

Modeling of Electron Transport in Thin Films with Quantum and Scattering Effects

Anuradha Bulusu

Advisor: Prof. D. G. Walker

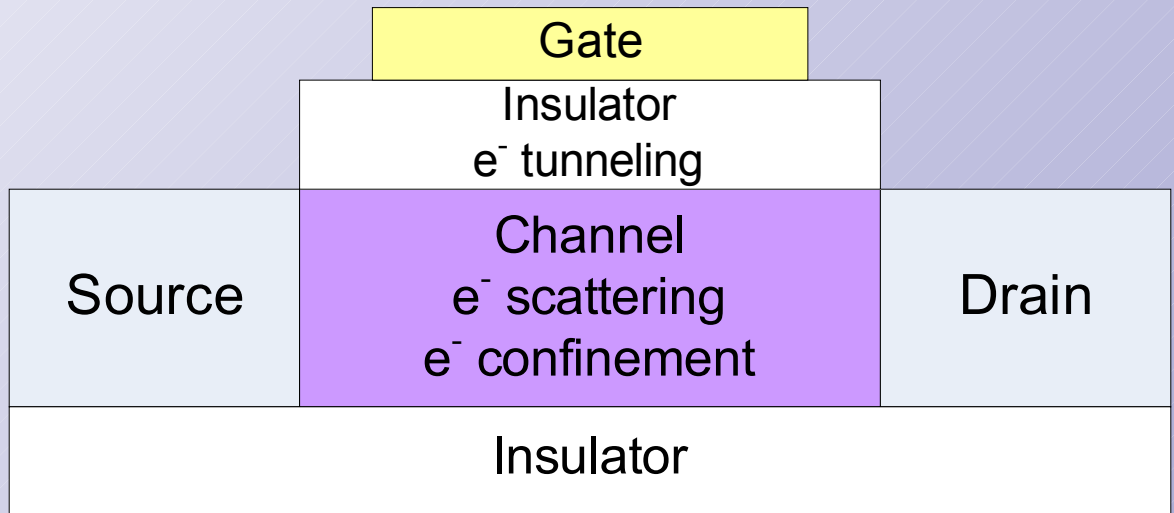
Interdisciplinary Program in Material Science

