Simulating Resonant Tunneling Diodes with the Wigner-Poisson Equations

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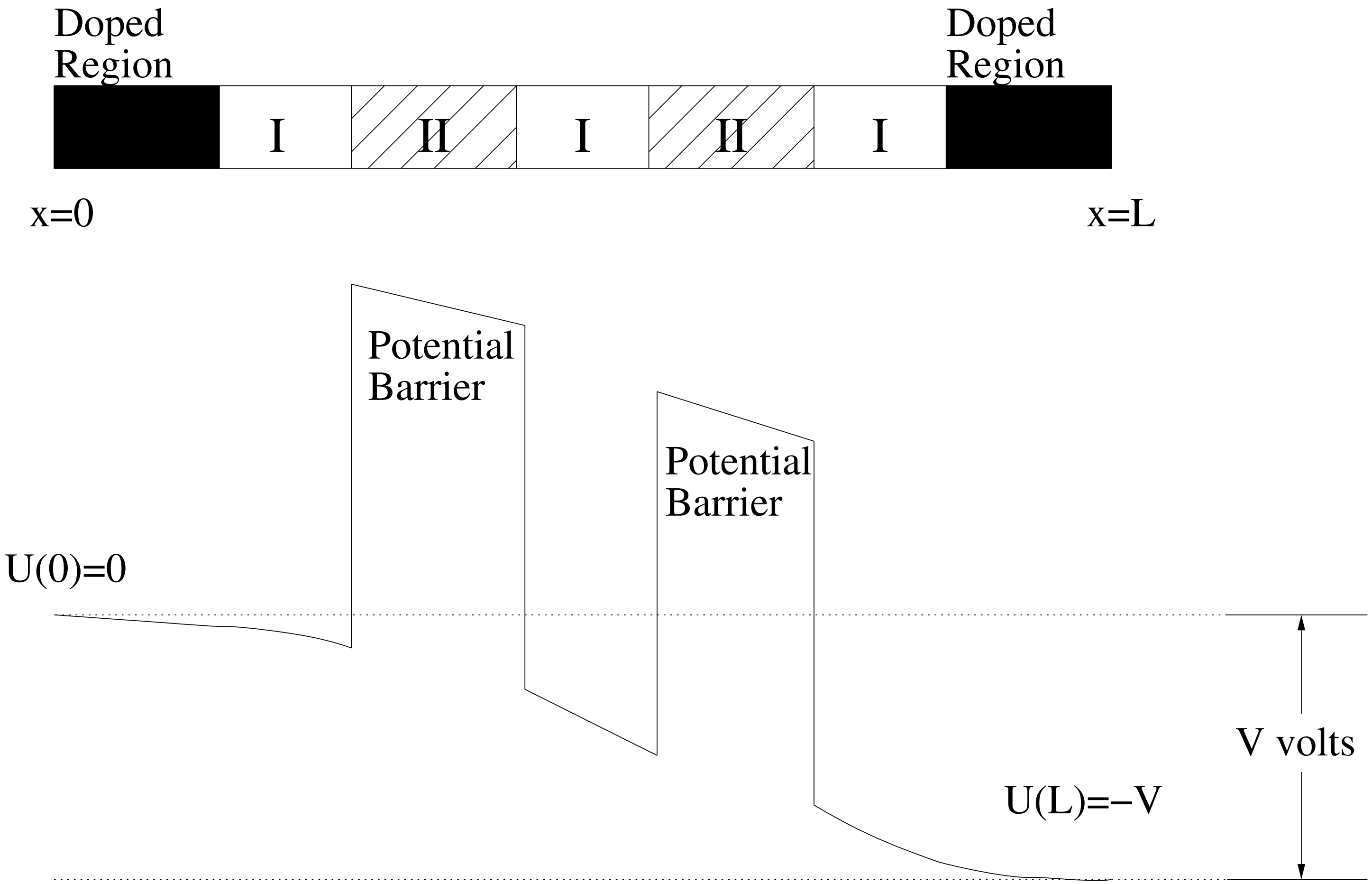
Outline

