NEMO1D: Implementation of NEGF Scattering Theory

NCN

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Optical/E&M Analogies to Quantum Mech

$$\nabla^2 \vec{E} = -\omega^2 \mu \varepsilon \vec{E}$$

$$k^2 = \omega^2 \mu \varepsilon$$

Physics are similar:

- Propagation as a wave phenomenon:
  - » Antennas
  - » Waveguides
- Propagation as a scattering problem:
  - » Diffraction gratings
  - » Radar cross-sections

- Green functions as propagators
- Finite difference, finite elements

$$\nabla^2 \Psi = -\frac{2m}{\hbar}(E-U)\Psi$$

$$k^2 = \frac{2m}{\hbar}(E-U)$$

But:

- Scattering is coherent & elastic rather than incoherent & inelastic
- Photons do not interact with themselves:
  - Calculate the propagation
  - Do not calculate the occupation
  - Exception is a laser!

- Electron and Laser Simulation need:
  Dynamics & Kinetics -
  States & Bean-counting

What are the Concepts?

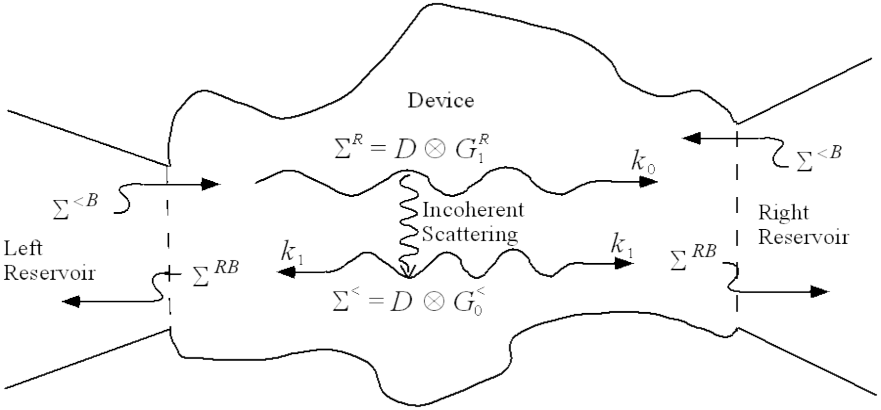
- Dynamics - States of the System
  - » Need to solve a form of the Schrodinger Wave Equation. Relatively simple problem.
- Kinetics - Occupation of states - transfer of carriers
  - » Need to account for many electrons, injection from contacts, scattering etc.
    This is the harder part of the problem.

- In general:
  - » Pauli exclusion principle couples the dynamics and the kinetics!
    - ✓ Expl:
      1) electron scatters into state and remains there (relatively long).
      2) higher energetic electrons cannot scatter into the full state,
         -> their scattering rate is reduced
         -> the available states are modified.
  - » We punted on the proper treatment of the coupled kinetics and dynamics and found approximations.

What are the Simulation Targets?

- Dynamics - States of the System - NEGF: G^R
  - » Need to solve a form of the Schrodinger Wave Equation.
    $(E-H-\Sigma^R_{bound}-\Sigma^R_{scatt})\, G^R = 1$ — G^R impulse response
    $\Sigma^R_{bound} = \Gamma^{left} + \Gamma^{right}$ — Σ^R_{bound} out-scattering to contacts
    $\Sigma^R_{scatt} = DxG^R$ — Σ^R_{scatt} out-scattering to other channels
- Kinetics - Occupation of states - transfer of carriers - NEGF: $G^<$
  - » Need to account for many electrons, injection from contacts, scattering etc.
    $(E-H-\Sigma^R_{bound}-\Sigma^R_{scatt})\, G^< = (\Sigma^<_{bound}+\Sigma^<_{scatt})\, G^A$
    $\Sigma^<_{scatt} = G^<$
- In general:
  - » Pauli exclusion principle couples the dynamics and the kinetics!
    - ✓ Expl:
      1) electron scatters into state and remains there (relatively long).
      2) higher energetic electrons cannot scatter into the full state,
         -> their scattering rate is reduced
         -> the available states are modified.
  - » We punted on the proper treatment of the coupled kinetics and dynamics and found approximations.

