# Semiclassical and quantum mechanical modeling of tunnel FET devices

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Many thanks to
D.Esseni, M.Iellina, P.Osgnach, A.Revelant, L.Selmi, (UD)
L.De Michielis (EPFL)

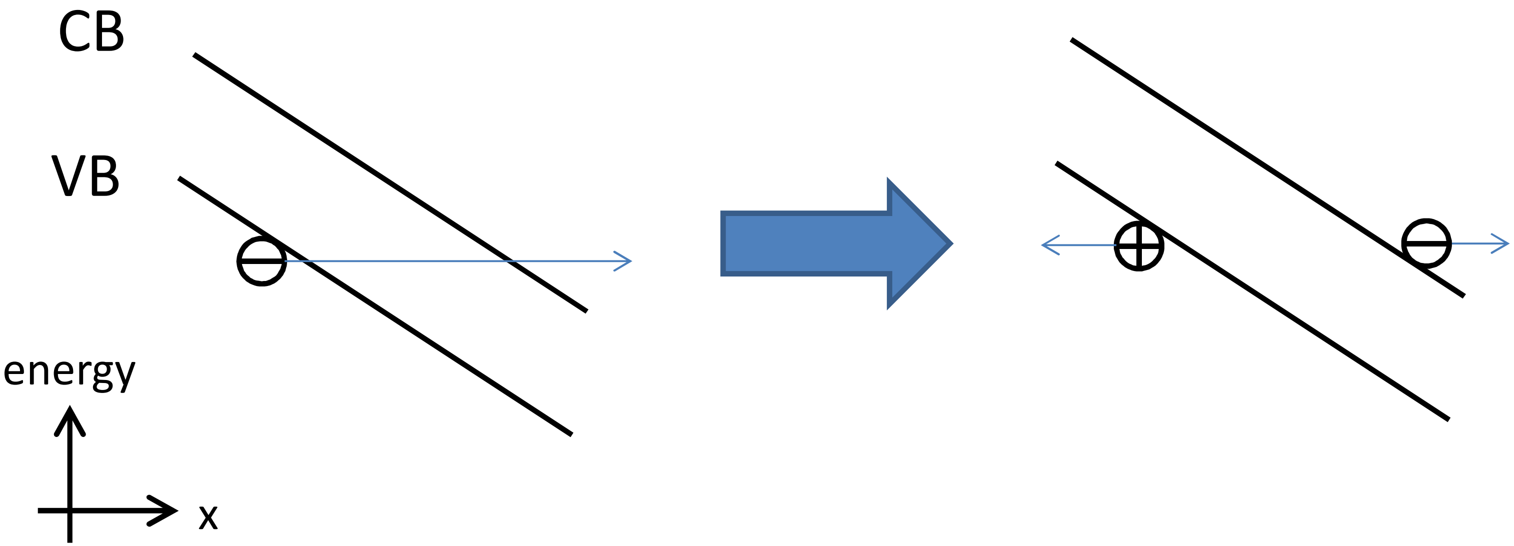
# Aim of the lecture

- to understand where the models for band-to-band tunneling come from
- to review the models employed in commercial TCAD simulators
- to understand the main limitation of such models

# OUTLINE

- band-to-band tunneling current
- direct tunneling:
  - local model
  - non-local model
- phonon assisted tunneling
- tunneling path
- impact of size-induced quantization
- application examples

# What is Band-to-band tunneling ?



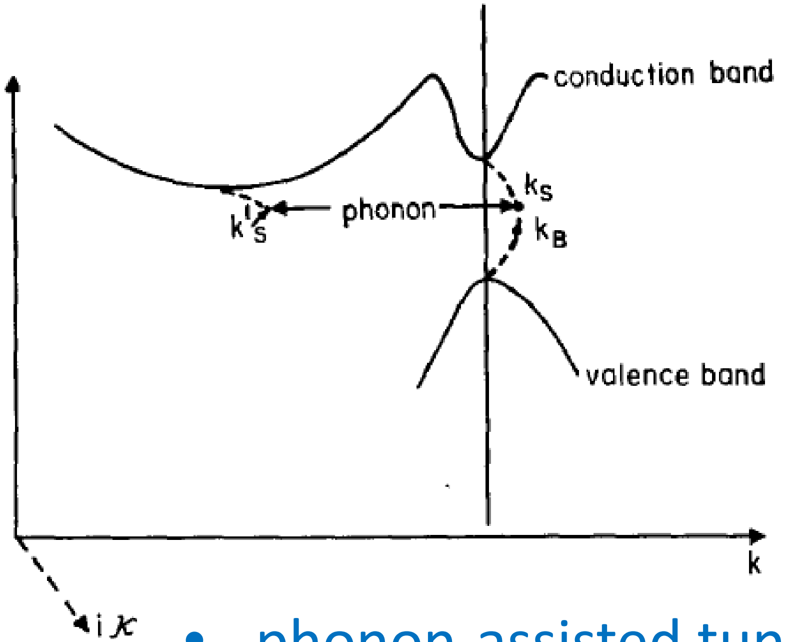

- electrons in the valence band tunnel into the conduction band
- this tunneling current generates e-h pairs

# Direct vs. phonon assisted

JOURNAL OF APPLIED PHYSICS VOLUME 32, NUMBER 1 JANUARY, 1961

**Theory of Tunneling**

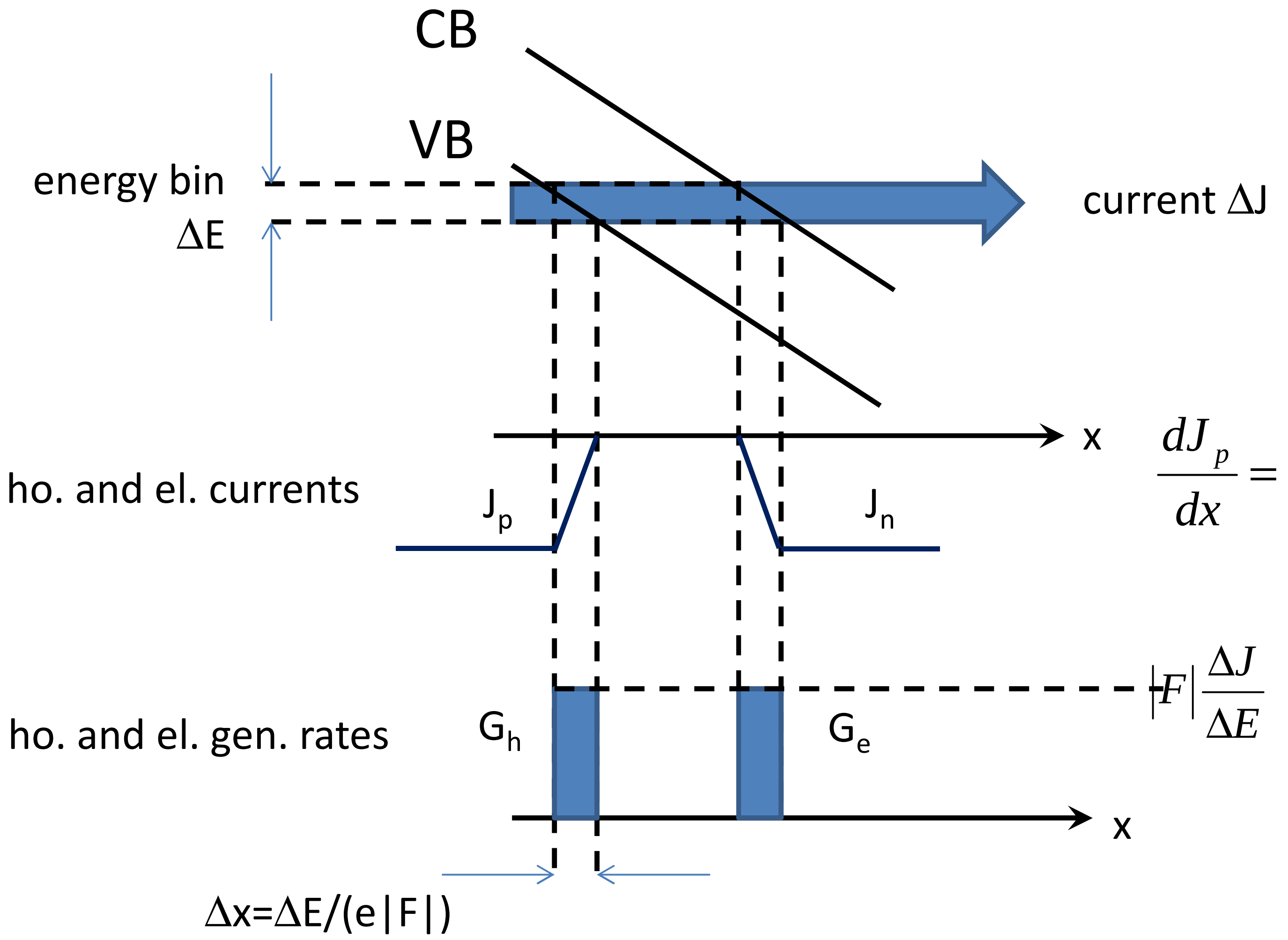
EVAN O. KANE
*Semiconductor Materials Department, Hughes Research Laboratories, Malibu, California*
(Received June 6, 1960)




