



NEGF Quantum Simulation of Field Emission Devices

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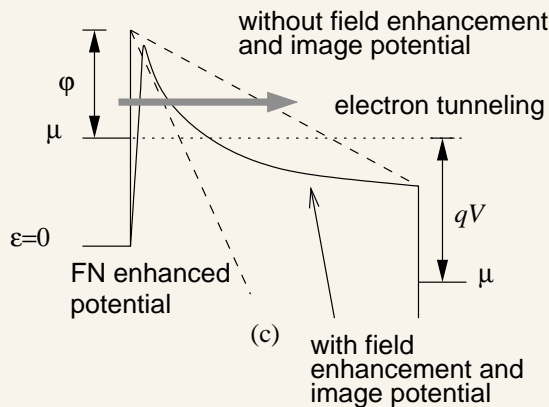
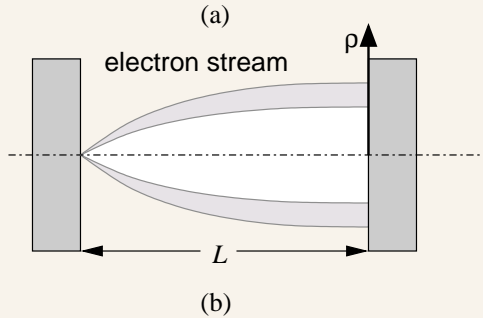
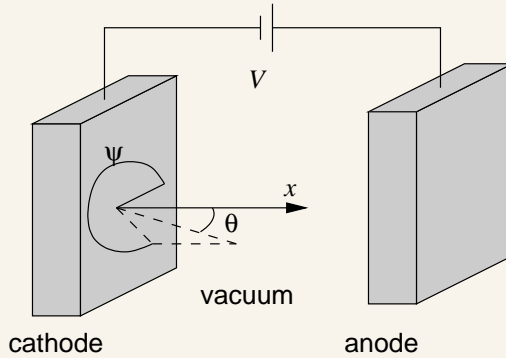
Terence D. Musho
Sarah M. Claiborne
D. Greg Walker
Vanderbilt University

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- Derived from quantum mechanics using the WKB approximation

$$I = A_{\text{eff}} K_1 \frac{(\beta F)^2}{\phi} \exp\left(-\frac{K_2 \phi^{3/2}}{\beta F}\right)$$

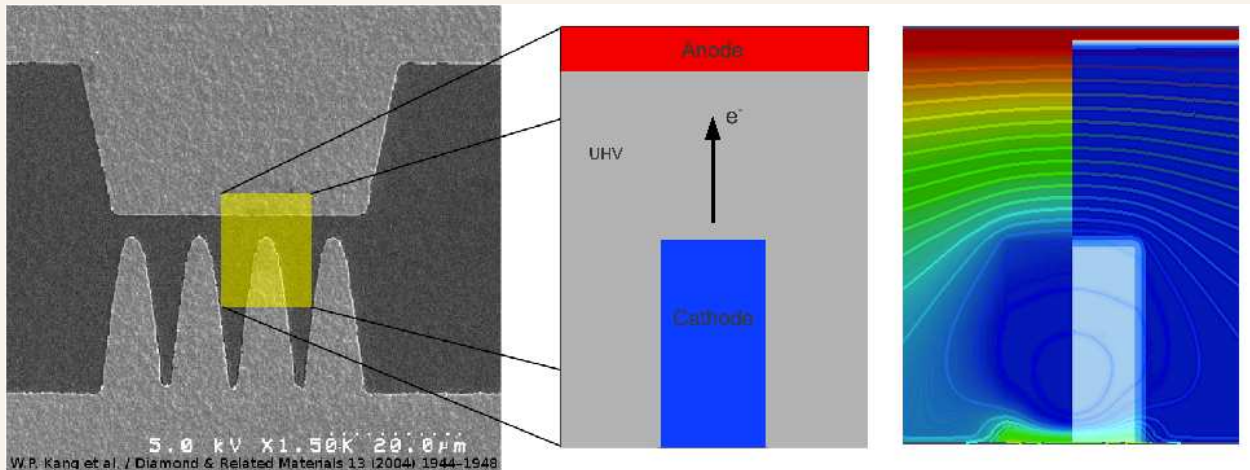
- Limitations:
 - metals only
 - absolute zero degrees
 - * Richardson's equation for thermionic emission
 - flat surfaces
 - * geometric enhancement factor β artificially increases the local field
 - Local effects: adsorbates on surface, grain boundaries, non-uniform emission area, work function variations, ...
 - uncertainty in parameters
- Benefits: Data plotted in Fowler-Nordheim coordinates are often linear



