Multi-Dimensional Tunneling in Density-Gradient Theory

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Introduction

- Density-gradient (DG) theory is widely used to analyze quantum confinement effects in devices.
  - Implemented in commercial codes from Synopsis, Silvaco and ISE.
- Similar use of DG theory for tunneling problems has not occurred. Why?
  - Issues of principle (including is it possible?).
  - Unclear how to handle multi-dimensions.
- Purpose of this talk: DG theory of tunneling and how to apply it in multi-dimensions.

Some Basics

- DG theory is a continuum description that provides an approximate treatment of quantum transport.
  - Not microscopic and not equivalent to quantum mechanics so much is lost, e.g., interference, entanglement, Coulomb blockade, etc.
  - Foundational assumption: The electron and hole gases can be treated as continuous media governed by classical field theory.
- Continuum assumption often OK even in ultra-small devices:
  - Long mean free path doesn't necessarily mean low density.
  - Long deBroglie λ means carrier gases are probability density fluids.
- Apparent paradox: How can a classical theory describe quantum transport? A brief answer:

  DG theory is only macroscopically classical. Hence:
  - Only <u>macroscopic</u> violations of classical physics must be small.
  - Material response functions can be quantum mechanical in origin.

Density-Gradient Theory

- DG theory approximates quantum non-locality by making the electron gas equation of state depend on both *n* and *grad*(*n*):

$$\varepsilon_n = \varepsilon_n(n, \nabla n) = \varepsilon_n^0(n) - \frac{b_n}{2}\frac{\nabla n \cdot \nabla n}{n^2} \qquad \text{where} \quad b_n = \frac{\hbar^2}{4 m_n^* q r_n}$$

- Form of DG equations depends on importance of scattering just as with classical transport:

	Continuum theory of classical transport	*Continuum theory of quantum transport*
With scattering	DD theory	DG quantum confinement
No scattering	Ballistic transport	DG quantum tunneling

Electron Transport PDEs

- General form of PDEs describing macroscopic electron transport:

Density Gradient

Ballistic Transport

(scattering-dominated)

(ballistic regime)

negligible gen/recomb

Charge/mass conservation: $\frac{d^n n}{dt} + n\nabla\cdot\mathbf{v}_n = -R_n$

inertia negligible

Momentum conservation: $m^* n\frac{d^n \mathbf{v}_n}{dt} = \nabla\cdot\tau_n + qn\mathbf{E} - qn\mathbf{E}_n$

negligible scattering

$\mathbf{E}_n = -\mathbf{v}_n/\mu_n$

$\tau_n = -\hat{\mathbf{p}}_n = -n^2\frac{\partial\varepsilon_n}{\partial n}\mathbf{I} - n\nabla\left(\frac{\zeta_n}{n}\right)$

$\zeta_n = -n^2\frac{\partial\varepsilon_n}{\partial\nabla n} \cong b_n\nabla n$

$\mathbf{J}_n = -n\mu_n\mathbf{E} - D_n\nabla n$

Electrostatics: $\nabla\cdot\mathbf{D} = -q(n - N)$

$\mathbf{D}=\varepsilon_d\mathbf{E}$

$\mathbf{E} = -\nabla\psi$

$\mathbf{J}_n = -n\mu_n\mathbf{E} - D_n\nabla n + 2b_n\mu_n\nabla\left(\frac{\nabla^2 s}{s}\right)$ with $s \equiv \sqrt{n}$

These equations describe quantum tunneling through barriers.