- Resonant Tunneling Diodes (RTDs)
- Wigner-Poisson Equations
- Continuation Methods (LOCA)
- Stability and Hopf Bifurcation
- Numerical Results
- Summary and Future Work

Resonant Tunneling Diode



Goal: Determine current output for a given voltage difference V

History of RTDs

- High frequency oscillator (THz)
- Failure due to power lost in lower frequency modes
- Searching for intrinsic oscillation
- Size of diode is measured in ångströms $(10^{-10}m)$
- Device physics dominated by quantum mechanics

Why Are We Interested in RTDs

- Novel device design
- Better understanding of quantum mechanical effects
- Potential benefits include:
  - Sensor technology: THz radiation for biological/chemical identification
  - Speed: Faster data transmission/processing

Wigner-Poisson Equation

$$\frac{\partial f(x,k,t)}{\partial t} = W(f) = K(f) + P(f) + S(f)$$

f is the electron distribution in RTD, as a function of the electron's position x, momentum k, and time t

First Term: Kinetic Energy Effects

$$K(f) = \frac{-hk}{2\pi m^*}\frac{\partial f}{\partial x}$$

h : Planck's Constant m^* : Electron's Effective Mass

Wigner-Poisson Equation

$$\frac{\partial f(x,k,t)}{\partial t} = W(f) = K(f) + P(f) + S(f)$$

Second Term: Potential Energy Effects

$$P(f) = \frac{-4}{h}\int_{-\infty}^{\infty} f(x,j)T(x,k-j)dj$$

$$T(x,k-j) = \int_0^{\frac{L_c}{2}} [U(x+y) - U(x-y)]\sin(2y(k-j))dy$$

This term is nonlinear because $U(x)$ depends on f.

U : Electric Potential L_c : Coherence Length

Wigner-Poisson Equation

$$\frac{\partial f(x,k,t)}{\partial t} = W(f) = K(f) + P(f) + S(f)$$

<u>Third Term: Scattering Effects</u>

$$S(f) = \frac{1}{\tau}[\frac{f_0(x,k)}{\int_{-\infty}^{\infty} f_0(x,j)dj} \int_{-\infty}^{\infty} f(x,j)dj - f(x,k)]$$

τ : Relaxation Time f_0 : Equilibrium Distribution

Boundary Conditions

The boundary conditions of f specify the distribution of the electrons that are entering the device.

(Adapted from Frensley, Phys. Rev. B, Vol. 36, 1987)

Obtaining U for Potential Energy Term

To obtain U from f, you need to solve the Poisson equation for $z(x)$, the electrostatic potential created by the electrons:

$$\frac{d^2z}{dx^2} = \frac{q^2}{\epsilon}\left[N_d(x) - \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x,j)dj\right]$$

