NEMO1D:

Hole Bandstructure in Quantum Wells and Hole Transport in RTDs

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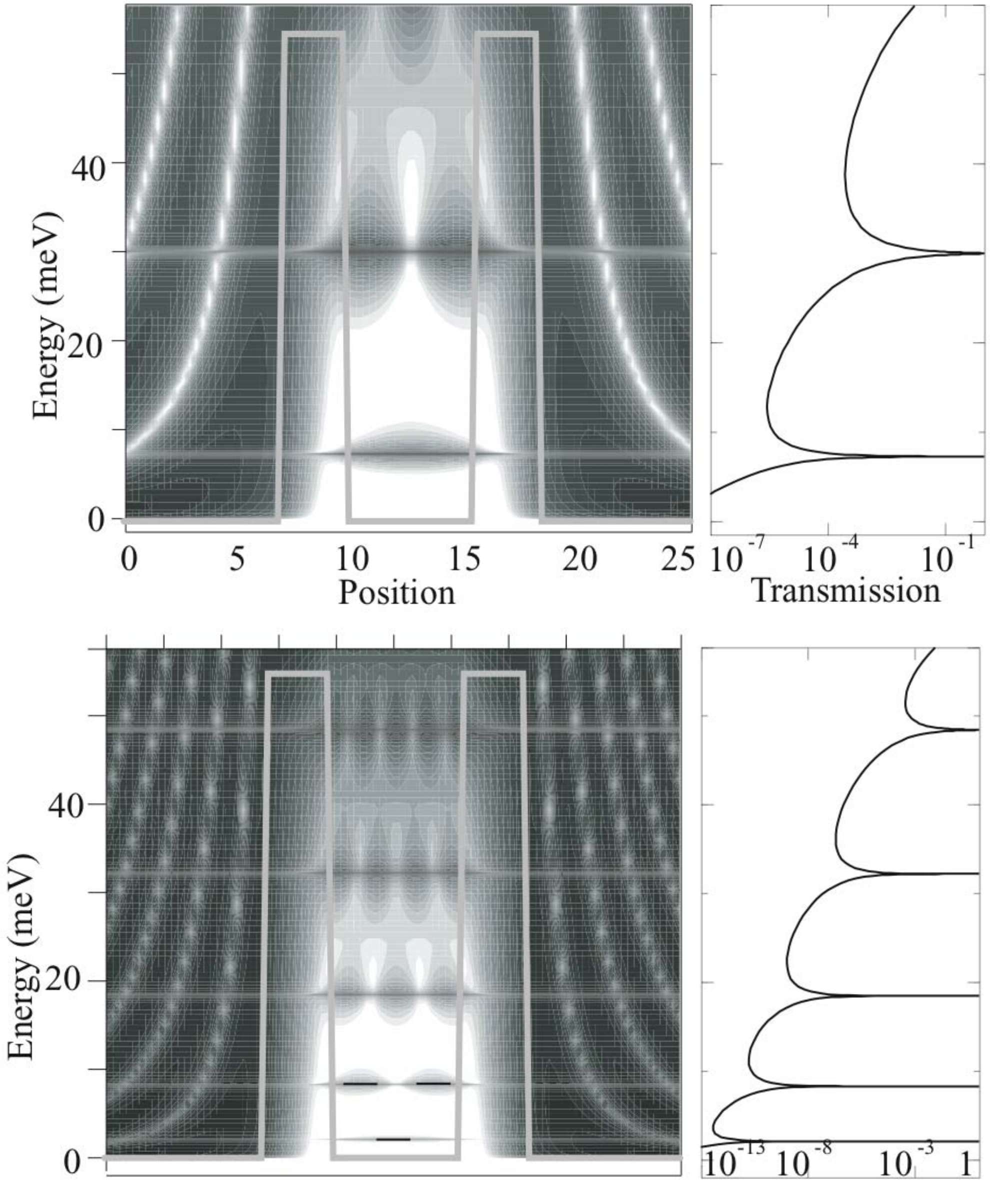
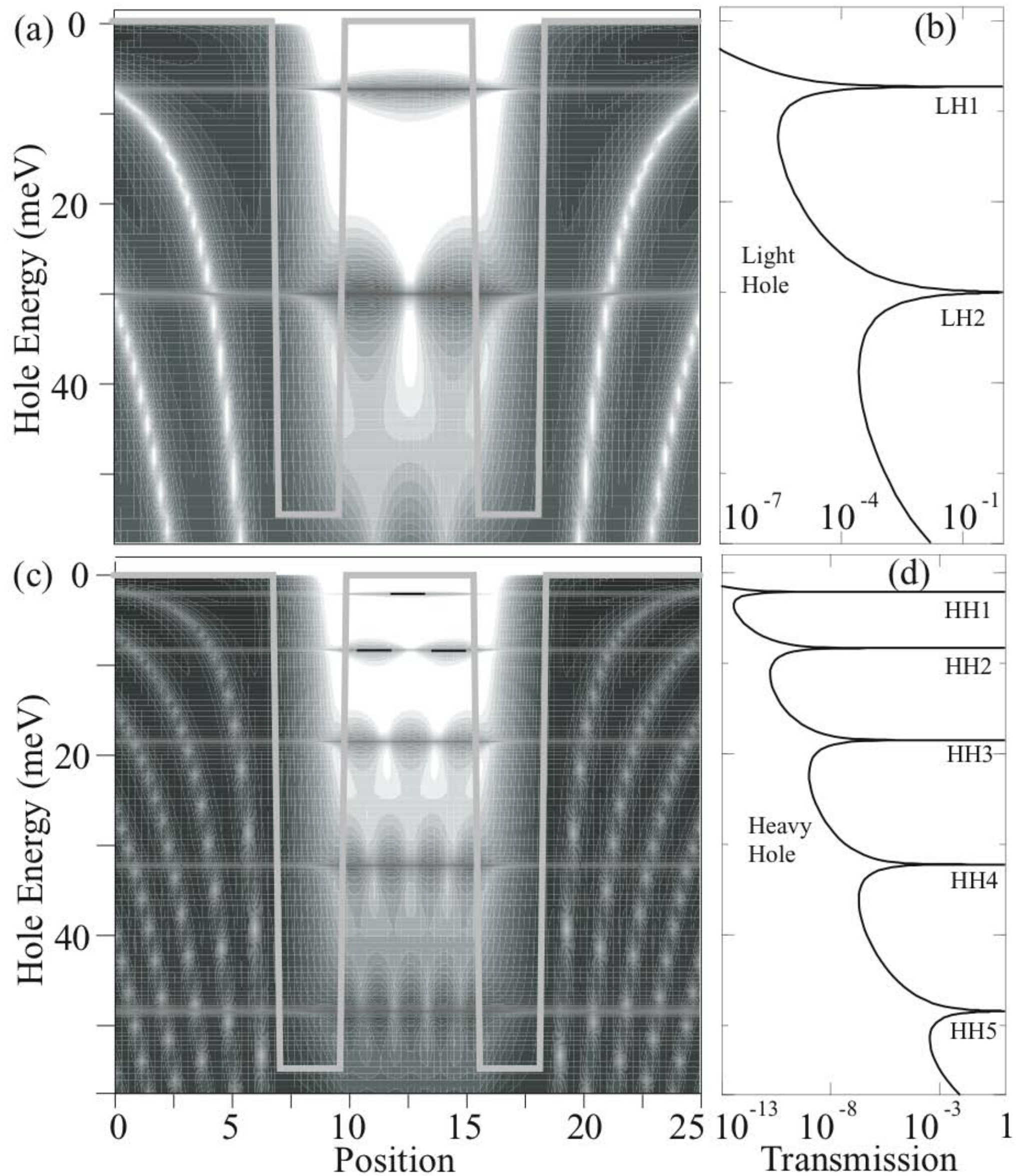
Electron transport in RTDs: Density of States and Transmission