PDEs for DG Tunneling

- Transformations of the DG equations:
  - Convert from gas pressures to chemical potentials.
  - Introduce a velocity potential defined by $\mathbf{v}_n \equiv \nabla \vartheta_n$
- Governing equations in steady-state:

$$\nabla \cdot \left(s^2 \nabla \vartheta_n \right) = 0 \qquad \nabla \vartheta_n \cdot \nabla \Psi_n^{DG} = 0 \qquad \nabla^2 \psi = \frac{qn}{\varepsilon_d}$$

$$\nabla \cdot \left(b_n \nabla s \right) + \frac{s}{2} \left(\psi + \Psi_n^{DG} \right) = 0$$

where $$\Psi_n^{DG} = \varphi_n^{DG} + \psi - \frac{m_n^*}{2q} \mathbf{v}_n \cdot \mathbf{v}_n$$

Boundary Conditions

- Lack of scattering implies infinite mobility plus a lack of mixing of carriers.
  - => Carriers injected from different electrodes must be modeled separately.
  - => Different physics at upstream/downstream contacts represented by different BCs.
- Upstream conditions are continuity of ψ, J_n, Ψ_n^{DG}, s, $\mathbf{n}\cdot\nabla(b_n s)$, ϑ_n
- Downstream conditions are continuity of ψ and J_n plus "tunneling recombination velocity" conditions:

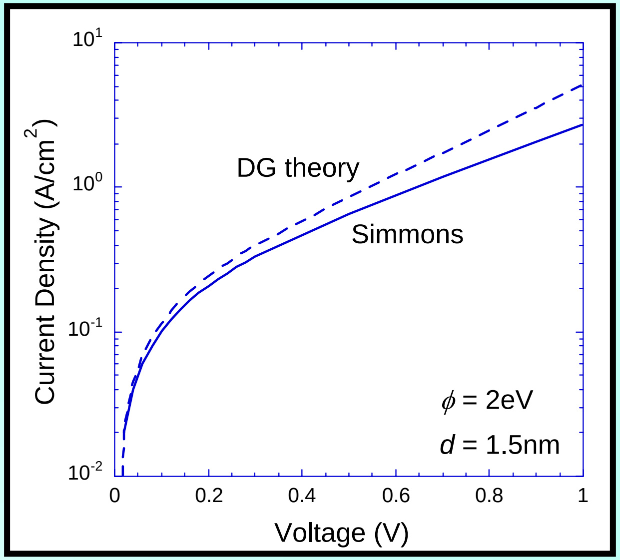
$$\mathbf{n}\cdot\nabla(b_n s) = 0 \quad \text{and} \quad \mathbf{n}\cdot\nabla\vartheta_n = v_{trv}$$

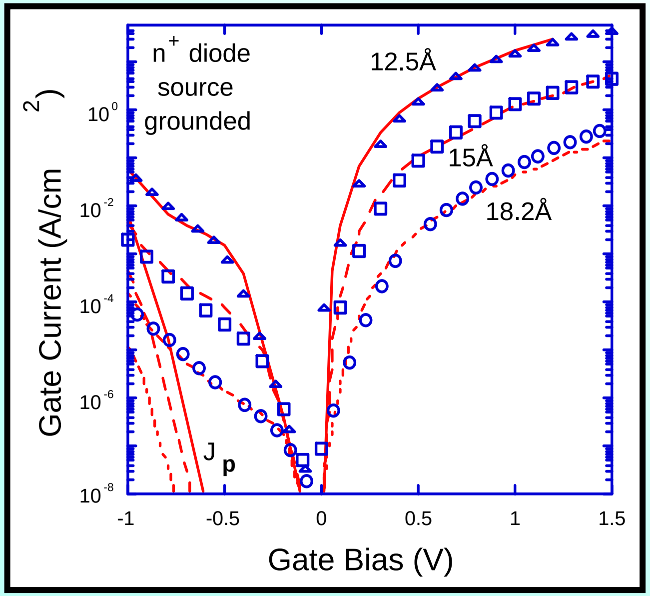
where v_{trv} is a measure of the density of final states.