$$z(0) = 0,\ z(L) = -V$$

Once $z(x)$ is known, $U(x) = z(x) + \Delta_c(x)$

q : Charge of Electron ϵ : Dielectric Permittivity

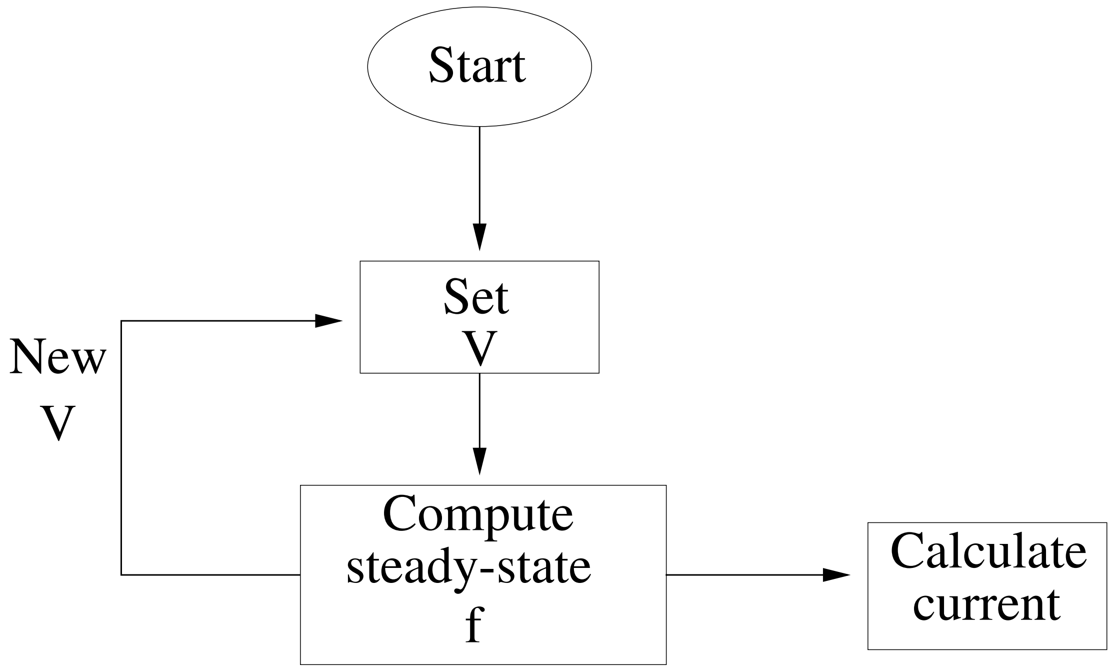
$N_d(x)$: Doping Profile $\Delta_c(x)$: Potential Barriers

V : Voltage Difference

Current Output

Want to analyze the steady-state current output as V is varied.

Basic idea is to:



Discretization

- Use finite difference method for approximation
- n_x, n_k - Number of x, k points on the grid
- Upwind difference scheme for $\frac{\partial f}{\partial x}$
- Quadrature formula to approximate integrals
- Centered differences for Poisson's solve
- Leads to nonlinear ODE in $\mathbb{R}^{n_x * n_k}$

Continuation Methods

Solve nonlinear equation $W(f, V) = 0$ for $f \in \mathbb{R}^{n_x * n_k}$.

- Determine solution branches $f(V)$ as a parameter V varies.
- Generates $\{V_i\}$ (parameters) and corresponding $\{f_i\}$ (solutions)
- Use LOCA (Library of Continuation Algorithms)

LOCA

- Part of Trilinos - Sandia's parallel solver project
- Makes use of several other parts of Trilinos:
  - NOX : Nonlinear solver
  - AztecOO : Preconditioned Krylov linear solvers
  - Anasazi : Eigensolver
  - Epetra : Data Structure

Stability of Nonlinear ODEs

- Nonlinear ODE: $\frac{dz}{dt} = g(z)$
- Steady-state solution: z^*
- How can we tell if z^* is dynamically stable?
- The eigenvalues (λ's) of the Jacobian $g'(z^*)$ determine stability
  - If $Re(\lambda) < 0$ for all λ, z^* is stable
  - If $Re(\lambda) > 0$ for any λ, z^* is unstable
- LOCA incorporates an eigensolver to calculate eigenvalues

We Want Instability

- As the parameter is varied, the eigenvalues of the Jacobian will change
- A change in stability of equilibirum is called a bifurcation
- Want: stable steady-state to go to oscillatory behavior
- This change is a Hopf bifurcation

Hopf Bifurcation (By Example)

Consider the two-dimensional nonlinear ODE [Kuznetsov, 1998],

$$\begin{pmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \end{pmatrix} = \begin{pmatrix} px - y - x(x^2 + y^2) \\ x + py - y(x^2 + y^2) \end{pmatrix}$$