- Density of States:
  Shows the
  spatial and
  energetic “location”
  of possible states
- Transmission:
  shows spikes where the
  DOS is strong in the central RTD
- Small effective mass:
  large state separation
- Large effective mass:
  “heavy” electrons
  - » small state separation
  - » Sharp peaks - strong confinement
    weak coupling to outside
  - » Deep background/peak ratio: 10^{13}
    strong confinement
    weak coupling to outside

Hole transport in RTDs: Simplified Density of States and Transmission



- Holes

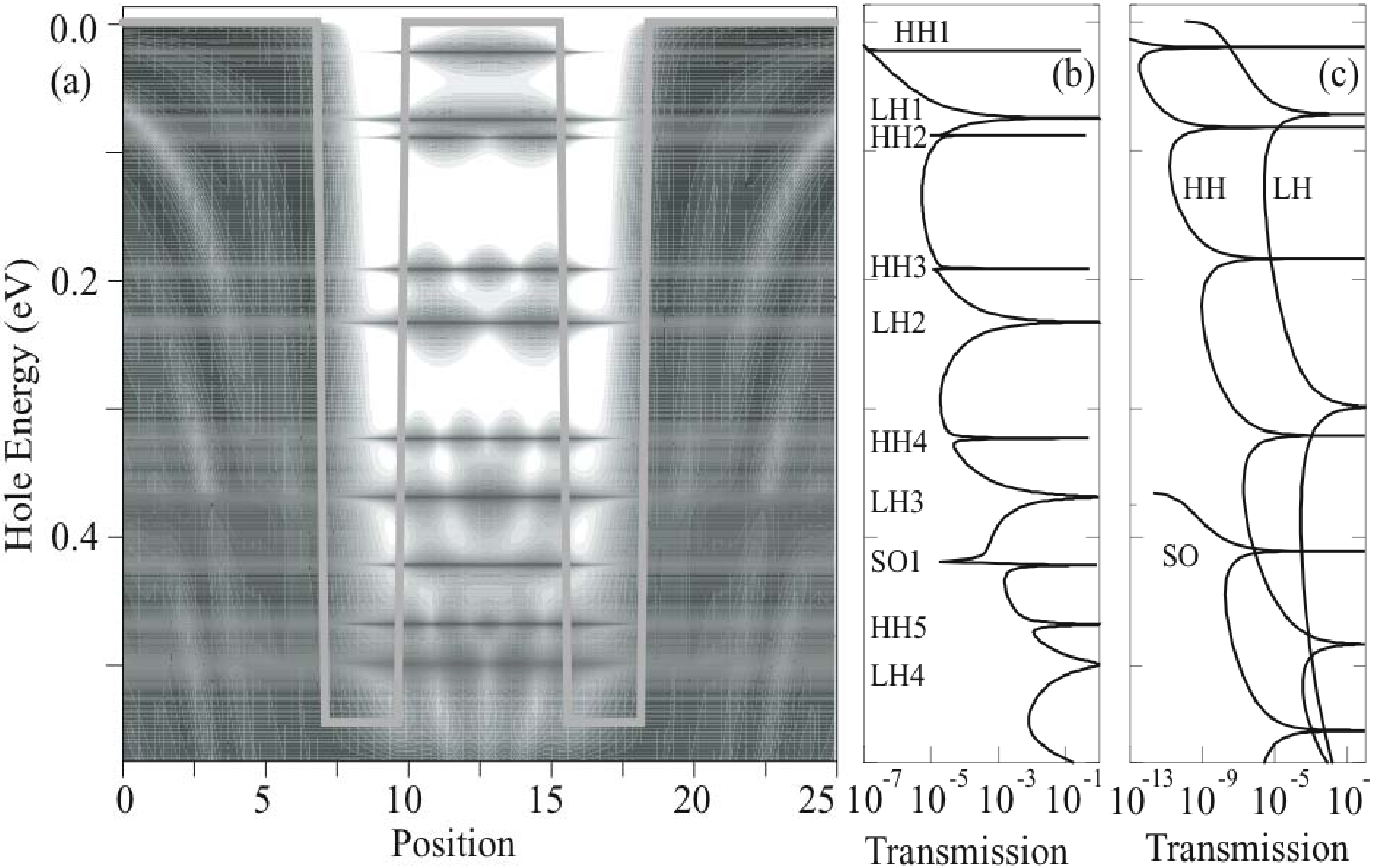
  Are just

  electrons

  upside-down????