DG Tunneling in 1D

Ancona, *Phys. Rev. B* (1990)

MIM



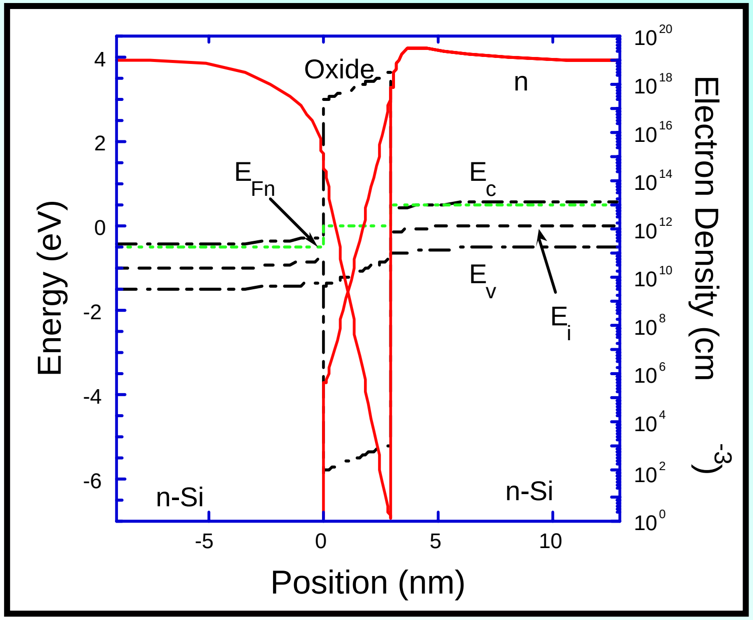


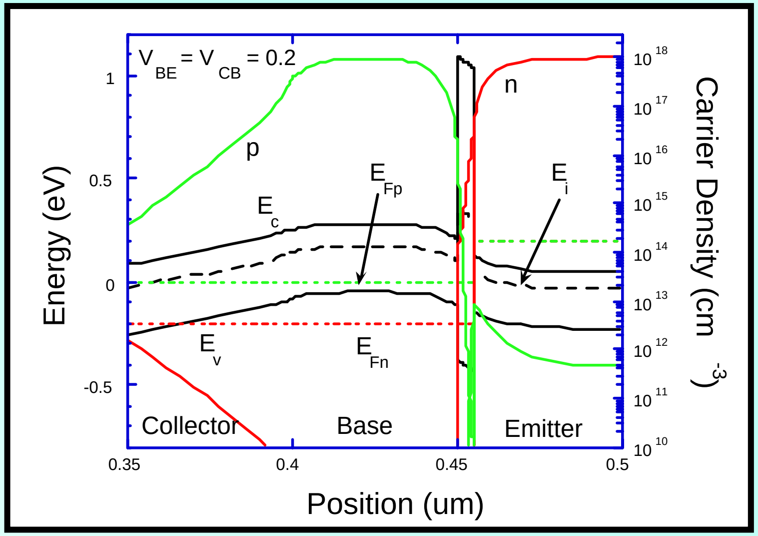
Ancona et al, *IEEE Trans. Elect. Dev.* (2000)

MOS

Ancona et al, *IEEE Trans. Elect. Dev.* (2000)