- direct tunneling: the ***k***-vector normal to tunneling is conserved;
- tunneling from top of the VB into CB minima in $\Gamma$ → important in direct semiconductors (III-V)

- phonon-assisted tunneling: scattering with phonons allows to tunnel from VB to CB minima other than $\Gamma$ → relevant in Si and Ge

# BBT current vs. BBT generation




$$\frac{dJ_p}{dx} = eG_h \qquad \frac{dJ_n}{dx} = -eG_e$$

# Semiclassical models

- translate the tunneling current into suitable generation rates
- these rates are used in trasnport models for electrons in CB and holes in VB (e.g. DD model in TCAD simulators)
- simplified treatment of BBT w.r.t. full quantum approaches (e.g. equilibrium distribution, WKB approximation, …)
- more efficient treatment of carrier transport after tunneling → can handle much larger devices w.r.t. full-quantum models
- challenge: include as much quantum effects as possible

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# Kane Model (1)

*J. Phys. Chem. Solids* Pergamon Press 1959. Vol. 12. pp. 181–188. Printed in Great Britain.

ZENER TUNNELING IN SEMICONDUCTORS

E. O. KANE

Local model
(i.e. *F*=const.)
for direct BBT

original derivation by Kane is based on the Schrödinger equation in ***k***

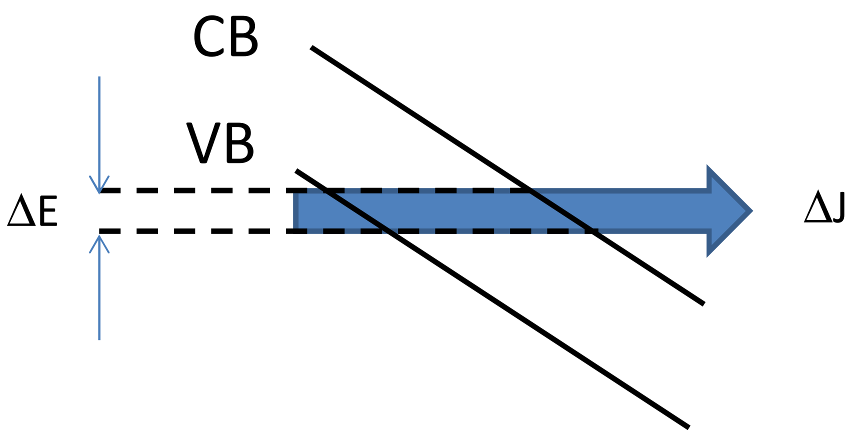
$$\left[E_n(k) - iF\frac{\partial}{\partial k_x} - E\right] a_n(k) - \sum_{n'} F X_{nn'} a_{n'}(k) = 0 \qquad (1)$$

the well know expression for $G_{bbt}$ (called *n* in the paper) is obtained

$$n = \frac{F^2 m_r^{\frac{1}{2}}}{18\pi \hbar^2 E_G^{\frac{1}{2}}} \exp\left\{\frac{-\pi m_r^{\frac{1}{2}} E_G^{\frac{3}{2}}}{2\hbar F}\right\} \qquad (39)$$

# Kane Model (2)

- we derive here Kane's equation in a simpler way using Landauer formula and WKB approximation for tunneling




- since the field is constant, we have the same $\Delta J$ in each bin $\Delta E$
- $G_e = G_h = G_{bbt}$ does not depend on $x$ and it is:

$$G_{bbt} = |F| \frac{\Delta J}{\Delta E}$$

- Landauer formula :

tunneling prob.

$$J = \frac{2e}{2\pi\hbar \mathrm{Area}} \int \sum_{\mathbf{k}_\perp} T(E, \mathbf{k}_\perp)[f_v - f_c] dE$$

normalizing area

occupation of VB and CB

k-normal to the tunneling direction

# Kane Model (3)

$$G_{bbt} = |F| \frac{\Delta J}{\Delta E} = \frac{e|F|}{\pi\hbar \mathrm{Area}} \sum_{\mathbf{k}_\perp} T(E, \mathbf{k}_\perp)$$

- we set $f_v$=1 $f_c$=0

- the structure is uniform and thus *T* does not depend on *E*
- we also convert the sum over $\mathbf{k}_\perp$ into an integral:

$$G_{bbt} = \frac{e|F|}{4\pi^3\hbar} \int T(E, \mathbf{k}_\perp) d\mathbf{k}_\perp$$

- the tunneling probability is compute under the WKB approximation:

$$T = \frac{\pi^2}{9} \exp\left(-2\int \mathrm{Im}(k_x) dx\right)$$

… a long story… check Kane's paper

# Kane Model (4)

- the integral of Im($k_x$) must be computed over a path conserving the total energy $E$ and the normal wave-vector $\boldsymbol{k}_\perp$
- we need an E-k relation valid into the gap and linking the VB states to the CB ones
- **Kane's relation**:

$$E_\pm = \frac{E_G}{2} + \frac{\hbar^2 k^2}{2m_0} \pm \frac{1}{2}\sqrt{E_G^2 + \frac{E_G \hbar^2 k^2}{2m_r}}$$

the total energy is:

$$E = E_\pm - e|F|x$$

for small $k$ (real): $E_- \approx -\frac{\hbar^2 k^2}{2}\left(\frac{1}{2m_r} - \frac{1}{m_0}\right)$ $\quad E_+ \approx E_G + \frac{\hbar^2 k^2}{2}\left(\frac{1}{2m_r} + \frac{1}{m_0}\right)$

meaning that: $\frac{1}{m_r} = \frac{1}{m_c} + \frac{1}{m_v}$

# Kane Model (5)

$$E_{\pm} = \frac{E_G}{2} + \cancel{\frac{\hbar^2 k^2}{2m_0}} \pm \frac{1}{2}\sqrt{E_G^2 + \frac{E_G \hbar^2 k^2}{2m_r}} \qquad k^2 = (\mathrm{Re}\, k_x)^2 + (\mathrm{Im}\, k_x)^2 + |\mathbf{k}_\perp|^2$$

negligible inside the gap

- the non null $k_\perp$ make $k_x$ imaginary over a longer path compared to $E_G/(e|F|)$ → *larger effective gap for large $k_\perp$*
- setting $x=0$ where $E=0$, we have:

$$\mathrm{Im}(k_x) = \sqrt{\frac{m_r}{E_G \hbar^2}} \sqrt{E_G^2 + E_G \frac{\hbar^2 |\mathbf{k}_\perp|^2}{m_r} - 4\left(e|F|x - \frac{E_G}{2}\right)^2}$$

- for $x$ between

$$x_{\pm} = \frac{\frac{E_G}{2} \pm \frac{1}{2}\sqrt{E_G^2 + E_G \frac{\hbar^2 |\mathbf{k}_\perp|^2}{m_r}}}{e|F|}$$

# Kane Model (6)

$$T = \frac{\pi^2}{9}\exp\left(-2\int \mathrm{Im}(k_x)dx\right)$$ thus gives:

$$T = \frac{\pi^2}{9}\exp\left(-\pi\frac{\sqrt{m_r}E_G^{3/2}}{2\hbar e|F|}\right)\exp\left(-\frac{\pi\hbar|\mathbf{k}_\perp|^2}{2e|F|}\sqrt{\frac{E_G}{m_r}}\right)$$

$$G_{bbt} = \frac{e|F|}{4\pi^3\hbar}\int T(E,\mathbf{k}_\perp)d\mathbf{k}_\perp$$ finally gives:

$$\boxed{G_{bbt} = \frac{e^2|F|^2\sqrt{m_r}}{18\pi\hbar^2\sqrt{E_G}}\exp\left(-\pi\frac{\sqrt{m_r}E_G^{3/2}}{2\hbar e|F|}\right)}$$ that is Kane's formula

# Effect of the carrier gas dimensionality

- we have integrated over the transverse $\boldsymbol{k}_\perp$ assuming the gas to be free (3D total ***k***-vector)
- in quantized structures (wells, wires) the k vector is 2D or 1D
- we obtain:

$$G_{BBT} = A\exp(-B/F)$$

$$A_{3D} = \frac{\sqrt{m_r}e^2F^2}{18\pi\hbar^2\sqrt{E_G}}$$

$$A_{2D} = \frac{(eF)^{3/2}\sqrt{2}}{18\hbar^{3/2}}\sqrt[4]{\frac{m_r}{E_G}}\frac{1}{T_{well}}$$

$$A_{1D} = \frac{eF\pi}{9\hbar}\frac{1}{A_{wire}}$$

$$B = \frac{\pi^2\sqrt{m_r}E_G^{1.5}}{eh}$$

where all rates are in $1/(m^3 s)$

3D=no quantization
2D=quantum well
1D=nanowire

# Local models in TCAD (1)

- even if the electric field profile is not constant, a local $G_{bbt}$ is computed based on the local field.
- Example: Kane model in SentaurusDevice

$$G^{\mathrm{b2b}} = AF^{P}\exp\left(-\frac{B}{F}\right) \tag{372}$$

Depending on value of `Model`, $P$ takes the values $1$, $1.5$, or $2$.