Treatment of a single Incoherent Scattering Event



- Scattering:
  - »couples different propagation channels (k and E).
  - »modifies the quantum mechanical spectrum of states (damped oscillator has a different eigen frequency)
- Incoherent Scattering:
  - »Destroys phase memory

States

$$(E - H_0^D - \Sigma^{RB}) G_1^R = 1$$

$$\Sigma_0^R = D \otimes G_1^R$$

$$(E - H_0^D - \Sigma^{RB} - \Sigma_0^R) G_0^R = 1$$

$$G_0^< = G_0^R \Sigma^{<B} G_0^A$$

$$\Sigma_0^< = D \otimes G_0^<$$

$$G_1^< = G_1^R \Sigma_0^< G_1^A$$

Transport

Multiple Sequential Scattering

Begin with calculations of bare Green function for all transverse k.

$$G_0^R(E) = \left[E - H_o^D\right]^{-1}$$

$$\sigma_0^R(E) = D_{el} \otimes G_0^R(E)$$

$$G_1^R(E) = \left[E - H_o^D - \sigma_0^R(E)\right]^{-1}$$

$$\sigma_1^R(E) = D_{el} \otimes G_1^R(E)$$

$$\vdots$$

$$G_{N-1}^R(E) = \left[E - H_o^D - \sigma_{N-2}^R(E)\right]^{-1}$$

$$\sigma_{N-1}^R(E) = D_{el} \otimes G_{N-1}^R(E)$$

$$G_N^R(E) = \left[E - H_o^D - \sigma_{N-1}^R(E)\right]^{-1}$$

$$G_N^<(E) = G_N^R(E)\Sigma^{<B}(E)G_N^A(E)$$

$$\sigma_N^<(E) = D_{el} \otimes G_N^<(E)$$

$$G_{N-1}^<(E) = G_{N-1}^R(E)\sigma_N^<(E)G_{N-1}^A(E)$$

$$\sigma_{N-1}^<(E) = D_{el} \otimes G_{N-1}^<(E)$$

$$\vdots$$

$$G_1^<(E) = G_1^R(E)\sigma_2^<(E)G_1^A(E)$$

$$\sigma_1^<(E) = D_{el} \otimes G_1^<(E)$$

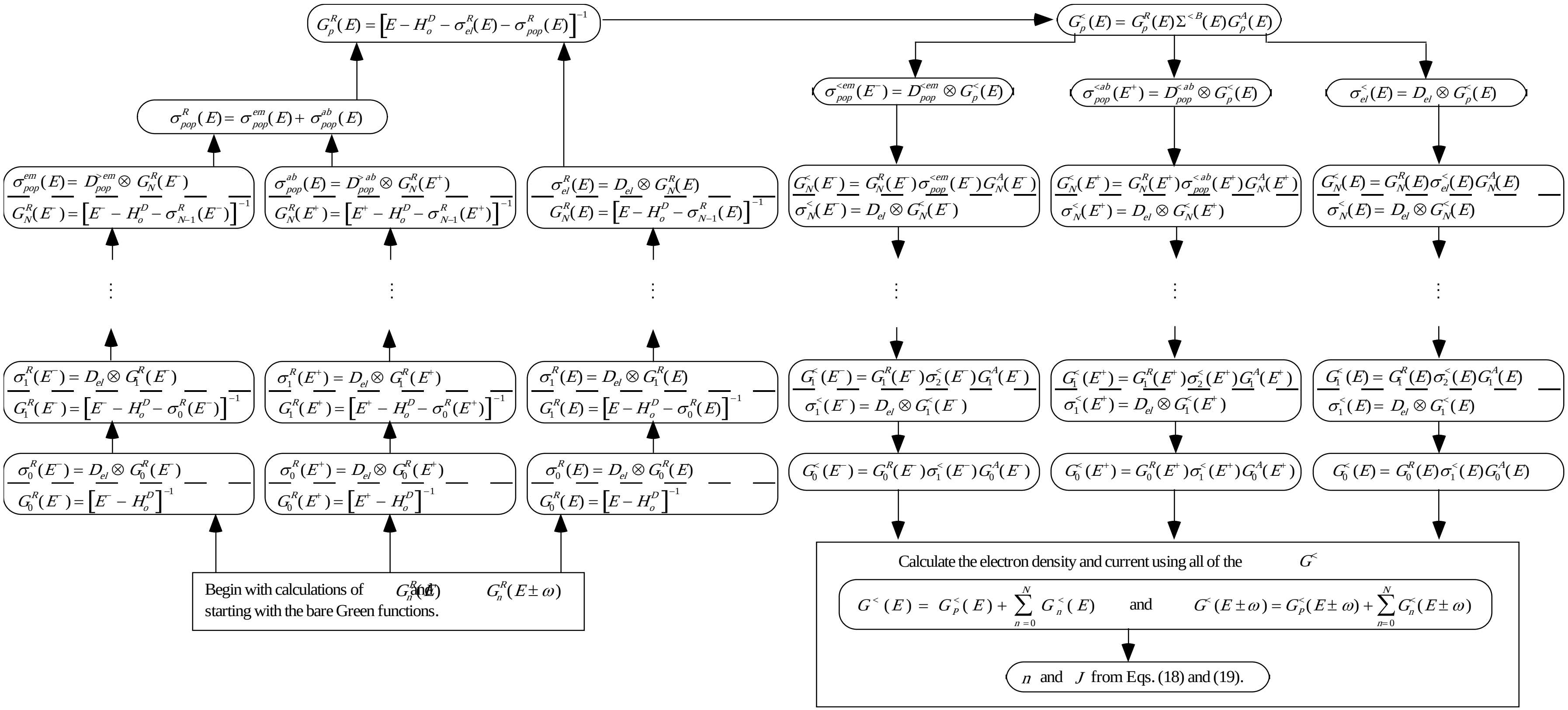
$$G_0^<(E) = G_0^R(E)\sigma_1^<(E)G_0^A(E)$$