Vanderbilt University

Nashville, TN

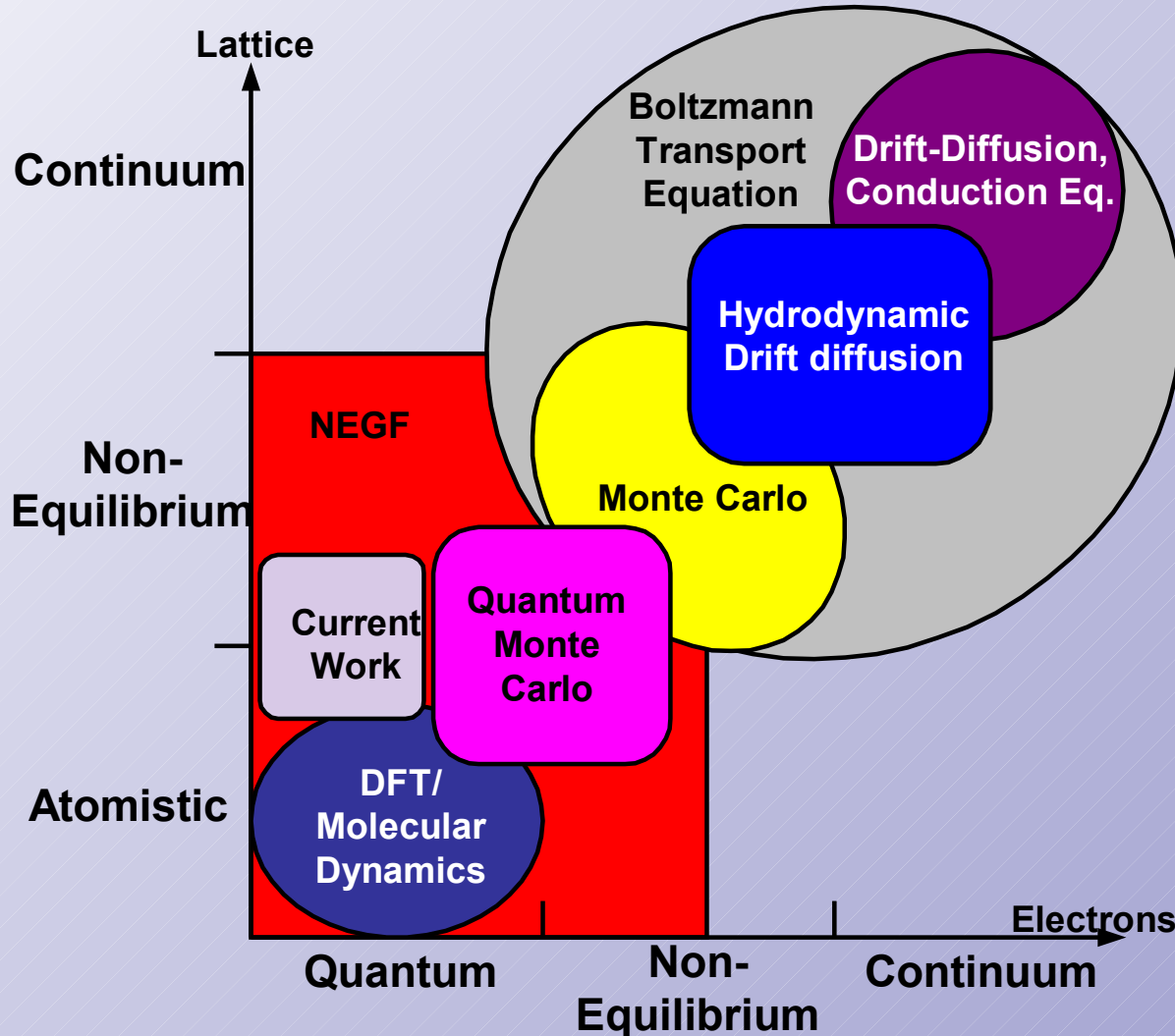
Motivation

- $L_{\text{Device}} \approx \lambda_{\text{de Broglie}} \Rightarrow$
quantum and scattering effects cannot be ignored.



- $L_{\text{device}} < \tau_r \Rightarrow$ **assumption of minimal deviation from local equilibrium no-longer valid \Rightarrow BTE moments cannot be applied to extreme non-equilibrium.**
- **Increased need for microelectronic device simulation models that incorporate both quantum and scattering effects without being computationally intensive.**

Nanoscale Device Models



NEGF: Non-Equilibrium Green's function

Advantages of Non-Equilibrium Green's Function Method

- Incorporation of quantum interference effects such as tunneling and diffraction, not possible through the Boltzmann equation.
- Mathematically accurate approach to include rigorous scattering (electron-phonon scattering, surface scattering etc).
- Eliminates periodic boundary conditions as outgoing waves are planar.
- Multiscale formulation: Can be used to solve atomistic systems to mesoscopic systems.

Non-Equilibrium Green's Function Formalism

Original Schrödinger wave equation

$$(H + U)\psi_{\alpha}(\mathbf{r}) = \varepsilon_{\alpha}\psi_{\alpha}(\mathbf{r})$$

Modified wave equation with self-energy terms

$$(H + U + \Sigma_1 + \Sigma_2 + \Sigma_s)\psi_{\alpha}(\vec{r}) = \varepsilon_{\alpha}\psi_{\alpha}(\vec{r})$$