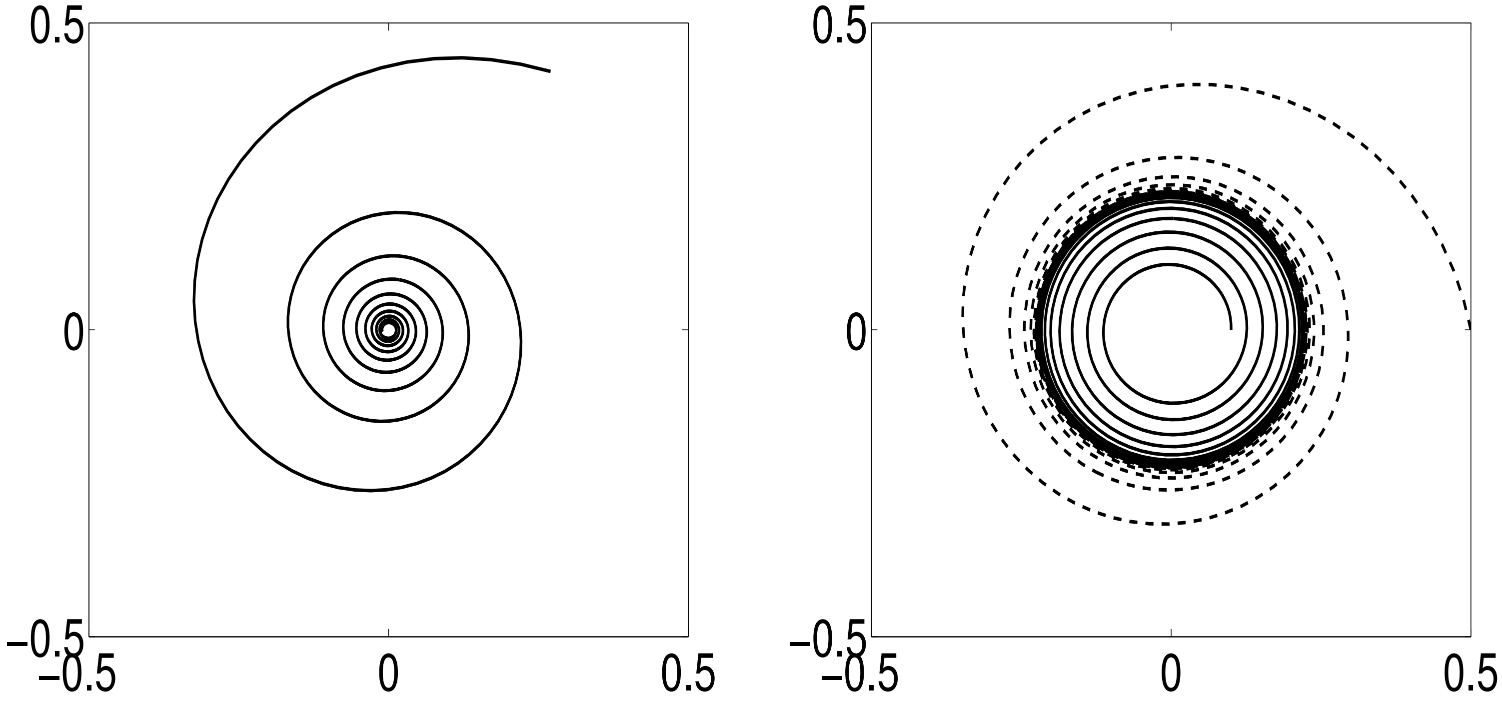
where p is a parameter

- For any p, $\binom{x}{y} = \binom{0}{0}$ is a steady-state solution
- The Jacobian at this steady-state is