Calculate the electron density and current using all of the $G^<$

$$G^<(E) = \sum_{n=0}^{N} G_n^<(E)$$

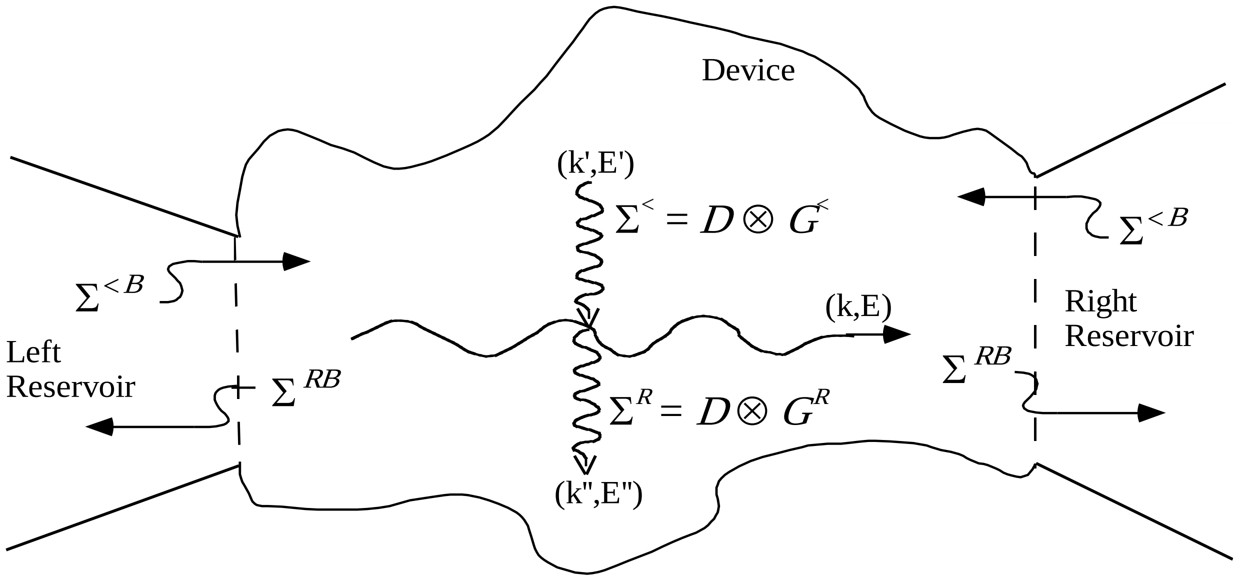
$n_L(E)$ and $J_L(E)$ from Eqs. (18) and (19).

Multiple Sequential Scattering with POP



- Elastic scattering couples all momenta (k)
- Inelastic scattering couples different total energies (E,E+hv,E-hv)
- Polar optical phonons are treated as a single scattering event in NEMO