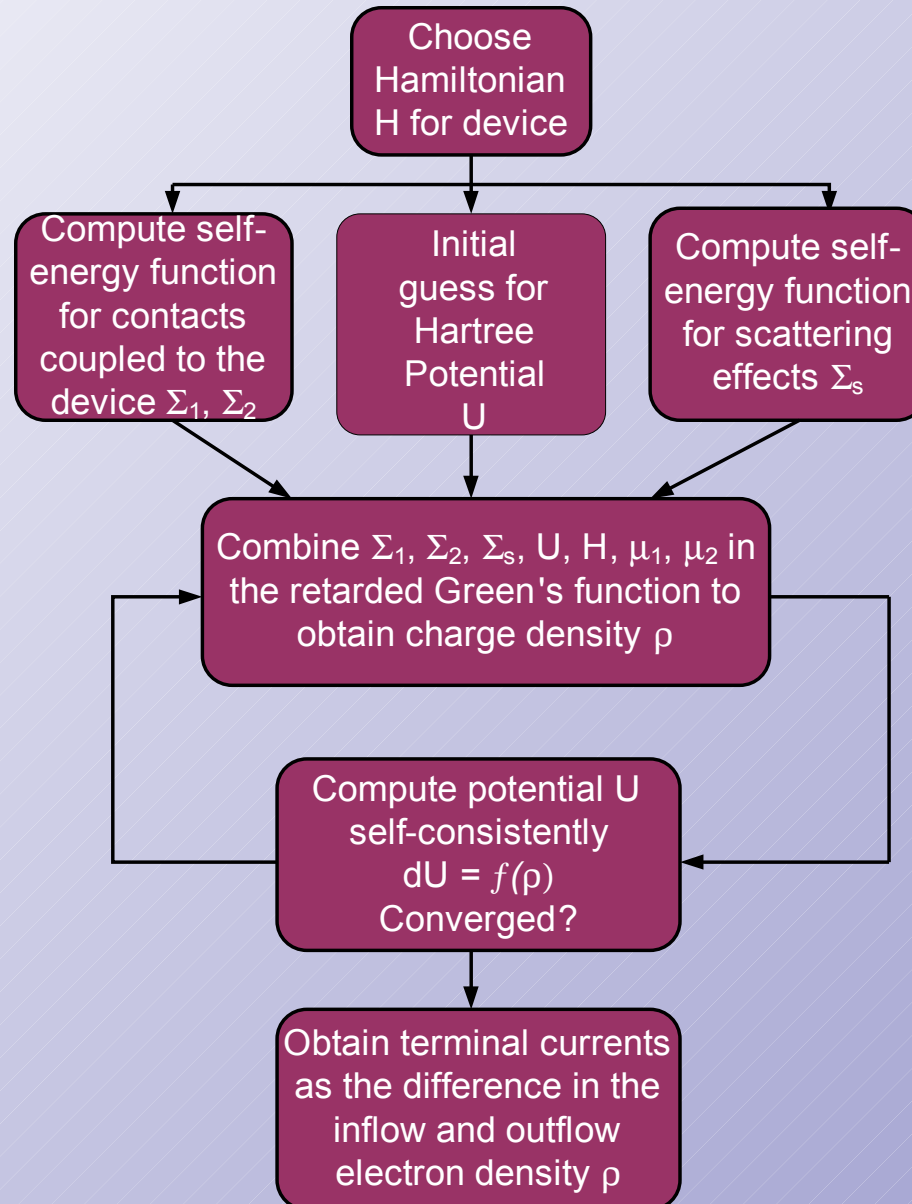
Green's function

$$G(E) = \left[\left(E - i\cdot^+ \right) I - H - \Sigma_v - \Sigma_r - \Sigma_s \right]^{-1}$$

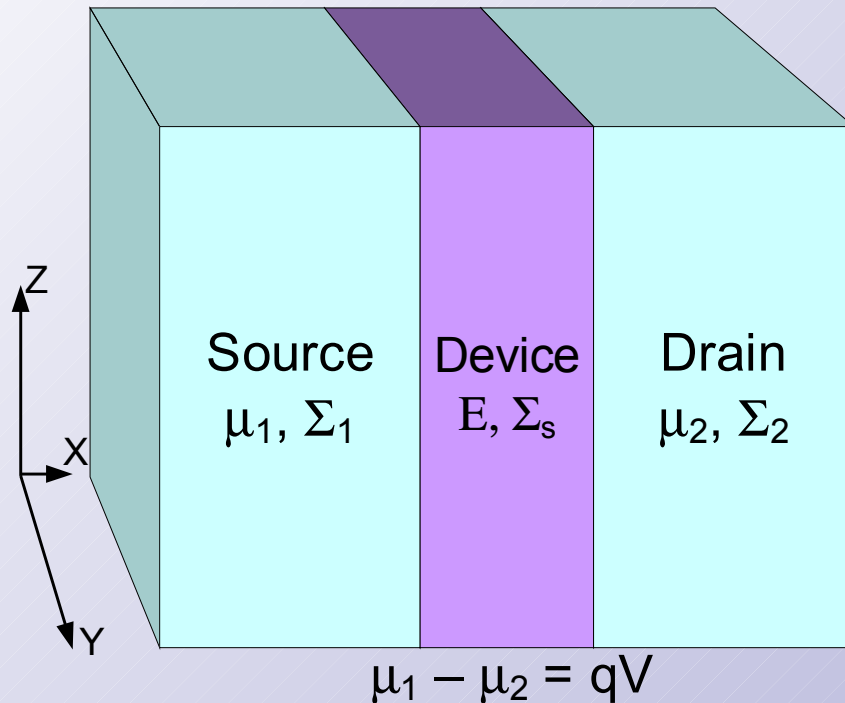
Device Current

$$I_i = \frac{-q}{\hbar} \int_{-\infty}^{+\infty} \text{Trace}[\Gamma_i A] f_i - \text{Trace}[\Gamma_i G^n]$$

Nonequilibrium Green's Function Method



Example of a Very-Small Scale Device Problem



2-D nanoresistor
connected to source
and drain contacts.