$$\begin{pmatrix} p & -1 \\ 1 & p \end{pmatrix}$$

- Eigenvalues are $\lambda = p \pm i \implies Re(\lambda) = p$

Solutions to ODE



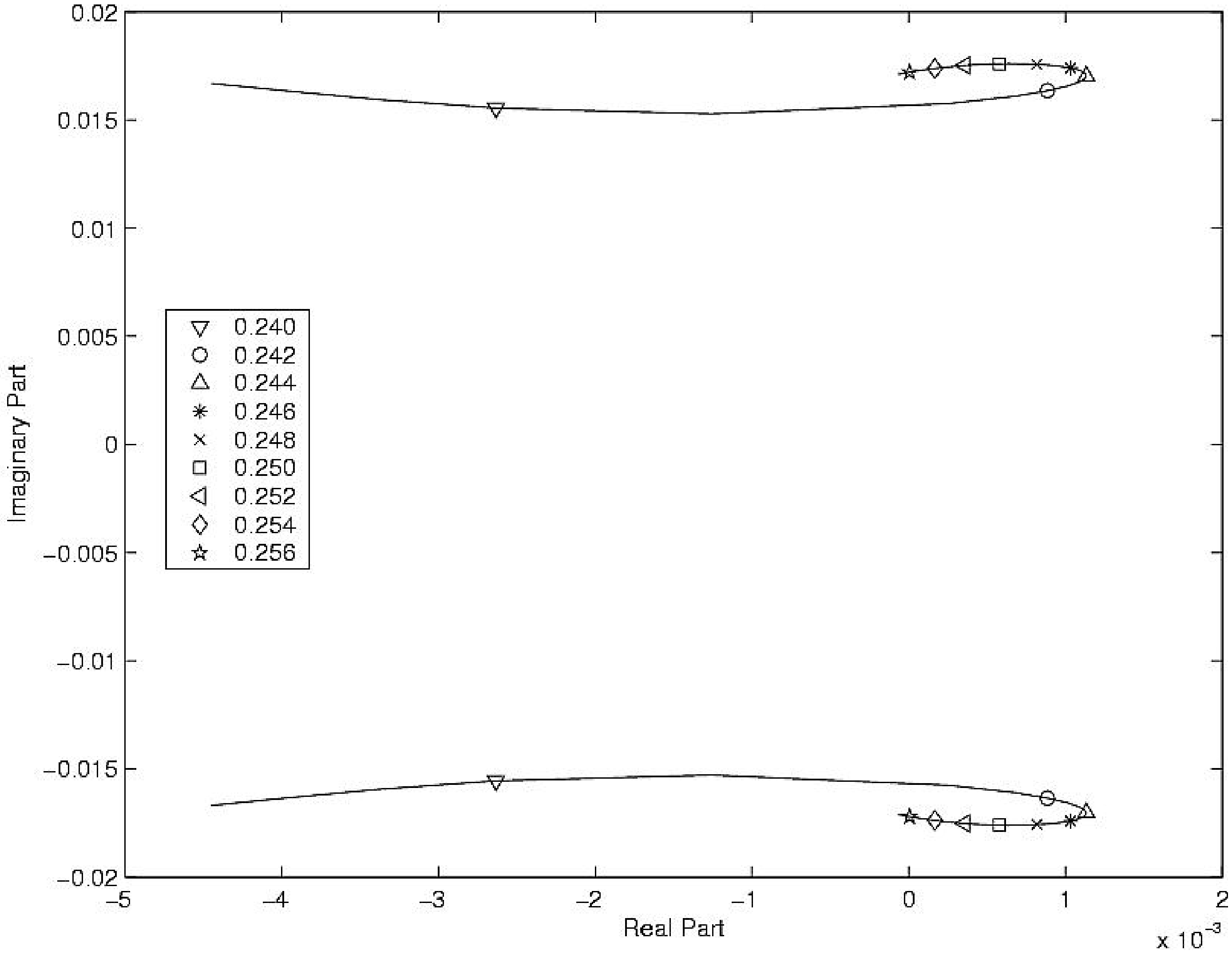
Solution when $p < 0$ Solutions when $p > 0$

- $p < 0 \implies$ origin is stable
- $p > 0 \implies$ origin is unstable and **oscillatory solution**