MOS



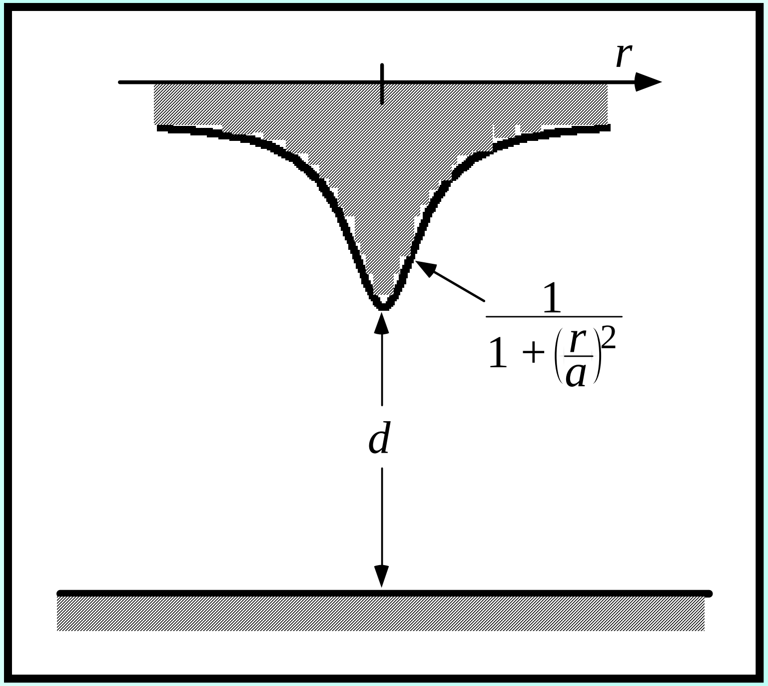


Ancona, unpublished (2002)

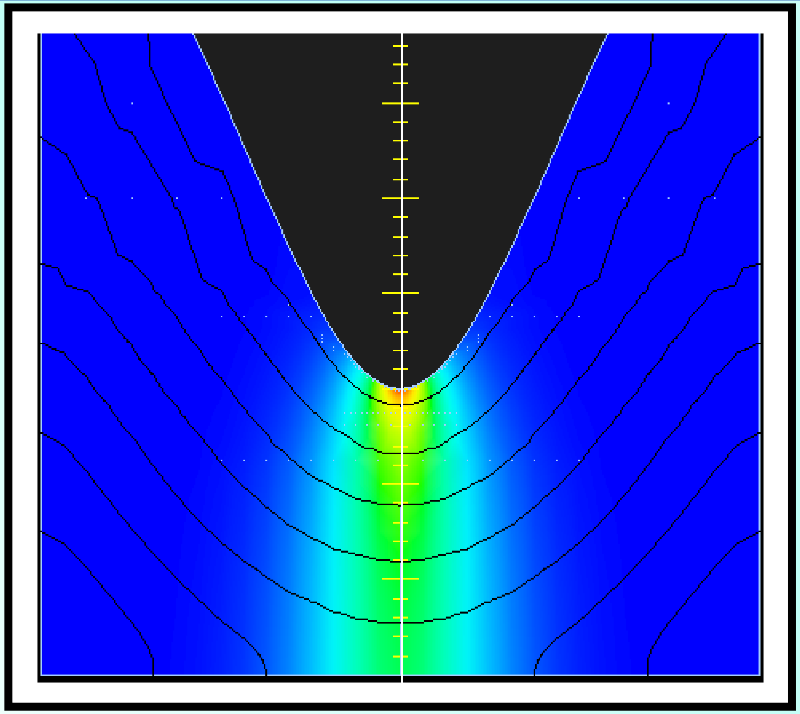
THBT

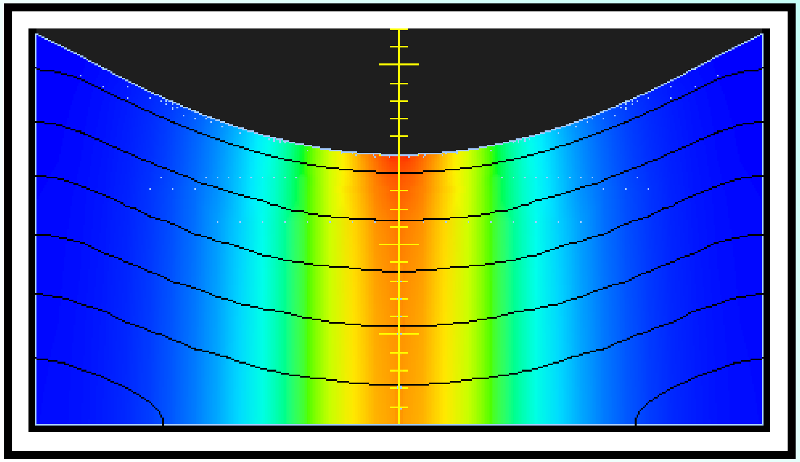
DG Tunneling in Multi-D

- Test case: STM problem, either a 2D ridge or a 3D tip.
- That electrodes are metal implies:
  - Can ignore band-bending in contacts (ideal metal assumption).
  - High density means strong gradients and space charge effects.
- Goal here is illustration and qualitative behavior, so ignore complexities of metals.
- Solve the equations using PROPHET, a powerful PDE solver based on a scripting language (written by Rafferty and Smith at Bell Labs).