370 Sentaurus Device User Guide
E-2010.12

- since the BBT rate only depend on *F*, we have current also for $V_{DS}$=0V ☹
- the ($f_v$-$f_c$) term of the Landauer equation must be included

# Local models in TCAD (2)

- Example: Hurks model in Sentaurus Device

$$R_{\mathrm{net}}^{\mathrm{bb}} = A \cdot D \cdot \left(\frac{F}{1\ \mathrm{V/cm}}\right)^{P} \exp\left(-\frac{BE_{\mathrm{g}}(T)^{3/2}}{E_{\mathrm{g}}(300\mathrm{K})^{3/2} F}\right) \qquad (373)$$

where:

$$D = \frac{np - n_{\mathrm{i,eff}}^{2}}{(n + n_{\mathrm{i,eff}})(p + n_{\mathrm{i,eff}})}(1 - |\alpha|) + \alpha \qquad (374)$$

  - we can have both generation and recombination
  - zero net rate at equilibrium (meaning zero current at $V_{DS}$=0V ☺ )

- Limitation of the local models: the electric field profile is not uniform → they largely overestimate the BBT generation

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# Non-local models in TCAD

- example: dynamic non-local path band-to-band model in Sentaurus

$$R_{\mathrm{net}}^{\mathrm{d}} = |\nabla E_{\mathrm{V}}(0)| C_{\mathrm{d}} \exp\left(-2\int_0^l \kappa dx\right)\left[\left(\exp\left[\frac{\varepsilon - E_{\mathrm{F},n}(l)}{kT(l)}\right] + 1\right)^{-1} - \left(\exp\left[\frac{\varepsilon - E_{\mathrm{F},p}(0)}{kT(0)}\right] + 1\right)^{-1}\right] \tag{375}$$

$$C_{\mathrm{d}} = \frac{g\pi}{36h}\left(\int_0^l \frac{dx}{\kappa}\right)^{-1}\left[1 - \exp\left(-k_{\mathrm{m}}^2 \int_0^l \frac{dx}{\kappa}\right)\right] \tag{376}$$

$$\kappa = \frac{1}{\hbar}\sqrt{m_{\mathrm{r}} E_{\mathrm{g,tun}}(1-\alpha^2)}$$

$$k_{\mathrm{m}}^2 = \min(k_{\mathrm{vm}}^2, k_{\mathrm{cm}}^2)$$

$$\frac{1}{m_{\mathrm{C}}} = \frac{1}{2m_{\mathrm{r}}} + \frac{1}{m_0}$$

$$\alpha = -\frac{m_0}{2m_{\mathrm{r}}} + 2\sqrt{\frac{m_0}{2m_{\mathrm{r}}}\left(\frac{\varepsilon - E_{\mathrm{V}}}{E_{\mathrm{g,tun}}} - \frac{1}{2}\right) + \frac{m_0^2}{16m_{\mathrm{r}}^2} + \frac{1}{4}}$$

$$k_{\mathrm{vm}}^2 = \frac{2m_{\mathrm{V}}(\varepsilon_{\max} - \varepsilon)}{\hbar^2}$$

$$\frac{1}{m_{\mathrm{V}}} = \frac{1}{2m_{\mathrm{r}}} - \frac{1}{m_0}$$

$$\frac{1}{m_{\mathrm{r}}} = \frac{1}{m_{\mathrm{V}}} + \frac{1}{m_{\mathrm{C}}}$$

$$k_{\mathrm{cm}}^2 = \frac{2m_{\mathrm{C}}(\varepsilon - \varepsilon_{\min})}{\hbar^2}$$

# “Simple“ derivation of the non-local model (1)

$$\kappa = \frac{1}{\hbar}\sqrt{m_r E_{g,tun}(1-\alpha^2)}$$

$$\alpha = -\frac{m_0}{2m_r} + 2\sqrt{\frac{m_0}{2m_r}\left(\frac{\varepsilon - E_V}{E_{g,tun}} - \frac{1}{2}\right) + \frac{m_0^2}{16m_r^2} + \frac{1}{4}}$$

$$\frac{1}{m_r} = \frac{1}{m_V} + \frac{1}{m_C}$$

- is the inverse of Kane’s relation

$$E_\pm = \frac{E_G}{2} + \frac{\hbar^2 k^2}{2m_0} \pm \frac{1}{2}\sqrt{E_G^2 + \frac{E_G \hbar^2 k^2}{2m_r}}$$

with $k=j\kappa$

quasi-electric field to convert current into gen/rec rate

$f_c$-$f_v$ assuming Fermi-Dirac statistics

$$R_{net}^d = |\nabla E_V(0)| \underbrace{C_d \exp\left(-2\int_0^l \kappa dx\right)}_{dJ/dE \text{ (Landauer + WKB)}} \left[\left(\exp\left[\frac{\varepsilon - E_{F,n}(l)}{kT(l)}\right] + 1\right)^{-1} - \left(\exp\left[\frac{\varepsilon - E_{F,p}(0)}{kT(0)}\right] + 1\right)^{-1}\right]$$

*dJ/dE* (Landauer + WKB)

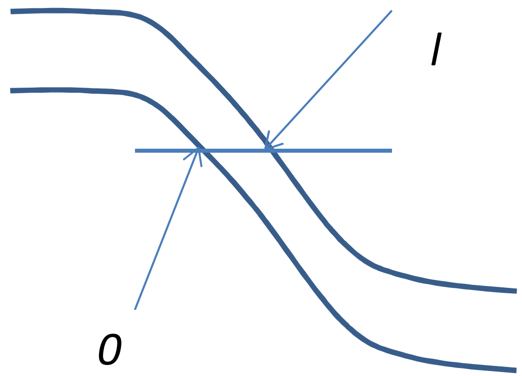
# "Simple" derivation of the non-local model (2)

$$\frac{dJ}{dE} = \frac{e}{4\pi^3\hbar}\int T(E,\mathbf{k}_\perp)d\mathbf{k}_\perp \qquad T = \frac{\pi^2}{9}\exp\left(-2\int \mathrm{Im}(k_x)dx\right)$$

since $k=j\kappa$ → $\mathrm{Im}(k_x) = \sqrt{\kappa^2 + |\mathbf{k}_\perp|^2} \approx \kappa + \frac{|\mathbf{k}_\perp|^2}{2\kappa}$

$$T = \frac{\pi^2}{9}\exp\left(-2\int \kappa dx\right)\exp\left(-|\mathbf{k}_\perp|^2\int\frac{dx}{\kappa}\right)$$

the tunneling path would depend on $\mathbf{k}_\perp$, but it is computed only for $\mathbf{k}_\perp=0$ and kept constant when integrating $T$ over $\mathbf{k}_\perp$



# "Simple" derivation of the non-local model (3)

integration over $\boldsymbol{k}_{\perp}$, gives

$$\frac{dJ}{dE} = \frac{e}{36\hbar}\left(\int \frac{dx}{\kappa}\right)^{-1}\left[1-\exp\left(-k_m^2\int\frac{dx}{\kappa}\right)\right]\exp\left(-2\int \kappa dx\right)$$