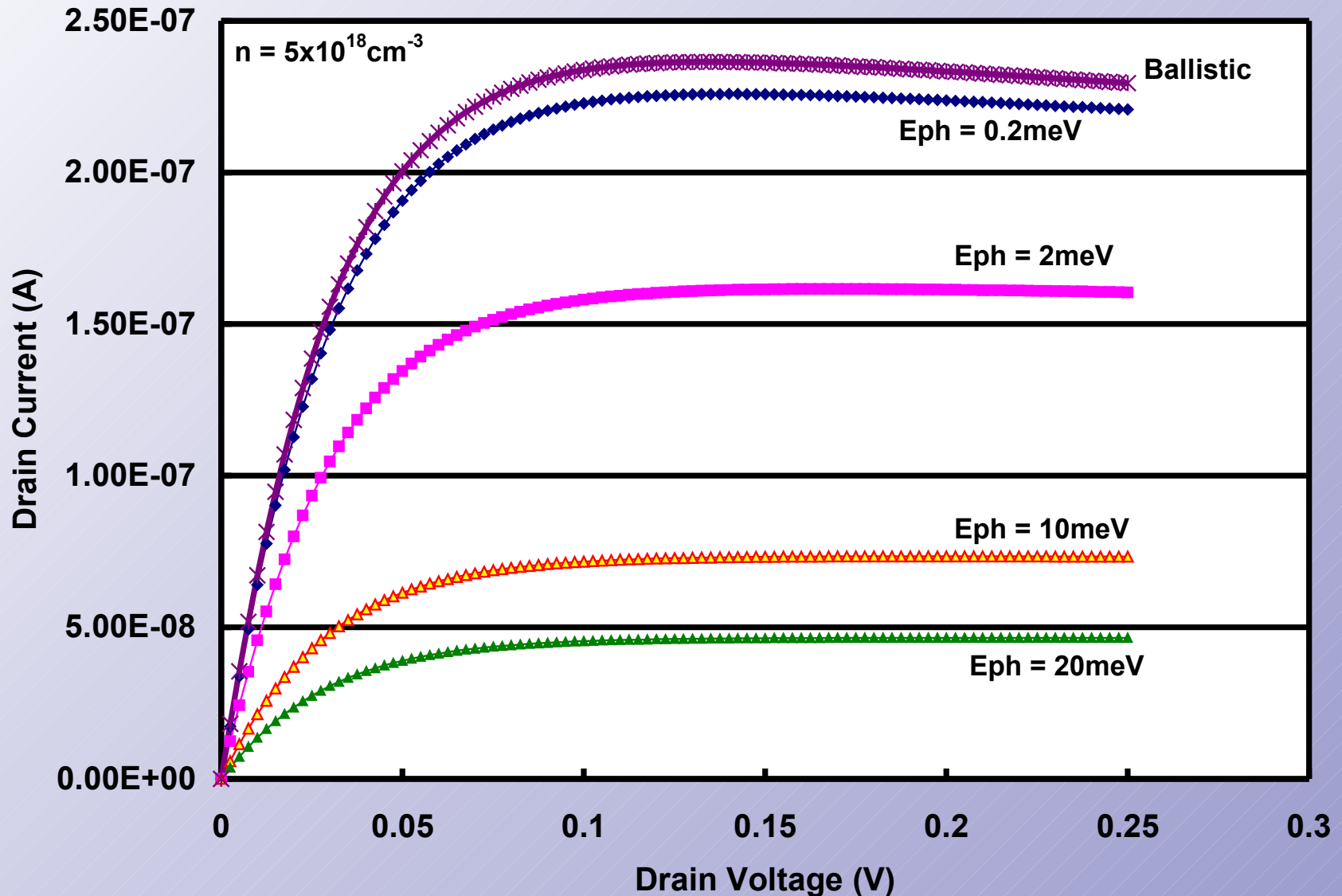
μ_1, μ_2 - source and drain
chemical potentials.