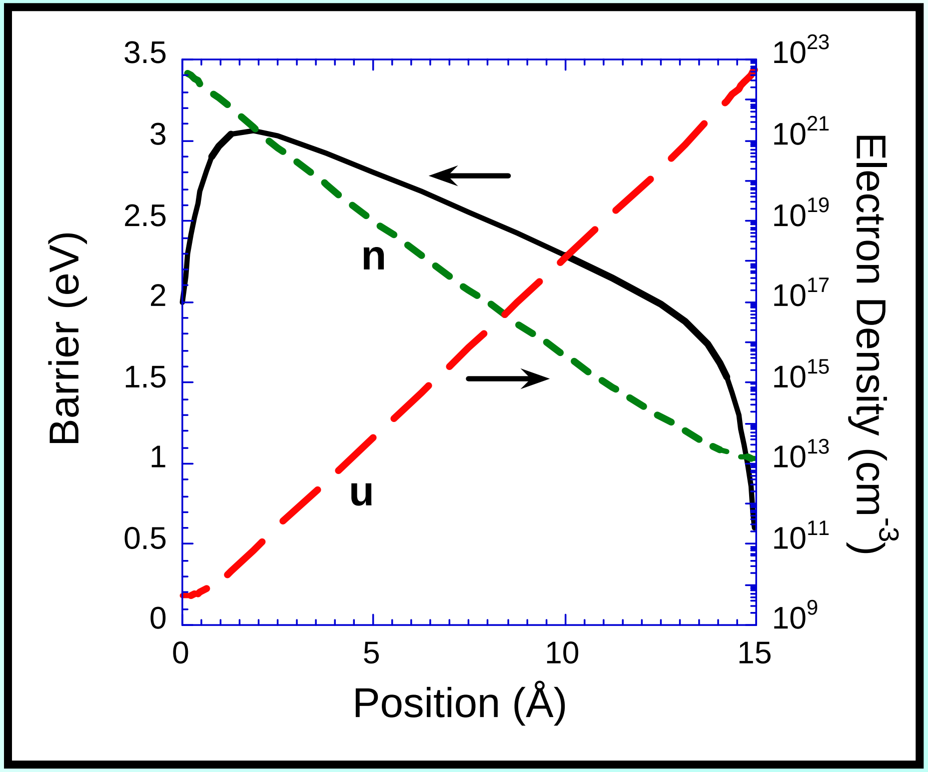


Solution Profiles



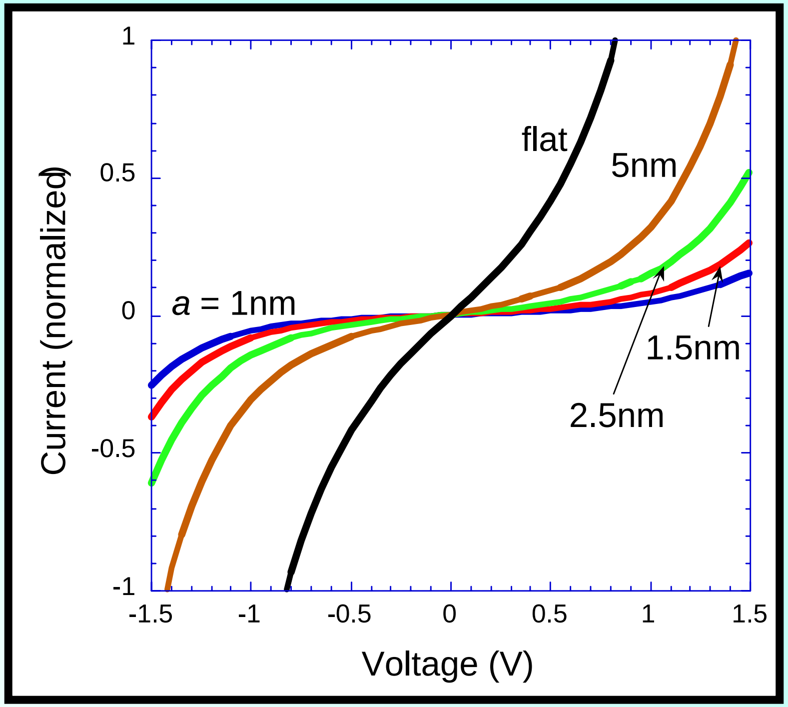