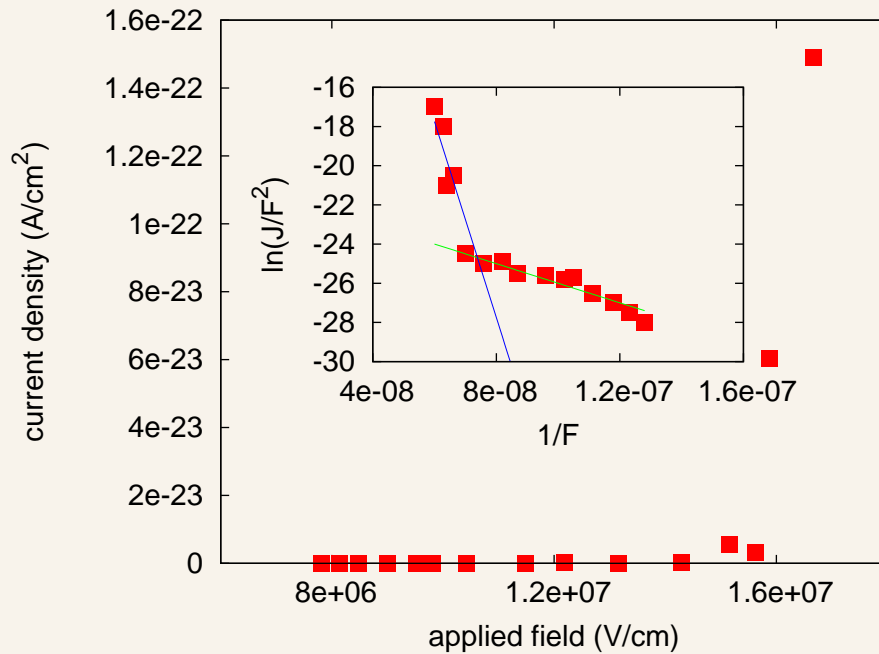
- Unenhanced potential (flat surface) is simply qV
- Enhanced FN potential is βqV
 - does not satisfy anode boundary condition
 - does not include image potential
 - does not have appropriate curvature
- more physical potentials have been developed to include local enhancement and image potential
- We will solve it numerically

- Three mathematical models
 - Use non-equilibrium Green's function to determine ballistic electron transport
 - Discretized Fowler-Nordheim approach (no geometric enhancement)
 - Standard Fowler-Nordheim with geometric enhancement

- Device model



- diamond emitter (4 nm diameter), lightly doped ($N_d = 10^{14} \text{ cm}^{-3}$); palladium anode; band in vacuum is determined by the work function



Governing equation

$$[H + U]\Psi(\mathbf{r}) = \varepsilon_\alpha \Psi_\alpha(\mathbf{r})$$

Green's function

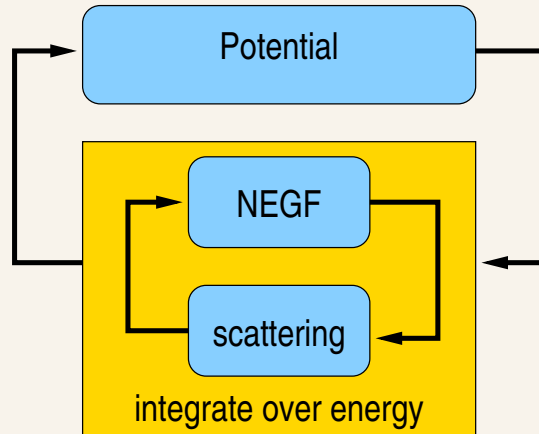
$$[G(E)] = [(E + i0^+)I - H - \Sigma_1 - \Sigma_2 - \Sigma_S(E)]^{-1}$$

Density of States

$$[A(E)] = 2\pi i([G(E)] - [G(E)]^+)$$

Density matrix

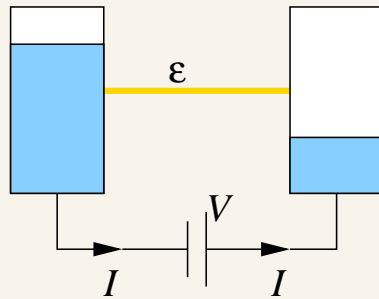
$$[\rho] = \int_{-\infty}^{\infty} F_0(E - \mu)[A(E)] dE$$



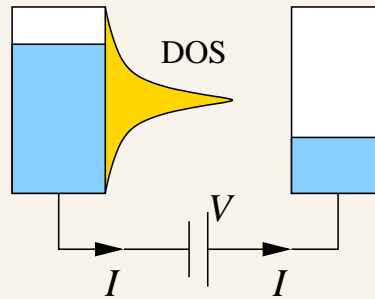
- Computational cost is in the inversion and in the integration
- integration loop is easily parallelizable

- Self-energy term $\Sigma_S(E)$ is derived from Fermi's golden rule, for example
- Transport is difference between incoming and outgoing quantities

Isolated channel



Level broadening



- Broadening of energy density of states near source and drain contacts leads to restricted current flow.