Energy states along
z-axis are quantized.

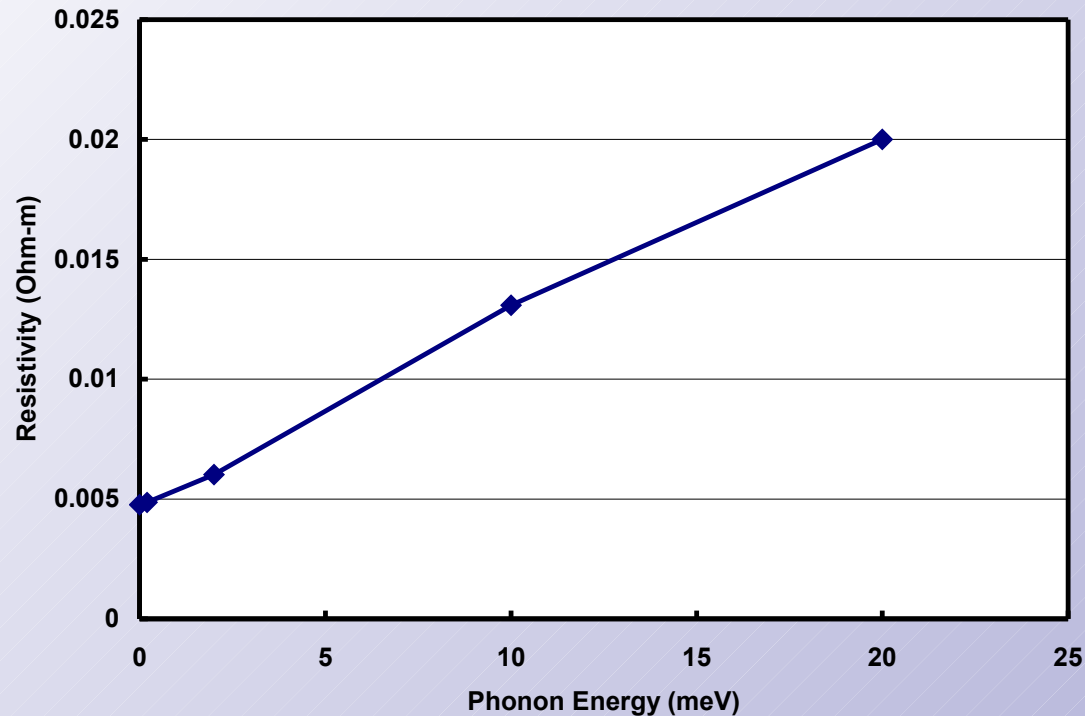
Electron-phonon scattering assumed to be independent of

electron energy. e.g. $D_0 = 0.1 \text{ eV}^2 \Rightarrow E_{\text{ph}} = 20 \text{ meV}$

I-V Characteristics of Silicon Thin Films with Incoherent Near-Elastic Scattering