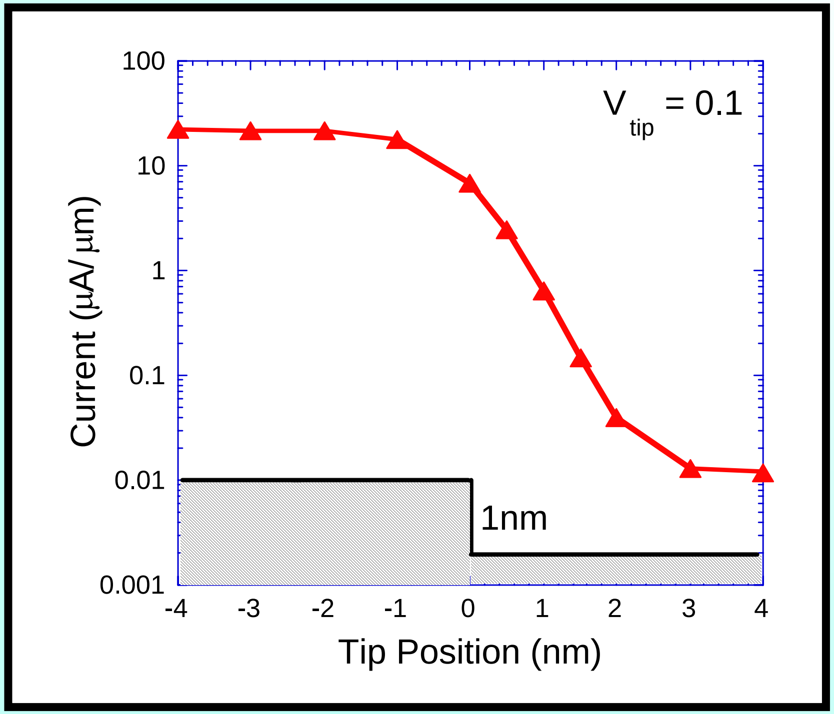
Densities are exponential and current is appropriately concentrated at the STM tip.