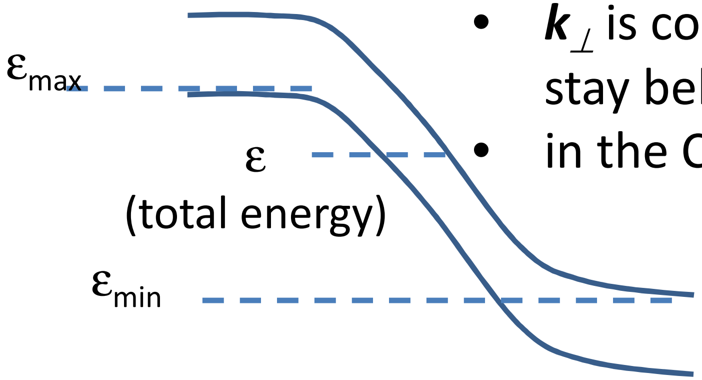
that is exactly the formula in the Sentaurus manual ☺

maximum transverse momentum

$$k_{\rm m}^2 = \min(k_{\rm vm}^2, k_{\rm cm}^2)$$

$$k_{\rm vm}^2 = \frac{2m_{\rm V}(\varepsilon_{\rm max}-\varepsilon)}{\hbar^2}$$

$$k_{\rm cm}^2 = \frac{2m_{\rm C}(\varepsilon-\varepsilon_{\rm min})}{\hbar^2}$$

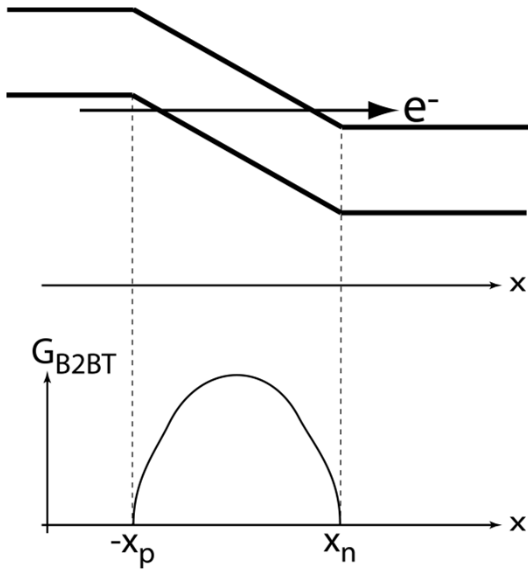


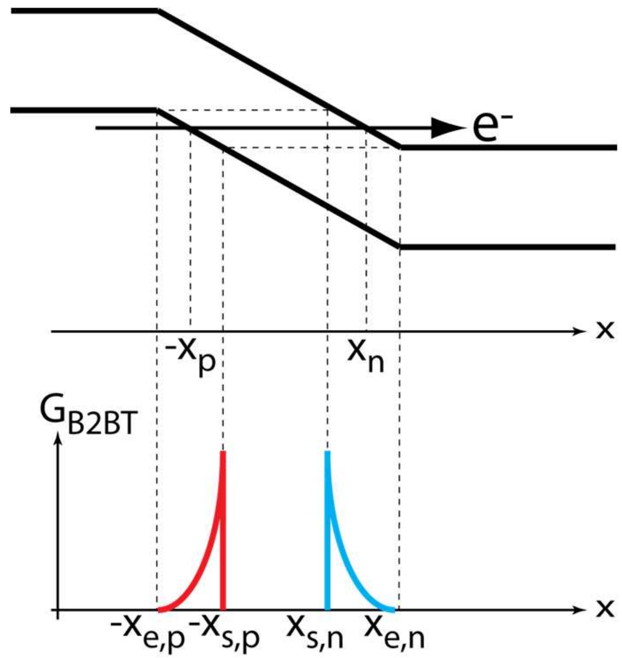

- in the CB and VB we can separate energy along $x$ and normal to $x$
- $\boldsymbol{k}_{\perp}$ is conserved, but energy along $x$ should stay below $\varepsilon_{max}$ in the VB and above $\varepsilon_{min}$
- in the CB

$$\varepsilon + \frac{\hbar^2|\mathbf{k}_{\perp}|^2}{2m_v} \le \varepsilon_{\rm max}$$

$$\varepsilon - \frac{\hbar^2|\mathbf{k}_{\perp}|^2}{2m_c} \ge \varepsilon_{\rm min}$$

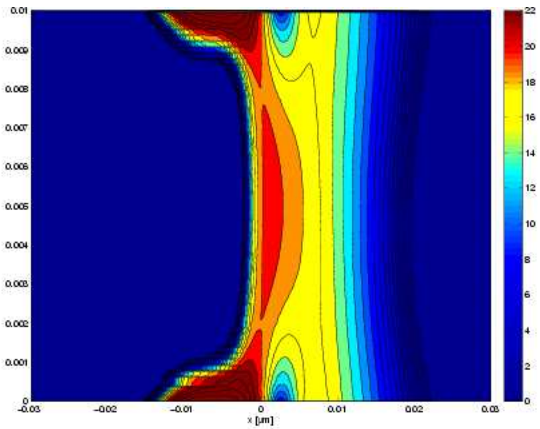
# Local vs. non-local (1)



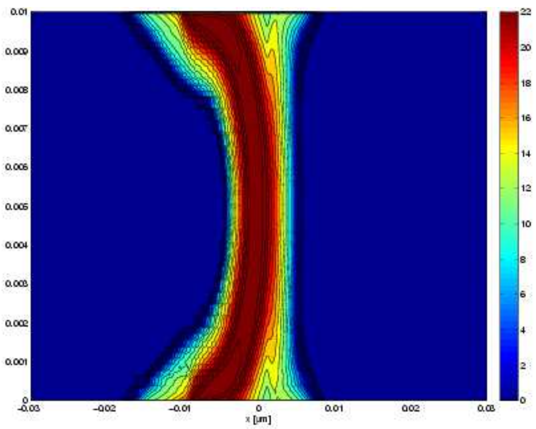




- in the local model el. and ho. generation profiles are the same
- in the non local ho. are generated at the beginning and electrons at the end of the tunneling path

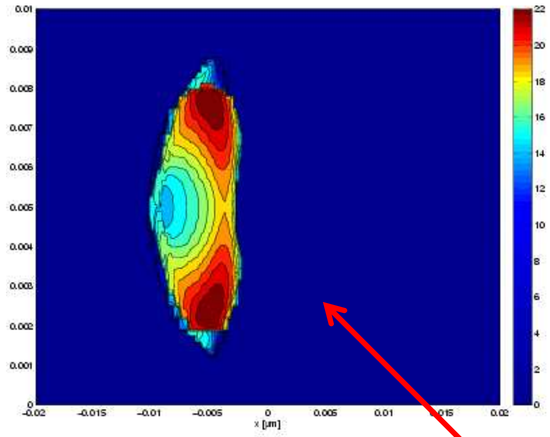
# Local vs. non-local (2)



local w/o $f_v$-$f_c$



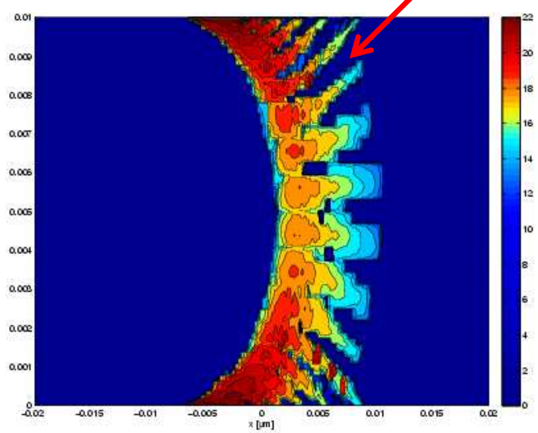
local w $f_v$-$f_c$

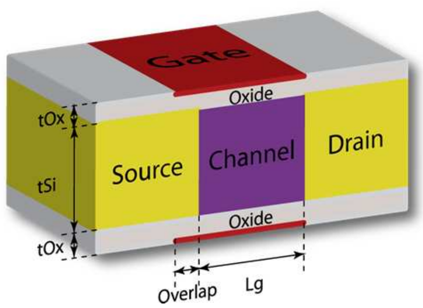


non-local w $f_v$-$f_c$

e

h






non local model: much lower generation, in particular close to the interfaces.

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# Phonon assisted BBT (1)

SOVIET PHYSICS JETP VOLUME 6 (33), NUMBER 4 APRIL, 1958

BEHAVIOR OF NON-METALLIC CRYSTALS IN STRONG ELECTRIC FIELDS

L. V. KELDYSH

JOURNAL OF APPLIED PHYSICS VOLUME 32, NUMBER 1 JANUARY, 1961

**Theory of Tunneling**

EVAN O. KANE
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(Received June 6, 1960)

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0038-1101/94 $7.00 + 0.00

A UNIFIED THEORY OF DIRECT AND INDIRECT INTERBAND TUNNELING UNDER A NONUNIFORM ELECTRIC FIELD

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the most complete and the "easy" to understand

JOURNAL OF APPLIED PHYSICS **109**, 124503 (2011)

**Generalized phonon-assisted Zener tunneling in indirect semiconductors with non-uniform electric fields: A rigorous approach**

William Vandenberghe,[1,a)] Bart Sorée,[2,b)] Wim Magnus,[2,c)] and Massimo V. Fischetti[3,d)]