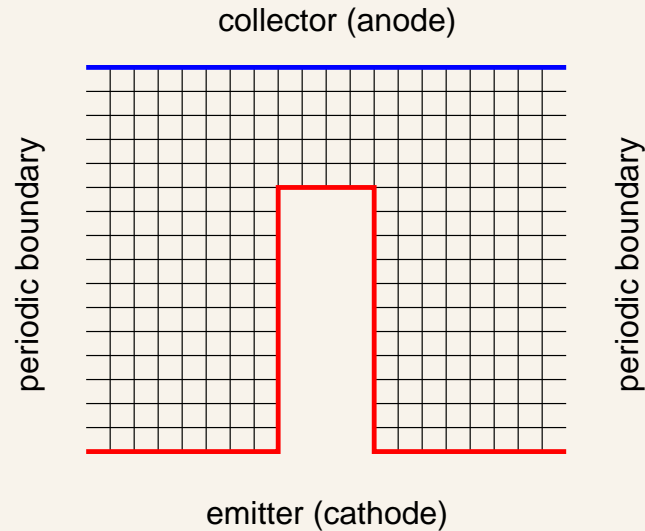
- NEGF method does not require a statistical distribution of carriers within the device, so not restricted to near equilibrium.
- Can be used to solve extreme non-equilibrium problems

$$E_{2D} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2}{2m^*} \left(\frac{n\pi}{d_z} \right)^2$$

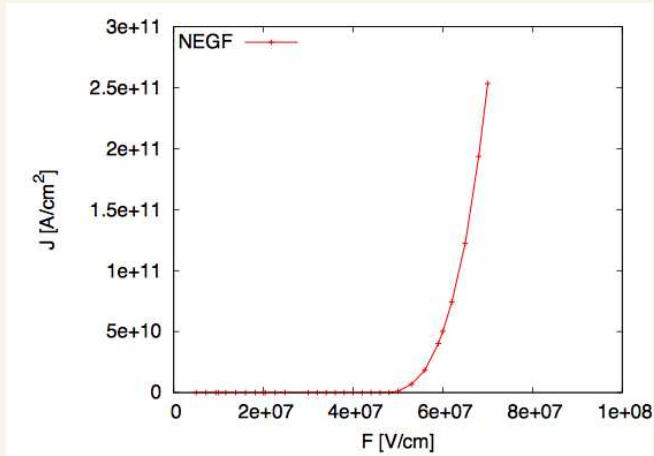
- Fermi functions are dependent on confined dispersions

$$E_{1D} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2}{2m^*} \left(\frac{m\pi}{dy} \right)^2 + \frac{\hbar^2}{2m^*} \left(\frac{n\pi}{d_z} \right)^2$$

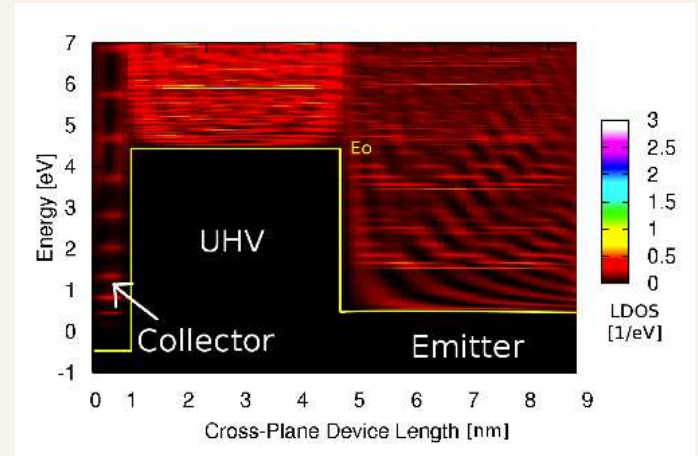
$$f_{2D}(E_{2D}) \quad f_{1D}(E_{1D})$$



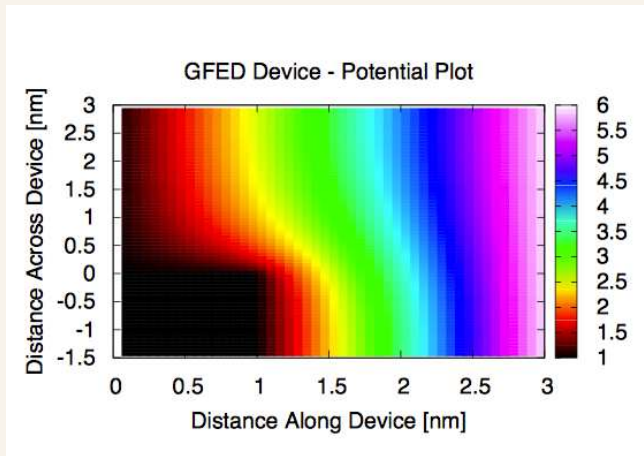
- At each element, Fowler-Nordheim is used without enhancement to estimate the local current.
- The contribution from every element on the tip is added to get the overall current