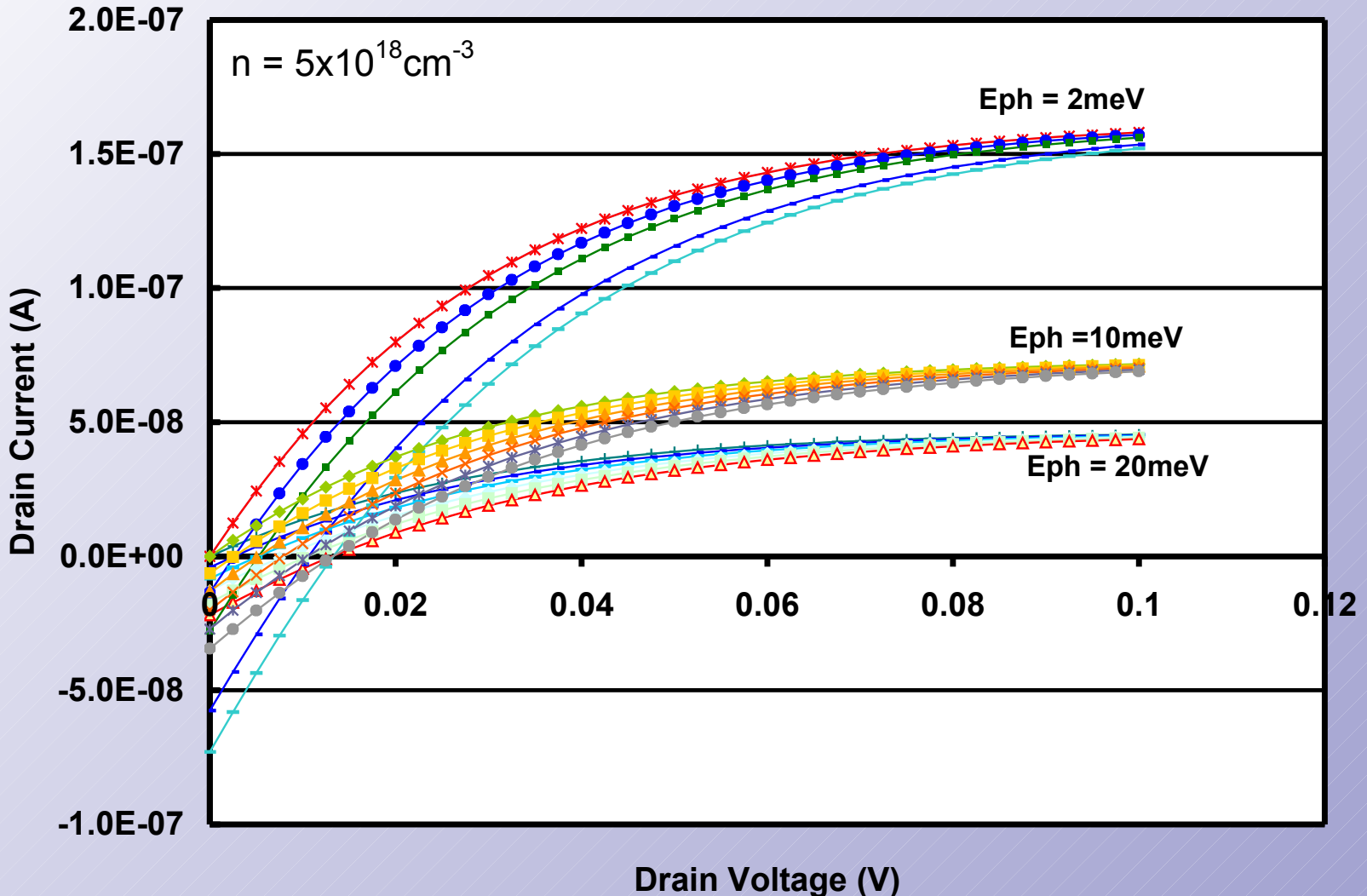
Effective Channel Resistivity with Incoherent Scattering



- **Continuous density of states from source and drain contacts spill over into the channel causing energy level broadening.**
- **Discrete energy states in narrow channel reduce the number of energy states available for the incoming electrons introducing resistance at the contacts.**