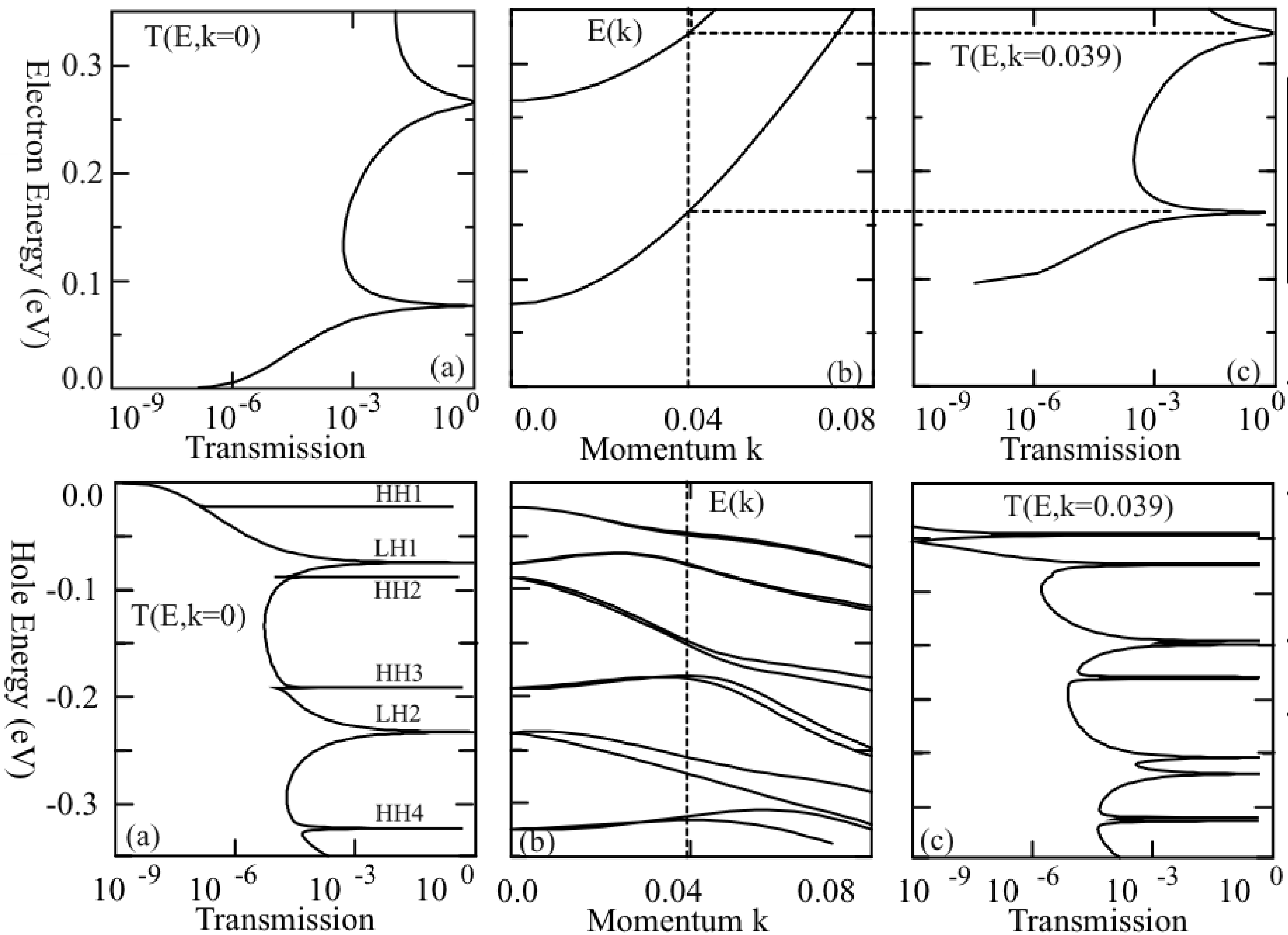
- Not quite!
  - » LH and HH are coupled
  - » Highly non-parabolic dispersion
  - » Highly anisotropic dispersion
- Very unintuitive transport behavior!