(a)

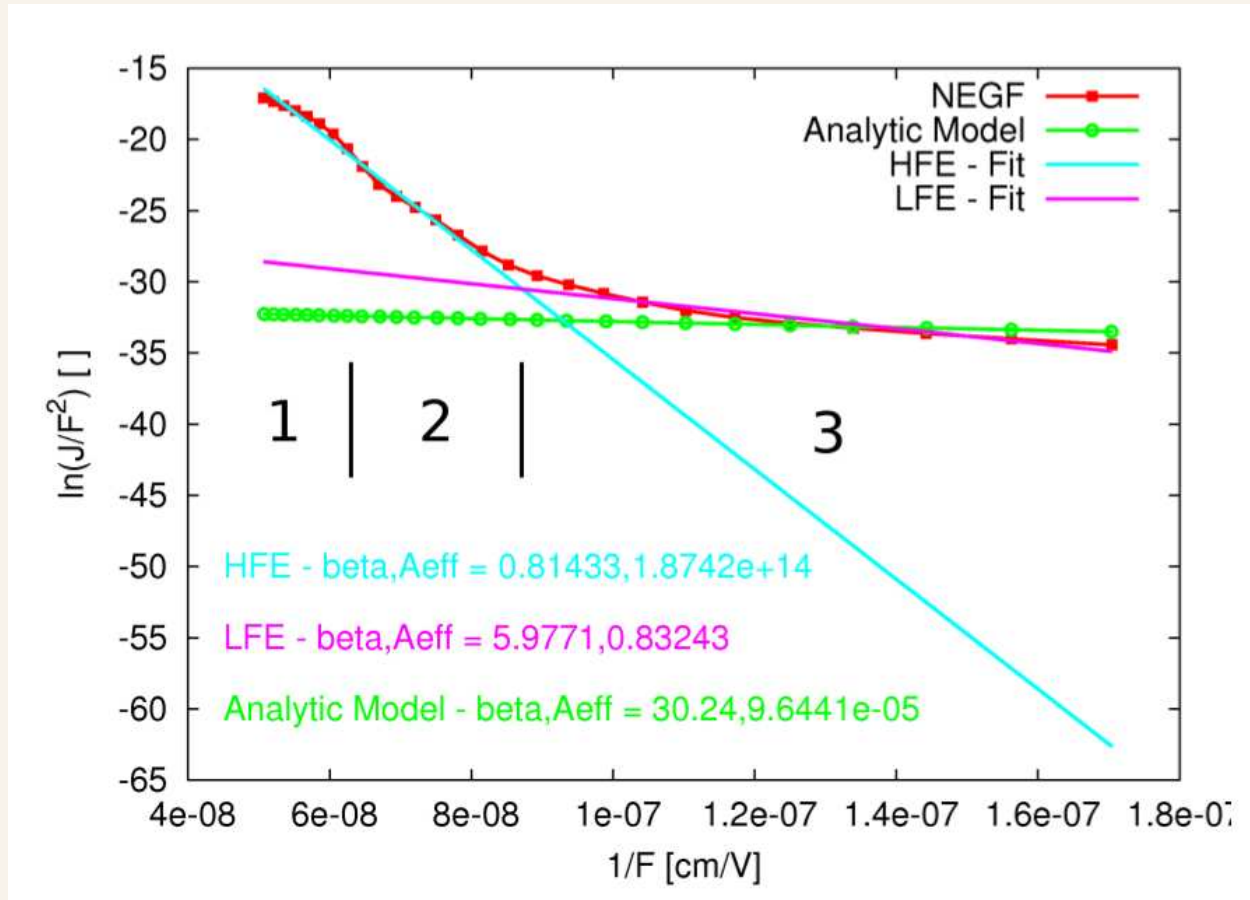


(b)



(c)

- (a) Current from FN model with enhancement
- (b) NEGF density of states
- (c) potential from discretized model



- work function was held constant for all models



- Green's function approach naturally captures the double exponential, but we are not sure of the origin of this artifact.
- Green's function also possibly captures Child-Langmuir transport
- The discretized FN does not capture the total emission very well.
 - possibly due to grid independence (we can solve the potential with good accuracy, but can not capture the field easily).