# Phonon assisted BBT (2)

- easiest way to see it: phonon scattering between evanescent states in the gap originating from the VB and the CB
- the E-k into the gap is less critical: we do not need to link the two branches, this is done by the phonon → the effective mass description may be used
- main equations (from Vandenberghe):

$$T_{\mathrm{v}}^{\mathrm{abs,\,em}}(E) = \Omega |M'_{\mathbf{k}_0}|^2 \int \mathrm{d}^3 r A_{\mathrm{v}}(\mathbf{r},\,\mathbf{r};\,E) A_{\mathrm{c}}(\mathbf{r},\,\mathbf{r};\,E \pm \hbar\omega_{\mathbf{k}_0}).$$

$$G_{\mathrm{v}}(x) = \frac{U'_{\mathrm{ext}}(x)}{\pi\hbar A} T_{\mathrm{v}}^{\mathrm{abs,\,em}}(U_{\mathrm{ext}}(x)). \quad *$$

where the spectral functions are:

$$A_{\mathrm{v,c}}(\mathbf{r},\,\mathbf{r}';\,E) = 2\pi\delta(E - H_{\mathrm{v,c}})$$

$$= 2\pi \sum_{\ell} \chi_{\mathrm{v,c}\ell}(\mathrm{r}) \delta(E - E_{\mathrm{v,c}\ell}) \chi^*_{\mathrm{v,c}\ell}(\mathbf{r}') \ .$$

$$\left(E_{\mathrm{c}0} - \frac{\hbar^2}{2m_{\mathrm{c}}^*}\nabla^2 + U_{\mathrm{ext}}(\mathbf{r})\right)\chi_{\mathrm{c}}(\mathbf{r}) = E\chi_{\mathrm{c}}(\mathbf{r}).$$

$$\left(E_{\mathrm{v}0} + \frac{\hbar^2}{2m_{\mathrm{v}}^*}\nabla^2 + U_{\mathrm{ext}}(\mathbf{r})\right)\chi_{\mathrm{v}}(\mathbf{r}) = E\chi_{\mathrm{v}}(\mathbf{r}).$$

*note: I suspect the phonon occupation is missing here

# Phonon assisted BBT (3)

- the equation is consistent with the phonon scattering as described in many books; the scattering rate with phonons is:

$$\frac{1}{\tau} \propto \sum_{\mathbf{q}} \left| \int \chi_i(\mathbf{r}) \exp(-\mathbf{q}\cdot\mathbf{r}) \chi_f(\mathbf{r}) d\mathbf{r} \right|^2 \delta(E_i - E_f \pm E_{ph})$$

i.e. the perturbation potential is a plane wave with wave-vector ***q*** and we sum over all phonons

- if $E_{ph}$ does not depend on **q** we may rework the term in $|\,|^2$ as

$$\int \chi_i(\mathbf{r}) \exp(-\mathbf{q}\cdot\mathbf{r}) \chi_f(\mathbf{r}) d\mathbf{r} \int \chi_i(\mathbf{r}') \exp(\mathbf{q}\cdot\mathbf{r}') \chi_f(\mathbf{r}') d\mathbf{r}' =$$

$$\iint \chi_i(\mathbf{r}) \chi_i(\mathbf{r}') \chi_f(\mathbf{r}) \chi_f(\mathbf{r}') \exp[\mathbf{q}\cdot(\mathbf{r}'-\mathbf{r})] d\mathbf{r} d\mathbf{r}'$$

integrated over ***q*** becomes $\propto \delta(\boldsymbol{r}-\boldsymbol{r}')$

- and thus $\frac{1}{\tau} \propto \int |\chi_i(\mathbf{r})|^2 |\chi_f(\mathbf{r})|^2 d\mathbf{r} \delta(E_i - E_f \pm E_{ph})$ i.e. the spectral functions appear

# Phonon assisted BBT (4)

- the difficult task is to compute the spectral functions *A(**r**,**r**,E)* that must include also the states normal to the tunneling direction
- example: 1D profile

$$\left(E_g - \frac{\hbar^2}{2m_c}\frac{d^2}{dx^2} + E_c^{\perp}(\mathbf{K}) + U_{ext}(x)\right)\chi_c(\mathbf{r};\mathbf{K},E) = E\chi_c(\mathbf{r};\mathbf{K},E).$$

$$E_{v,c}^{\perp}(\mathbf{K}) = \frac{\hbar^2|\mathbf{K}|^2}{2m_{v,c}}.$$

(idem for VB)

$$A_{v,c}(\mathbf{r},\,\mathbf{r};\,E) = \frac{m_v}{\hbar^2}\int_0^{\infty}\frac{dE_v^{\perp}}{2\pi}|\chi_{v,c}(\mathbf{r};\,E_{v,c}^{\perp},\,E)|^2$$

with $$\int_{-\infty}^{+\infty} d^3r\,\chi_{v,c}^{*}(\mathbf{r};\mathbf{K},E)\chi_{v,c}(\mathbf{r};\mathbf{K}',E') = (2\pi)^3\delta(E-E')\delta(\mathbf{K}-\mathbf{K}').$$

# Phonon assisted BBT: local model

- considering evanescent states along x and plane waves in the normal direction and assuming uniform field:

$$\chi_{\mathrm{v}}(\mathbf{r};\,\mathbf{K},\,E) = \sqrt{\frac{2\pi}{F x_{\mathrm{v}}^2}}\mathrm{Ai}\left(\frac{x}{x_{\mathrm{v}}} + \frac{E + E_{\mathrm{v}}^{\perp}(\mathbf{K})}{F x_{\mathrm{v}}}\right) e^{\mathrm{i}\mathbf{K}\cdot\mathbf{R}},$$

$$\chi_{\mathrm{c}}(\mathbf{r};\,\mathbf{K},\,E) = \sqrt{\frac{2\pi}{F x_{\mathrm{c}}^2}}\mathrm{Ai}\left(-\frac{x}{x_{\mathrm{c}}} - \frac{E - E_{\mathrm{g}} - E_{\mathrm{c}}^{\perp}(\mathbf{K})}{F x_{\mathrm{v}}}\right) e^{\mathrm{i}\mathbf{K}\cdot\mathbf{R}}$$

$$T_{\mathrm{v}}^{\mathrm{abs,\,em}}(E) \approx \frac{\Omega |M'_{\mathbf{k}_0}|^2 A (m_{\mathrm{c}} m_{\mathrm{v}})^{\frac{3}{2}} F^{\frac{3}{2}}}{2^{\frac{23}{4}} \pi^{\frac{3}{2}} \hbar^{\frac{7}{2}} (E_{\mathrm{g}} \mp \hbar\omega_{\mathbf{k}_0})^{\frac{7}{4}} \bar{m}^{\frac{5}{4}}} \exp\left(-\frac{4}{3}\frac{\sqrt{2\bar{m}}(E_{\mathrm{g}} \mp \hbar\omega_{\mathbf{k}_0})^{\frac{3}{2}}}{F\hbar}\right).$$

$$G_{\mathrm{v,\,Kane}}^{\mathrm{abs,\,em}} = G_0^{\mathrm{abs,\,em}} F^{\frac{5}{2}} \exp\left(-\frac{4}{3}\frac{\sqrt{2\bar{m}_x}(E_{\mathrm{g}} \mp \hbar\omega_{\mathbf{k}_0})^{\frac{3}{2}}}{F\hbar}\right)$$

with

$$G_0^{\mathrm{abs,\,em}} = A g_0 \Omega |M'_{\mathbf{k}_0}|^2 \frac{\sqrt{m_{\mathrm{v},x} m_{\mathrm{v},y} m_{\mathrm{v},z} m_{\mathrm{c},x} m_{\mathrm{c},y} m_{\mathrm{c},z}}}{2^{\frac{27}{4}} \pi^{\frac{5}{2}} \hbar^{\frac{7}{2}} (E_{\mathrm{g}} \mp \hbar\omega)^{\frac{7}{4}} \bar{m}_x^{\frac{5}{4}}}$$

as in Kane/Keldish papers

# Phonon assisted BBT: non-local model

- 1D profile
- evanescent states along *x* (WKB) and plane waves in the normal direction:

$$\chi_{\rm v}(\mathbf{r};\,\mathbf{K},E)=\frac{\exp\left(-\int_{x_{\rm tv}}^{x}{\rm d}x'\sqrt{\frac{2m_{\rm v}}{\hbar^2}(E-U_{\rm ext}(x')+E_{\rm v}^{\perp})}\right)}{\sqrt[4]{\frac{2\hbar^2}{m_{\rm v}}(E-U_{\rm ext}(x)+E_{\rm v}^{\perp})}}e^{{\rm i}\mathbf{K}\cdot\mathbf{R}},$$

$$\chi_{\rm c}(\mathbf{r};\mathbf{K},E)=\frac{\exp\left(\int_{x_{\rm tc}}^{x}{\rm d}x'\sqrt{-\frac{2m_{\rm c}}{\hbar^2}(E-E_{\rm g}-U_{\rm ext}(x')-E_{\rm c}^{\perp})}\right)}{\sqrt[4]{2\frac{\hbar^2}{m_{\rm c}}(E-E_{\rm g}-U_{\rm ext}(x')-E_{\rm c}^{\perp})}}e^{{\rm i}\mathbf{K}\cdot\mathbf{R}}$$