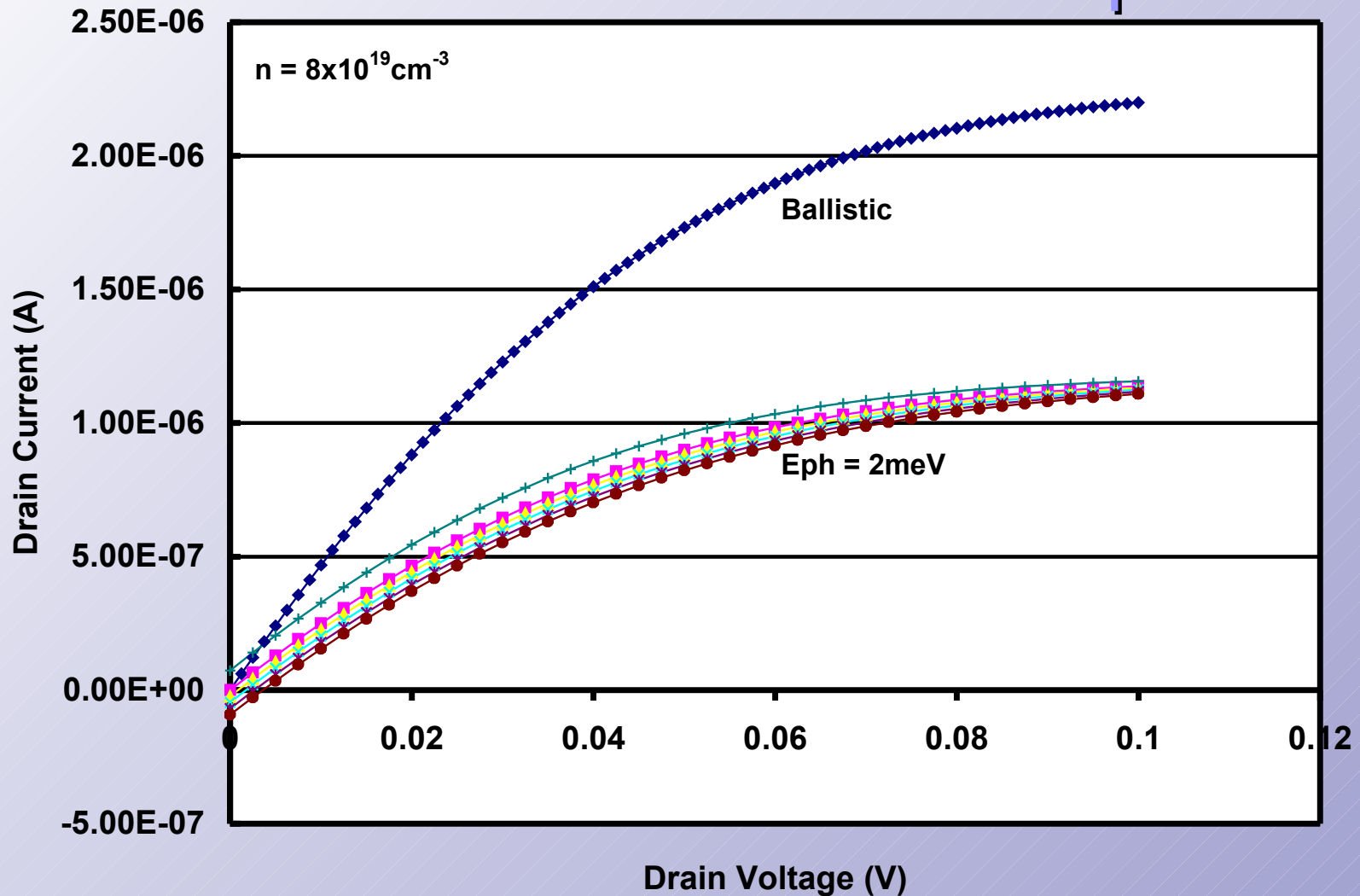
Increase in phonon energy from 0 to 20m eV for various resistors increases corresponding channel resistivity by a factor of 4.

Thermoelectric Properties of Silicon Thin Films



Predicted Seebeck coefficient value of $250 \mu \text{ V/K}$ matches well with experiments. (Geballe, T. H. et.al, *Physical Review*, 98, 4, 1955).

Seebeck Coefficient for SiGe Superlattices



Calculated Seebeck value of $100 \mu \text{ V/K}$ matched well with experimentally measured values of $312 \mu \text{ V/K}$ (B. Yang et. al. Applied Physics Letters, 80, 10, 2002).