Scattering: Self-Consistent Born Treatment



Dynamics

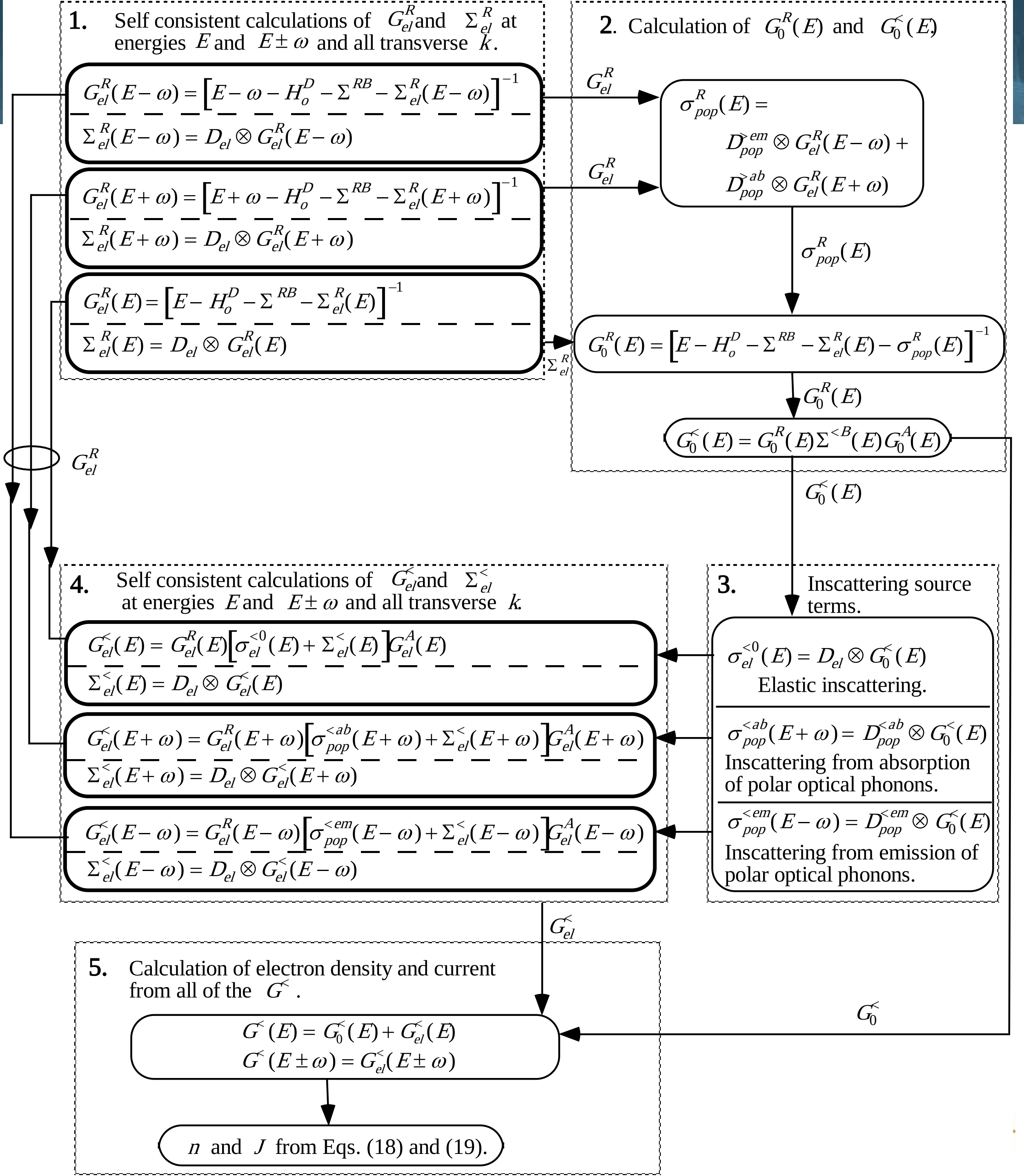
$$\left(E - H_0 - \Sigma^R_{SCATT} - \Sigma^R_{BOUND}\right) G^R = 1$$

Kinetics

$$\left(E - H_0 - \Sigma^R_{SCATT} - \Sigma^R_{BOUND}\right) G^< = \left(\Sigma^<_{SCATT} - \Sigma^<_{BOUND}\right) G^A$$

Infinite number of uncorrelated single scattering events.

Self-Consistent Born Scattering with POP



- **Elastic scattering couples all momenta (k)**
- **Inelastic scattering couples different total energies (E,E+hv,E-hv)**
- **Polar optical phonons are treated as a single scattering event in NEMO**

If you REALLY want to learn NEGF

- Supriyo Datta has an Excellent web Page on nanoHUB.org: https://nanohub.org/topics/negf
- Tutorials, On-Line seminars, Ph.D. theses, tool examples

- The implementations and equations mentioned here are described fully in:

"Single and multiband modeling of quantum electron transport through layered semiconductor devices",

Roger Lake, Gerhard Klimeck, R. Chris Bowen and Dejan Jovanovic,

J. of Appl. Phys. 81, 7845 (1997).

Question & Answer 1

Question & Answer 2