$$G_{\rm v,NU}^{\rm abs,em}=G_0^{\rm abs,em}\frac{\hbar^2(E_{\rm g}\mp\hbar\omega_{\mathbf{k}_0})\bar{m}_x}{m_{{\rm v},x}m_{{\rm c},x}\sqrt{U'_{\rm ext}(x_{\max})}}$$
$$\times\frac{\exp(-2\int_{x_{\rm tv0}}^{x_{\max}}{\rm d}x'\kappa_{\rm c}(x';\,E))}{\int_{x_{\rm tv0}}^{x_{\max}}{\rm d}x'/\kappa_{\rm v}(x';\,E)}$$
$$\times\frac{\exp(2\int_{x_{\rm tc0}}^{x_{\max}}{\rm d}x'\kappa_{\rm v}(x';\,E\pm\hbar\omega_{\mathbf{k}_0}))}{\int_{x_{\rm tc0}}^{x_{\max}}{\rm d}x'/\kappa_{\rm c}(x';\,E\pm\hbar\omega_{\mathbf{k}_0})}$$

with

$$\kappa_{\rm v}(x;\,E)=\sqrt{\frac{2m_{\rm v}}{\hbar^2}(E-U_{\rm ext}(x))},$$

$$\kappa_{\rm c}(x;\,E)=\sqrt{\frac{2m_{\rm c}}{\hbar^2}(E_{\rm g}+U_{\rm ext}(x)-E)}.$$

$$\kappa_{\rm v}(x_{\max}^{\pm};\,E)=\kappa_{\rm c}(x_{\max}^{\pm};\,E\pm\hbar\omega_{\mathbf{k}_0}).$$

$$1/\bar{m}=1/m_{\rm v}+1/m_{\rm c}.$$

somehow similar (but not equal) to the formula in Tanaka paper

# Non-local phonon assisted BBT in TCAD

- example: dynamic non-local model in Sentaurus

$$R_{\mathrm{net}}^{\mathrm{p}} = |\nabla E_{\mathrm{V}}(0)| C_{\mathrm{p}} \exp\left(-2\int_{0}^{x_0} \kappa_{\mathrm{V}} dx - 2\int_{x_0}^{l} \kappa_{\mathrm{C}} dx\right)\left[\left(\exp\left[\frac{\varepsilon - E_{\mathrm{F},n}(l)}{kT(l)}\right] + 1\right)^{-1} - \left(\exp\left[\frac{\varepsilon - E_{\mathrm{F},p}(0)}{kT(0)}\right] + 1\right)^{-1}\right] \quad (385)$$

$$C_{\mathrm{p}} = \int_{0}^{l} \frac{g(1+2N_{\mathrm{op}})D_{\mathrm{op}}^{2}}{2^{6}\pi^{2}\rho\varepsilon_{\mathrm{op}}E_{\mathrm{g,tun}}} \sqrt{\frac{m_{\mathrm{V}}m_{\mathrm{C}}}{hl\sqrt{2m_{\mathrm{r}}E_{\mathrm{g,tun}}}}}\, dx \left(\int_{0}^{x_0} \frac{dx}{\kappa_{\mathrm{V}}}\right)^{-1} \left(\int_{x_0}^{l} \frac{dx}{\kappa_{\mathrm{C}}}\right)^{-1} \left[1 - \exp\left(-k_{\mathrm{vm}}^{2} \int_{0}^{x_0} \frac{dx}{\kappa_{\mathrm{V}}}\right)\right] \left[1 - \exp\left(-k_{\mathrm{cm}}^{2} \int_{x_0}^{l} \frac{dx}{\kappa_{\mathrm{C}}}\right)\right] \quad (386)$$

$$\kappa_{\mathrm{V}} = \frac{1}{\hbar}\sqrt{2m_{\mathrm{V}}|\varepsilon - E_{\mathrm{V}}|}\,\Theta(\varepsilon - E_{\mathrm{V}})$$

$x_0$ is the location where $\kappa_{\mathrm{V}} = \kappa_{\mathrm{C}}$.

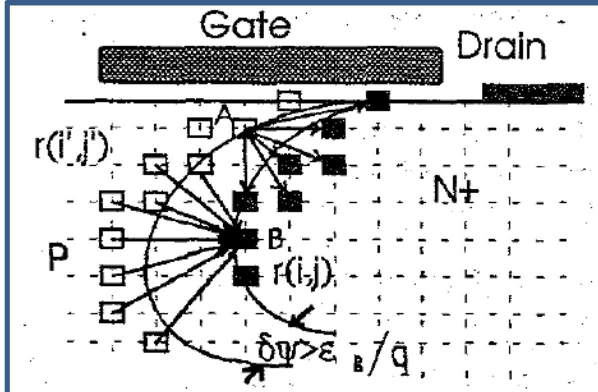
$$\kappa_{\mathrm{C}} = \frac{1}{\hbar}\sqrt{2m_{\mathrm{C}}|E_{\mathrm{C}} + \Delta_{\mathrm{C}} - \varepsilon|}\,\Theta(E_{\mathrm{C}} + \Delta_{\mathrm{C}} - \varepsilon)$$

# OUTLINE

- band-to-band tunneling current
- direct tunneling:
  - local model
  - non-local model
- phonon assisted tunneling
- **tunneling path**
- impact of size-induced quantization
- application examples

# The concept of *Tunneling path* (1)

- when going from 1D analysis to 2D devices one needs to define a tunneling path.
- Many possible approaches:
  - horizontal path (assumes tunneling is 1D from S to D)
  - shortest path btw VB and CB
  - gradient of the VB
  - semiclassical path
  - multiple path




all tunneling paths that fulfill the condition $\Delta V = E_G$ [Peng]

Follow the classical path (minimum action) and integrate the equations of motion in the gap (imaginary K) [Fischetti07]

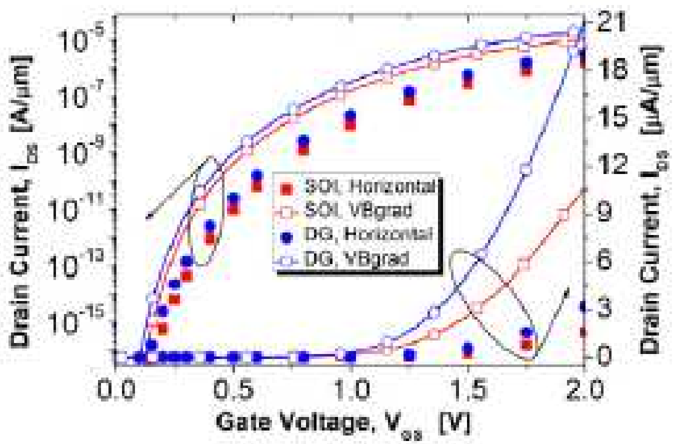
$$\frac{d\mathbf{r}}{dt} = \mathbf{v}\left[\mathbf{k}(t)\right] \qquad \frac{d\mathbf{k}}{dt} = -\frac{e}{\hbar}\mathbf{F}\left[\mathbf{r}(t)\right].$$

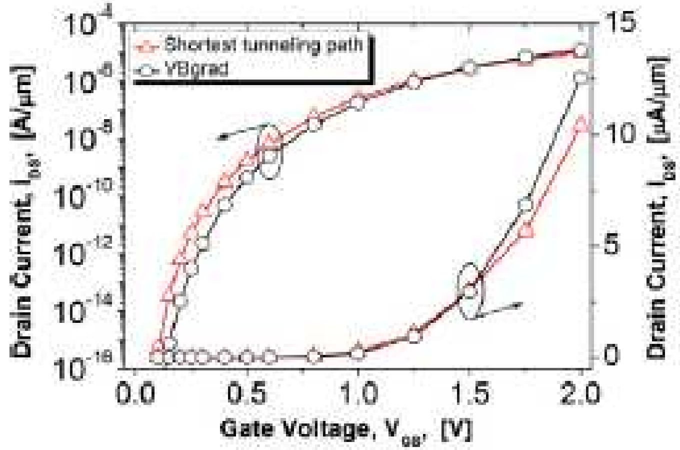
# The concept of *Tunneling path* (2)

Solid-State Electronics 71 (2012) 7–12

Effect of the choice of the tunnelling path on semi-classical numerical simulations of TFET devices

Luca De Michielis [a,b,*], Matteo Iellina [b], Pierpaolo Palestri [b], Adrian M. Ionescu [a], Luca Selmi [b]




- shortest path: highest current
- horizontal path: lowest current
- what’s the best one ? Comparison with full-quantum would be needed BUT … see next point …