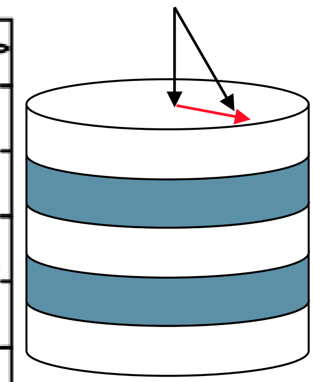
Hole Transport in RTDs sp3s* full band model



- Transmission coefficient at k_x=0
- sp^3s^* represents all bands simultaneously. Can identify LH, HH, and SO features

Dispersion in the Transverse Direction Electron vs. Hole Subbands





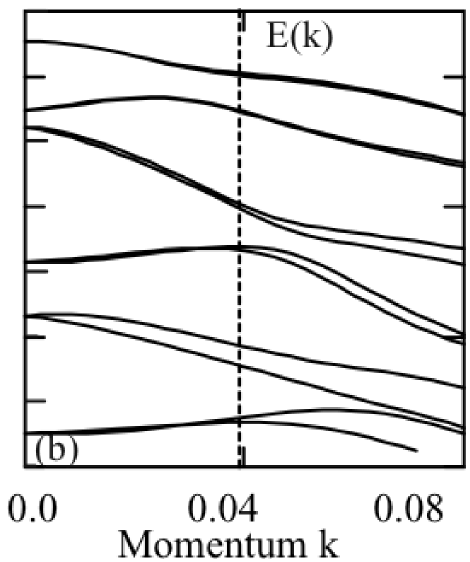
Electron:

- Dispersion "simple", almost parabolic
- Transmission simple "replica"

Holes:

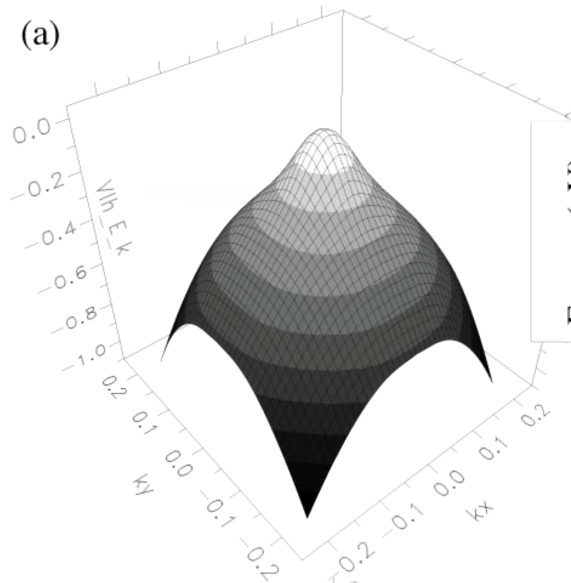
- Dispersion "complicated"
- Transmission dramatically altered