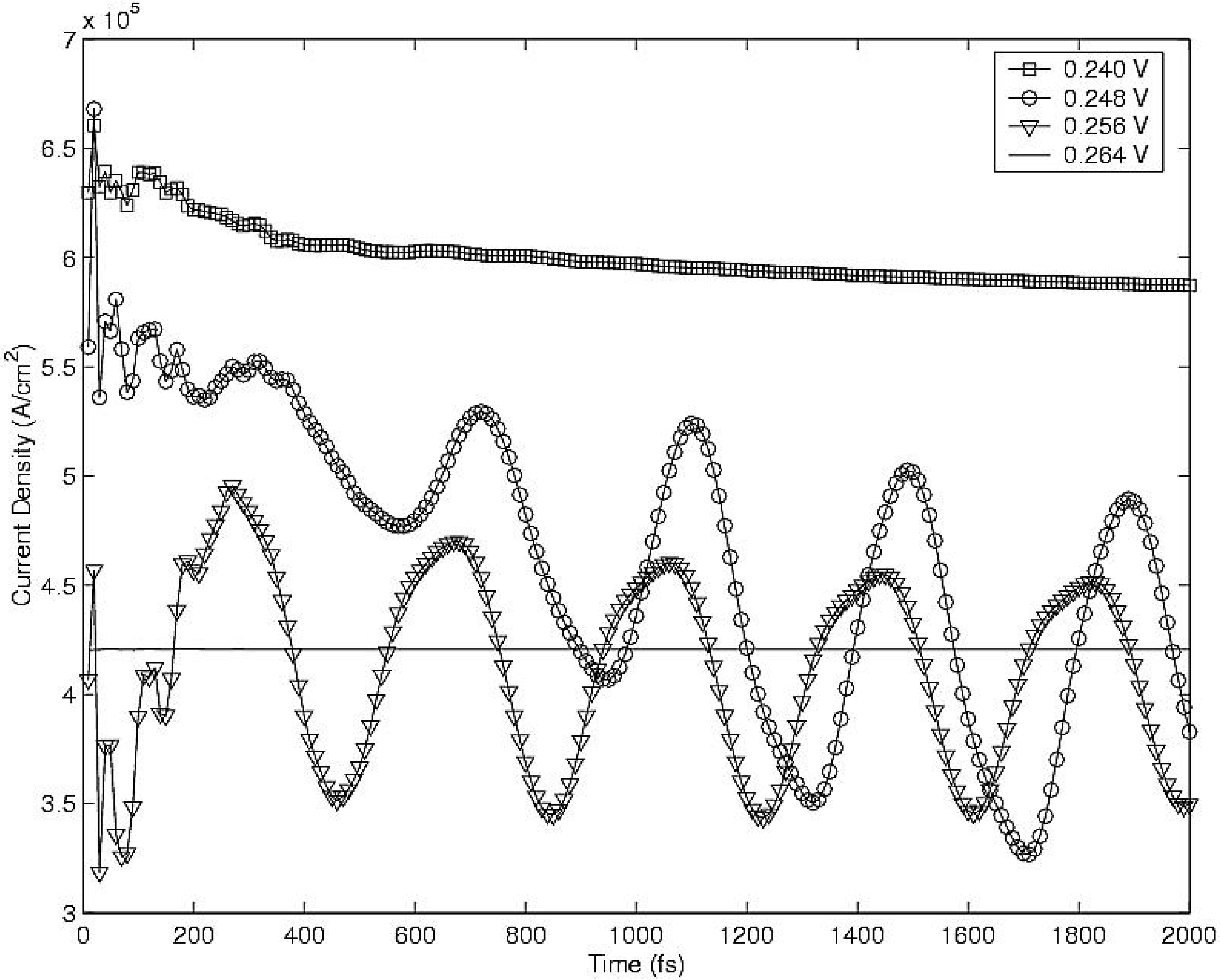
Eigenvalues Predict Hopf Bifurcation

- A Hopf bifurcation is characterized by a complex conjugate-pair of eigenvalues crossing the real axis
- Use LOCA to find such a pair as voltage is varied
- Verify Hopf's existence using time-integrator (Lawrence Livermore's VODEPK)

Eigenvalue Results



Time Integration Results



Summary

- Using Wigner-Poisson Equations to model RTDs
- LOCA is used to trace-out steady-state electron distributions as voltage varies
- Preliminary results show a voltage region where current oscillation can be expected

Future Work

- Grid convergence
- Hopf tracking with LOCA
- Analysis of equations/numerical methods