2D simulations

I-V Characteristics





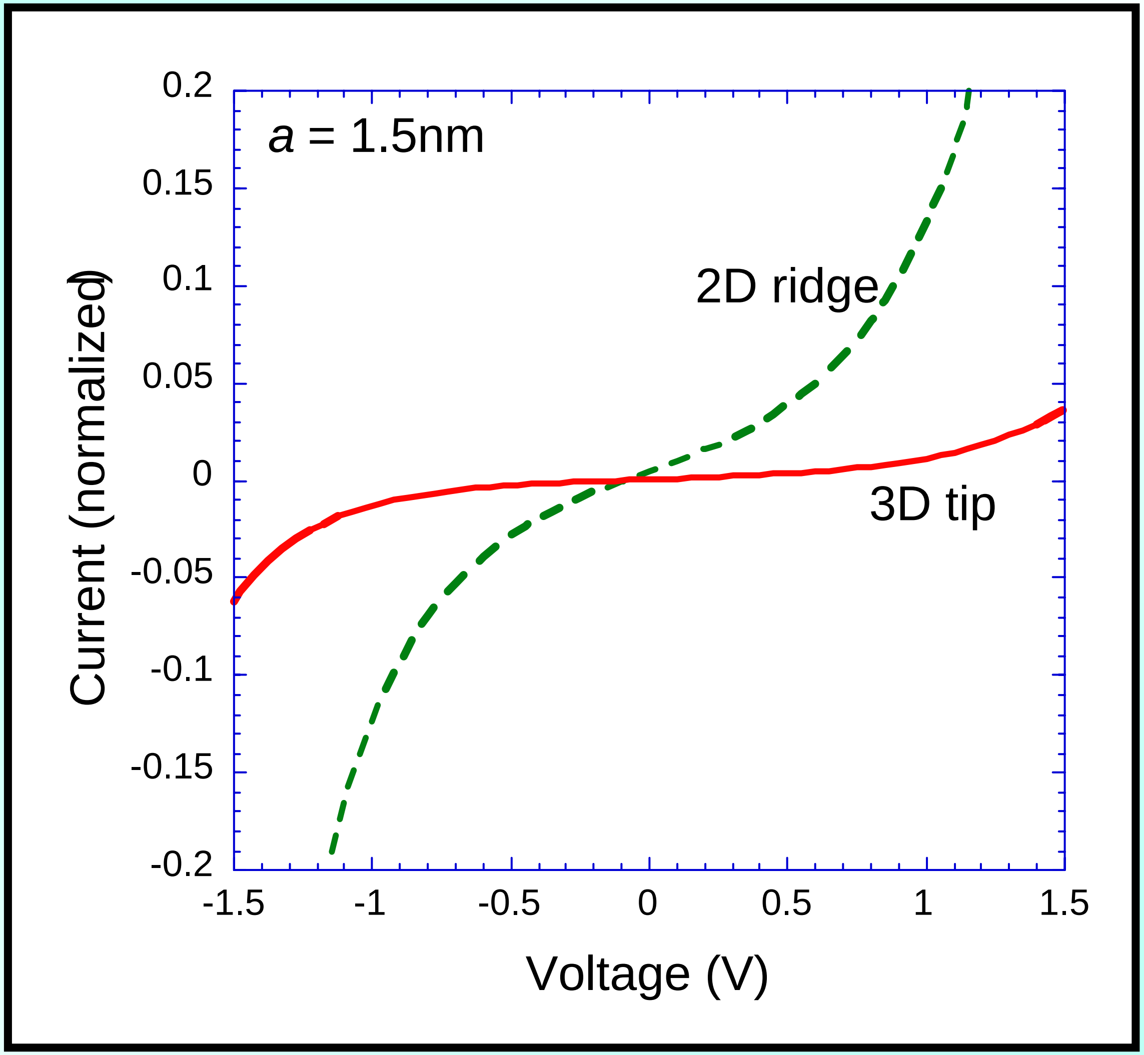
Current is exponential with strong dependence on curvature.

Asymmetrical geometry produces asymmetric I-V as is known to occur in STM.

Illustration: Estimate tip convolution --- the loss in STM resolution due to finite radius of curvature.

DG Tunneling in 3-D

- Main new issue in 3D is efficiency --- DG approach even more advantageous.
- As expected, asymmetry effect even stronger with 3D tip.



Final Remarks

- Application of DG theory to MIM tunneling in multi-dimensions has been discussed and illustrated.
- Qualitatively the results are encouraging, but quantitatively less sure.
  - DG confinement reasonably well verified in 1D and multi-D.
  - Much less work done verifying DG tunneling and all in 1D.
- Many interesting problems remain, e.g., gate current in an operating MOSFET.
- Main question for the future: Can DG tunneling theory follow DG confinement in becoming an engineering tool?
  - Need to address theoretical, practical and numerical issues.