# OUTLINE

- band-to-band tunneling current
- direct tunneling:
  - local model
  - non-local model
- phonon assisted tunneling
- tunneling path
- **impact of size-induced quantization**
- application examples

# Phonon assisted BBT: full 2D model (1)

- use directly the solution of the 2D Schrödinger equation to obtain the spectral functions *A*

IEDM11-99

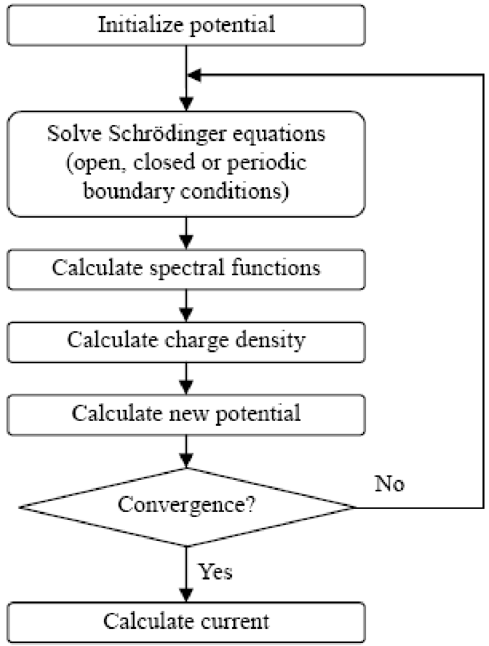
**Two-Dimensional Quantum Mechanical Modeling of Band-to-Band Tunneling in Indirect Semiconductors**

William G. Vandenberghe[1,2], Bart Sorée[1,3], Wim Magnus[1,3], Massimo V. Fischetti[4], Anne S. Verhulst[1] and Guido Groeseneken[1,2]

$$T_{\mathrm{v}}^{\mathrm{abs,em}}(\mathbf{R};E) = \Omega\,|M_0|^2 \sum_{\alpha,\alpha'} A_{\mathrm{v}\alpha}(\mathbf{r},\mathbf{r};E) \times A_{\mathrm{c}\alpha'}(\mathbf{r},\mathbf{r};E \pm \hbar\omega_0) \quad (\Omega = \text{total volume}), \quad (5)$$

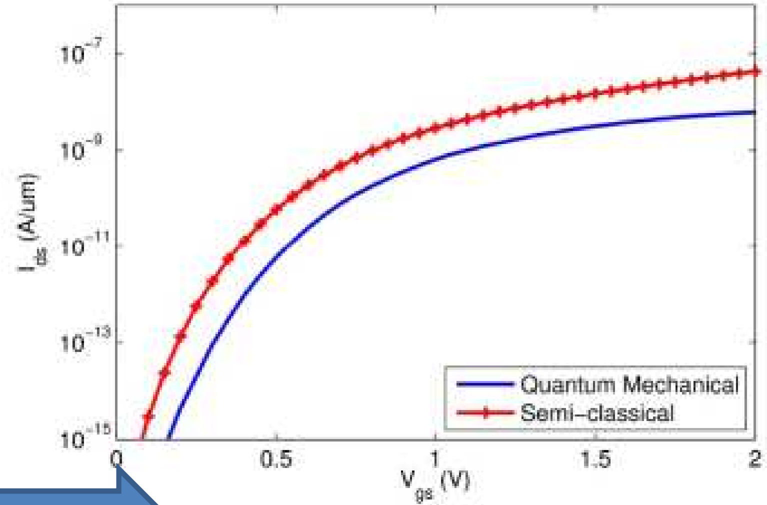
$$G(\mathbf{R}) = -\frac{2}{\hbar}\int \frac{\mathrm{d}E}{2\pi}\Big(\big(f_{\mathrm{v}}(E)(1-f_{\mathrm{c}}(E-\hbar\omega_0))(\nu(\hbar\omega_0)+1) - f_{\mathrm{c}}(E-\hbar\omega_0)(1-f_{\mathrm{v}}(E))\nu(\hbar\omega_0)\big)T_{\mathrm{v}}^{\mathrm{em}}(\mathbf{R};E) + \big(f_{\mathrm{v}}(E)(1-f_{\mathrm{c}}(E+\hbar\omega_0)\nu(\hbar\omega_0) - f_{\mathrm{c}}(E+\hbar\omega_0)(1-f_{\mathrm{v}}(E))(\nu(\hbar\omega_0)+1)\big)T_{\mathrm{v}}^{\mathrm{abs}}(\mathbf{R};E)\Big), \quad (6)$$

$$I_{\mathrm{ds}} = qW\int \mathrm{d}^2R\, G(\mathbf{R}). \quad (7)$$



# Phonon assisted BBT: full 2D model (2)

- in principle it is a full-quantum model
- limit (w.r.t. other full quantum approaches):
  - it assumes equilibrium, i.e. BBT is not perturbing the potential profile and the charge distribution
- advantages (w.r.t. TCAD):
  - no need to define a tunneling path
  - size and bias-induced quantization are accounted for




differences w.r.t. non-local model in TCAD

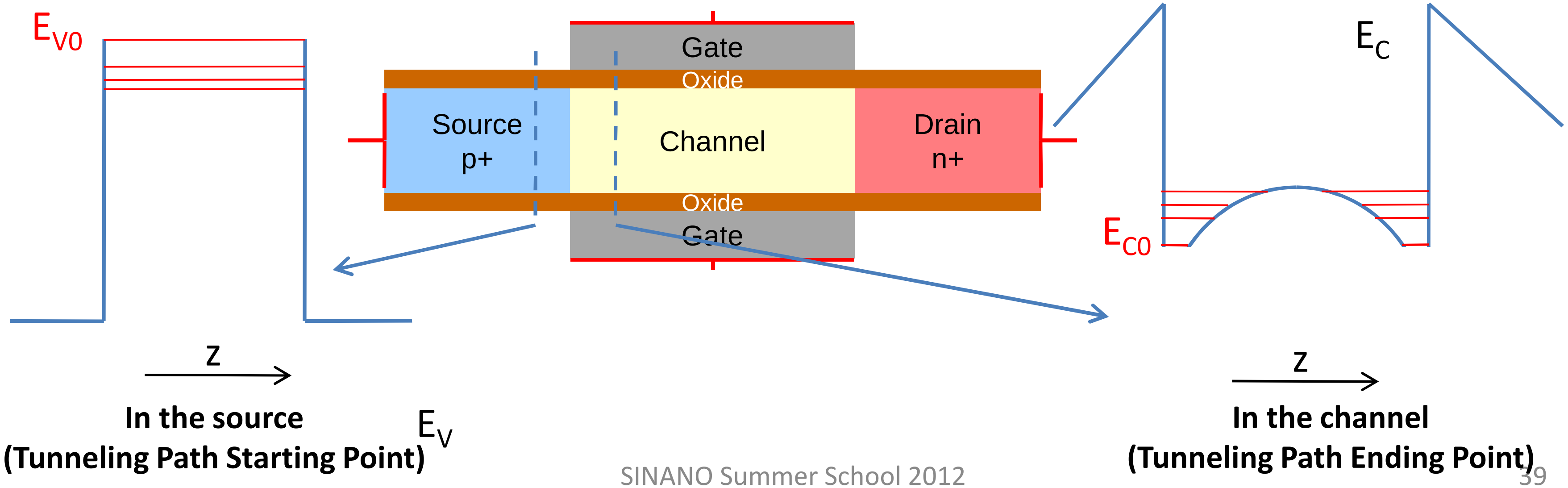
# Alternative approach to include quantization (1)

**Multi-Subband Semi-classical Simulation of n-type Tunnel-FETs**

ULIS 2012

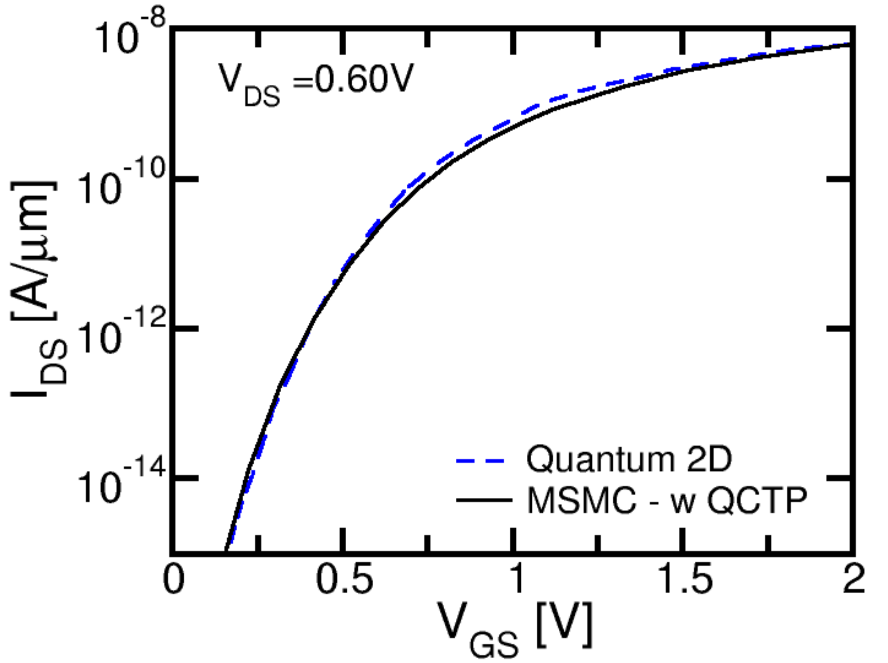
A. Revelant, P. Palestri and L. Selmi

- non-local tunneling path (as in TCAD) with effective gap from solution of 1D Schrödinger equation in each section
- cut everything in the VB above $E_{v0}$ and everything in CB below $E_{c0}$



