\|}{\|T(\eta_{i-2}) - \eta_{i-2}\|}$$

  then

$$\omega := \omega * 0.8 \,, \quad \omega' := \min(\omega, \frac{\|T(\eta_{i-1}) - \eta_{i-1}\|}{\|T(\eta_i) - \eta_i\|})$$

- $\eta_{i+1} = \omega' T(\eta_i) + (1 - \omega')\eta_i$
- until convergence
  $\rightarrow$ or ω decreases 5 times in a row
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Acceleration by Newton's Method

- Reformulation: $\eta_{i+1} = T(\eta_i) \rightsquigarrow \eta - T(\eta) = 0$
- Newton:
  $\rightarrow$ requires solution of linear system

$$[I - \nabla_\eta T(\eta_i)]d\eta = -[\eta_i - T(\eta_i)]$$

- $\nabla_\eta T(\eta_i)$ is the Jacobian matrix of T at η_i
  $\rightarrow$ not known explicitly
- solve system without generating the Jacobian
  $\rightarrow$ nonlinear version of GMRES (NLGMR)

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Derivative-free GMRES

- Solution of Newton's equation equivalent to minimization over $d\eta$ of
$$\|(I - T)(\eta_i) + [I - \nabla_\eta T(\eta_i)]d\eta\|_2$$
- GMRES: find approximate solution in Krylov subspace
$$K_m = span\{v_1, [I - \nabla_\eta T(\eta_i)]v_1, \ldots, [I - \nabla_\eta T(\eta_i)]^{m-1} v_1\}$$
- ONB of K_m easily gained by Arnoldi process, provided $v \mapsto [I - \nabla_\eta T(\eta_i)]v$ is available
- $\nabla_\eta T(\eta_i)$ never needed explicitly
$\rightarrow$ only matrix-vector multiplication $\nabla_\eta T(\eta_i)v$
- approximate by:
$$\nabla_\eta T(\eta_i)v \approx \frac{T(\eta_i + hv) - T(\eta_i)}{h}$$

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- adjust accuracy of solution to Newton's method adaptively
  $\rightarrow$ vary number m of steps in NLGMR
- η_0 : current approximate solution to $\eta - T(\eta) = 0$
- η_m : solution after m steps of GMRES
- nonlinear residual:

$$res_{nl} = \eta_m - T(\eta_m)$$

- linear residual:

$$res_{lin} = \eta_0 - T(\eta_0) + [I - \nabla_\eta T(\eta_0)](\eta_m - \eta_0)$$

- nonlinearity mild $\Rightarrow \|res_{nl}\| \approx \|res_{lin}\|$
- $\|res_{nl}\| \not\approx \|res_{lin}\|$
  $\rightarrow$ linearized model not good
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- η_m : solution after m steps of GMRES
- nonlinear residual:

$$res_{nl} = \eta_m - T(\eta_m)$$

- linear residual:

$$res_{lin} = \eta_0 - T(\eta_0) + [I - \nabla_\eta T(\eta_0)](\eta_m - \eta_0)$$

- nonlinearity mild $\Rightarrow \|res_{nl}\| \approx \|res_{lin}\|$
- $\|res_{nl}\| \not\approx \|res_{lin}\|$
  $\rightarrow$ linearized model not good
  $\rightarrow$ accurate solution of Newton's method wasteful

Adaption of NLGMR

- adjust accuracy of solution to Newton's method adaptively
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Resulting NLGMR Iteration

- set $m = 2$
- get initial guess η_0 for carrier density
- employ m steps of GMRES:
  $\rightarrow$ yields η_m
- adapt m:
  $\rightarrow \frac{2}{3} \leq \|res_{nl}\|/\|res_{lin}\| \leq \frac{3}{2} \Rightarrow m := \min(2m, 25)$
  $\rightarrow \frac{3}{2} \leq \|res_{nl}\|/\|res_{lin}\| \leq 5 \Rightarrow m := m$
  $\rightarrow$ else $m := \max(2, m/2)$
- perform linesearch for stepsize τ
  $\rightarrow$ guarantee decrease of $\|(\eta_0 + \tau d\eta) - T(\eta_0 + \tau d\eta)\|$
- until convergence
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Summary of the Algorithm

- take initial guess
- perform adaptive underrelaxation
- until 'close' to the solution
- perform NLGMR method
  $\rightarrow$ Newton's method; derivative-free GMRES
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Outline

1. Physical System
   - The Kohn-Sham System
2. Analytical Results
   - Existence and Uniqueness of Solutions
3. Numerics
   - The Kerkhoven Scheme
   - Results

General

Implementation:

- in the Framework of WIAS-pdelib2 (C++)
  $\longrightarrow$ www.wias-berlin.de/software/pdelib

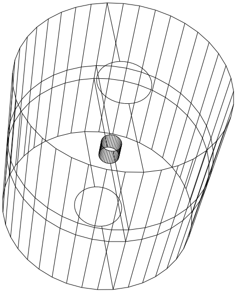
Discretization:

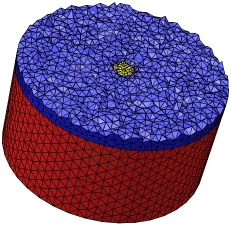
- Finite Volume Method
  $\longrightarrow$ TetGen: Tetrahedral Mesh Generator and 3D Delaunay Triangulator (tetgen.berlios.de)

Eigenvalues:

- ARPACK: Large Scale Eigenvalue Solver
  $\longrightarrow$ www.caam.rice.edu/software/ARPACK

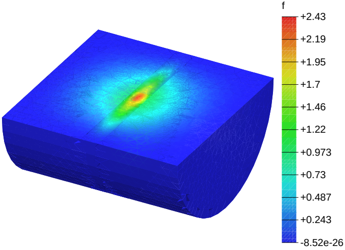
Grid

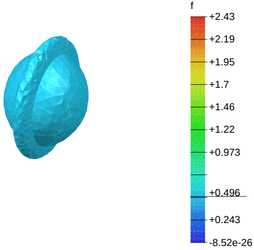




- Input: 320 points, 172 faces, 4 regions, 6 bregions
- Output: 4 regions, 12381 points, 70230 cells, 6 bregions, 9905 bfaces

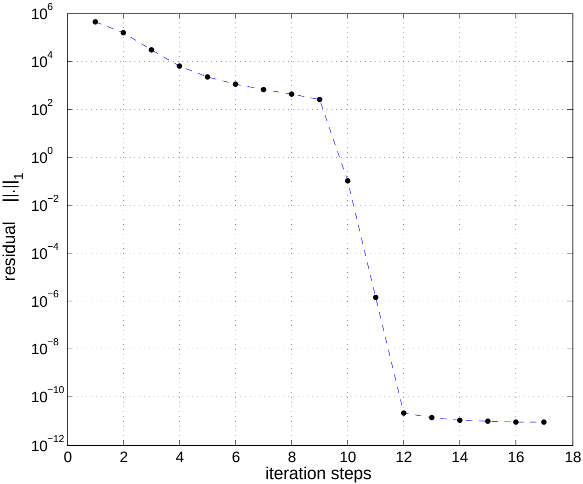
Single Electron





	cpu seconds	steps
total	1410	17
underrelaxed	100	9
Newton	1310	8

Residual Evolution



A.T. Galick, T. Kerkhoven, U. Ravaioli, J.H. Arends, Y. Saad
Efficient numerical simulation of electron states in quantum wires.
J. Appl. Phys., 68(7):3461-3469, 1990