Conclusions and Future Work

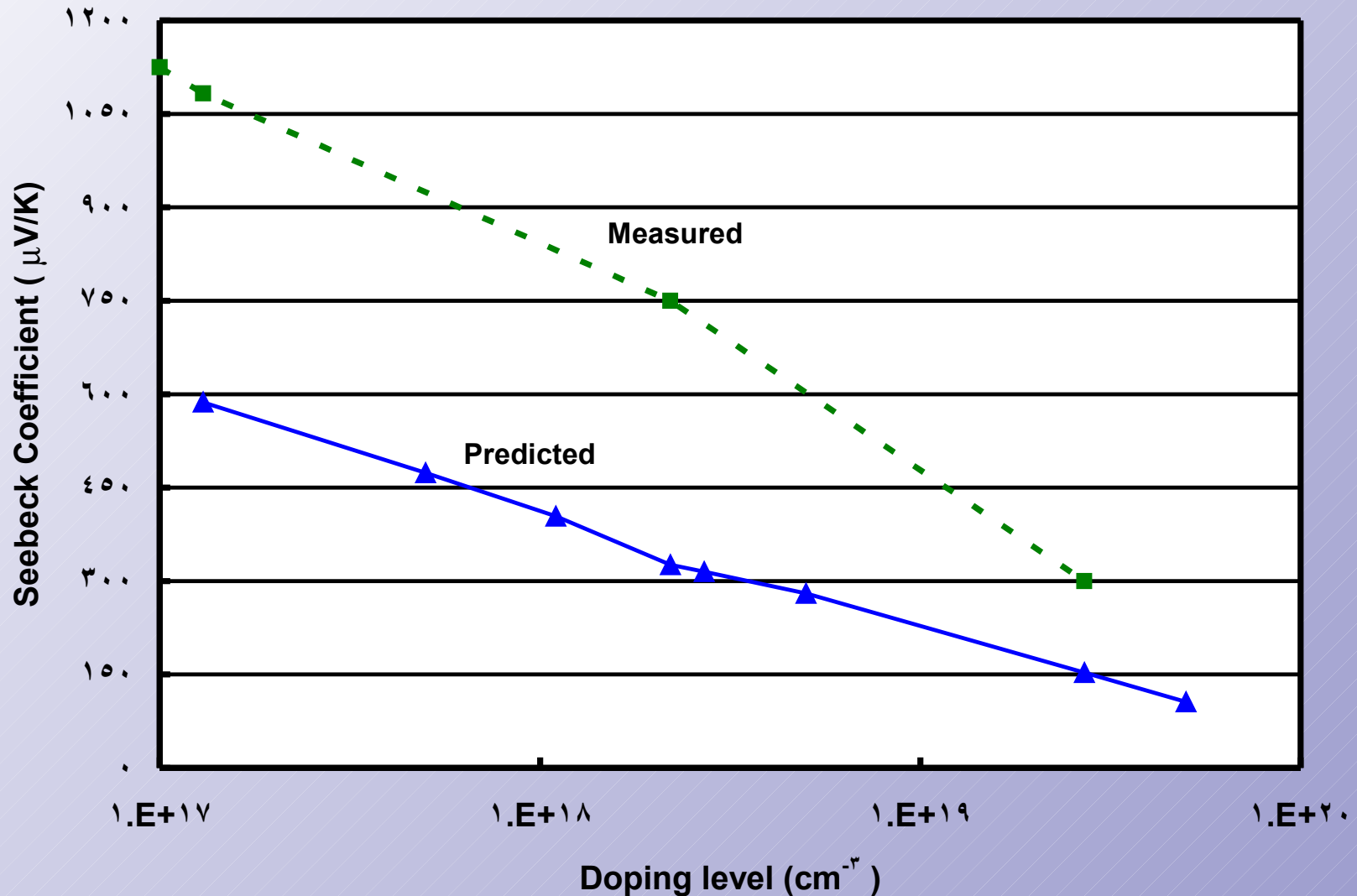
- The NEGF formalism successfully couples quantum effects with electron-phonon scattering.
- A 33% to 70% drop in channel current was noticed due to near-elastic electron-phonon scattering.
- Predicted Seebeck coefficient values are in good agreement with experiment for Silicon and SiGe superlattices.
- Extension of the present work to include energy-dependent electron-phonon scattering.

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Seebeck Coefficient of Silicon Thin Films

(submitted to Journal of Applied Physics)



Non-Equilibrium Green's Function Formalism

Modified wave equation with self-energy terms $(H + U + \Sigma_1 + \Sigma_2 + \Sigma_s)\psi_\alpha(\vec{r}) = \varepsilon_\alpha \psi_\alpha(\vec{r})$

Relation between lifetime of the eigen state and self energy $\frac{1}{\tau} = \frac{\gamma}{\hbar} = -\frac{\text{Im} \Sigma}{\hbar}$

Energy level broadening

$$\Gamma_{1,2,s} = i(\Sigma_{1,2,s} - \Sigma_{1,2,s}^+) \quad \Sigma_s(E) = D_o G(E)$$

Green's function

$$G(E) = \left[\left(E - i0^+ \right) I - H - \Sigma_1 - \Sigma_2 - \Sigma_s \right]^{-1}$$

Spectral function

$$\frac{A(E)}{\hbar\pi} = D(E) = i(G(E) - G^+(E)) = \frac{\gamma}{(E - \varepsilon')^2 + (\gamma/\hbar)^2}$$

Device Current

$$I_i = \frac{-q}{\hbar} \int_{-\infty}^{+\infty} \text{Trace}[\Gamma_i A] f_i - \text{Trace}[\Gamma_i G^n]$$