# Alternative approach to include quantization (2)

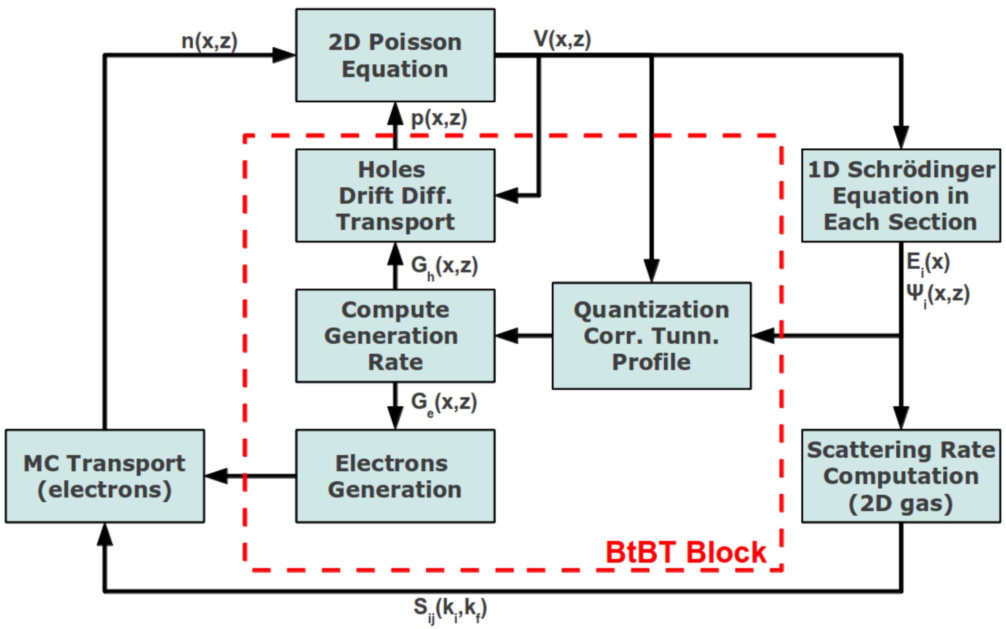
- good agreement vs. full 2D model [VandenbergheIEDM2011]



# OUTLINE

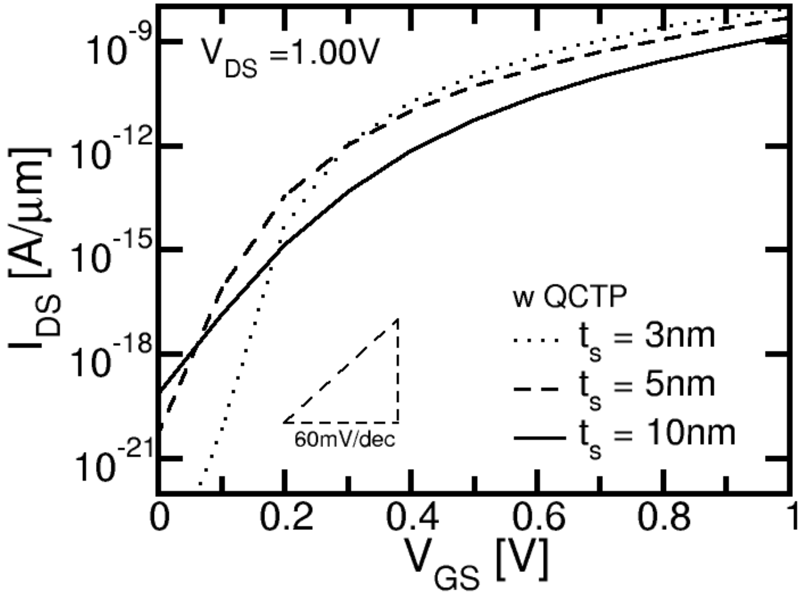
- band-to-band tunneling current
- direct tunneling:
  - local model
  - non-local model
- phonon assisted tunneling
- tunneling path
- impact of size-induced quantization
- **application examples**

# Modeling framework




- planar devices (uniform in the W direction)
- 2D carrier gas (inversion layer)
- MC transport of the generated electrons
- DD transport (with $v_{sat}$) of the generated holes
- BBT generation as in TCAD but with corrections to the tunneling profile

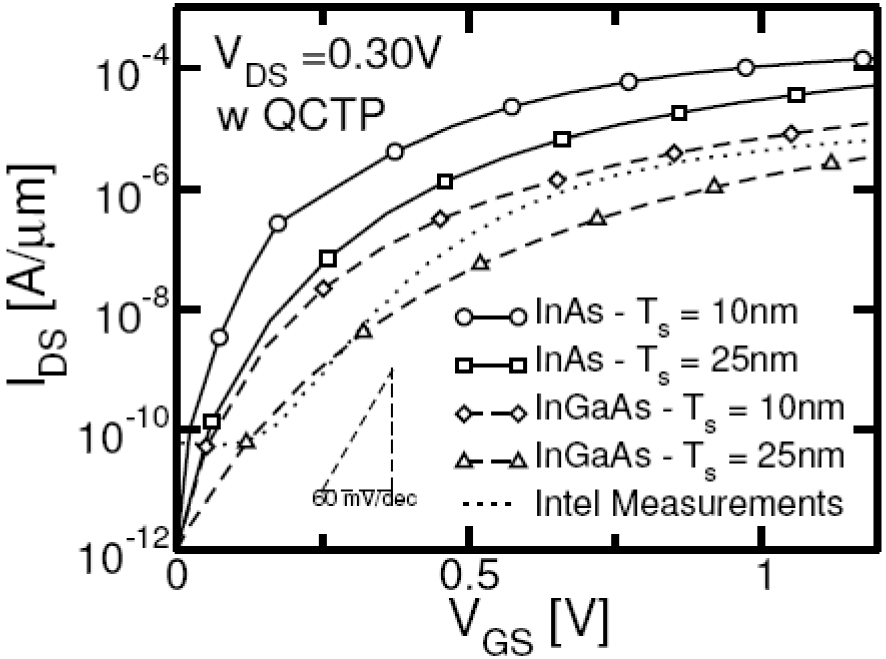
# Application example: SiOI TFETs




| $T_{Si}$ [nm] | EOT [nm] | SS [mV/dec] |
|---|---|---|
| 3 | 0.7 | 21 |
| 5 | 0.9 | 23 |
| 10 | 1.1 | 44 |

when $T_{si}$ is scales, electrostatic integrity wins vs. increased gap [Revelant, submitted to SSE]

# Application example: III-VTFETs




- Large $I_{on}$ in III-V channels.
- Scaling of $T_s$ helps

[Revelant, submitted to SSE] experiments from [Dewey,IEDM 2011]

# Summary and open issues

- important ingredients of BBT models are
  - band structure (EMA, Kane's relation…)
  - dimensionality of the gas (TCAD models only for 3D gas, so far)
  - local vs. non-local
- quantization effects "normal" to tunneling can be relevant
- choice of the tunneling path is not trivial in semiclassical models → benchmarking vs. full quantum will be needed
- trap-assisted BBT may be relevant in real devices but only local models are available
- direct and phonon assisted BBT are two separate process: how to "merge" them ? Relevant situations:
  - Ge (direct gap not too larger than indirect one)
  - hetero-junctions btw III-V  and indirect gap (e.g. InAs-Si nanowires)

# Assignment

- following the treatment in slides 9-14 (Kane's model for the 3D gas), demonstrate the expression in slide 15 for the 1D gas (assuming a single subband)
- Hint: essentially, all relevant formulas are in slide 14, just consider that $\boldsymbol{k}_{\perp}$ does not exist in a 1D gas (but it is not just putting $\boldsymbol{k}_{\perp}=0$ ...)