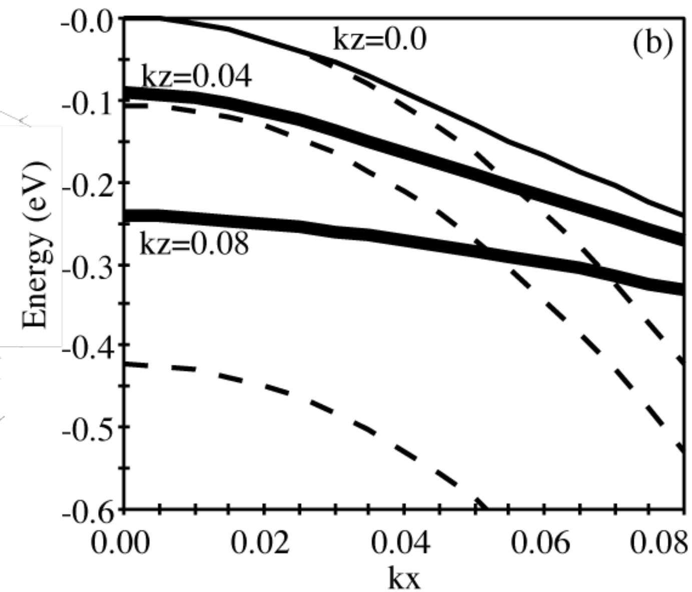
Where does this dispersion come from?

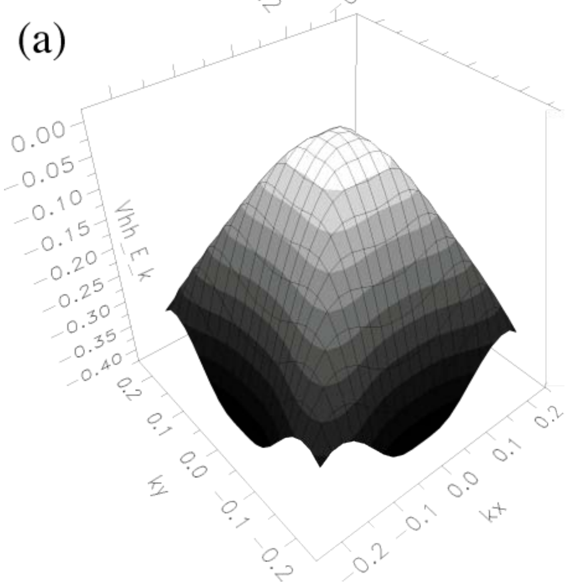


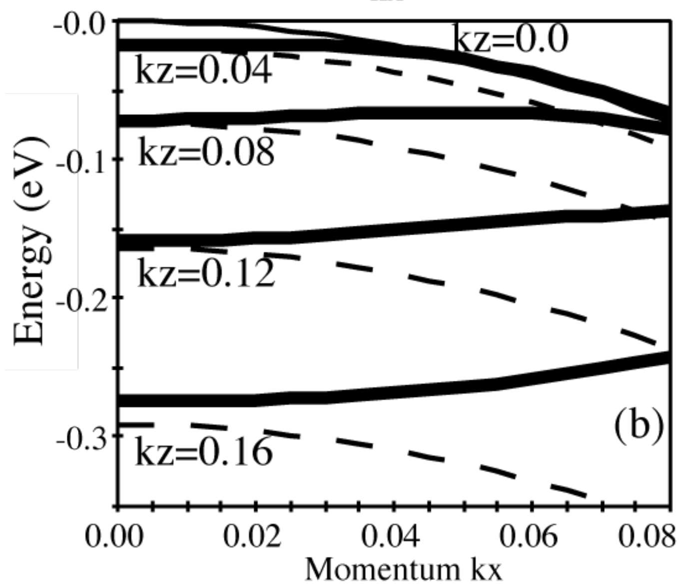
Property	GaAs exp.	GaAs sim.
E_g^{Γ}	1.4240	1.4240
Δ_{so}	0.3400	0.3664
m_{Γ}^*	0.0670	0.0679
$m_{lh}^*[001]$	-0.0871	-0.0708
$m_{lh}^*[011]$	-0.0804	-0.0662
$m_{lh}^*[111]$	-0.0786	-0.0649
$m_{hh}^*[001]$	-0.4030	-0.4105
$m_{hh}^*[011]$	-0.6600	-0.6929
$m_{hh}^*[111]$	-0.8130	-0.8750
m_{so}^*	-0.1500	-0.1440

HH and LH dispersions in bulk









LH band non-parabolic

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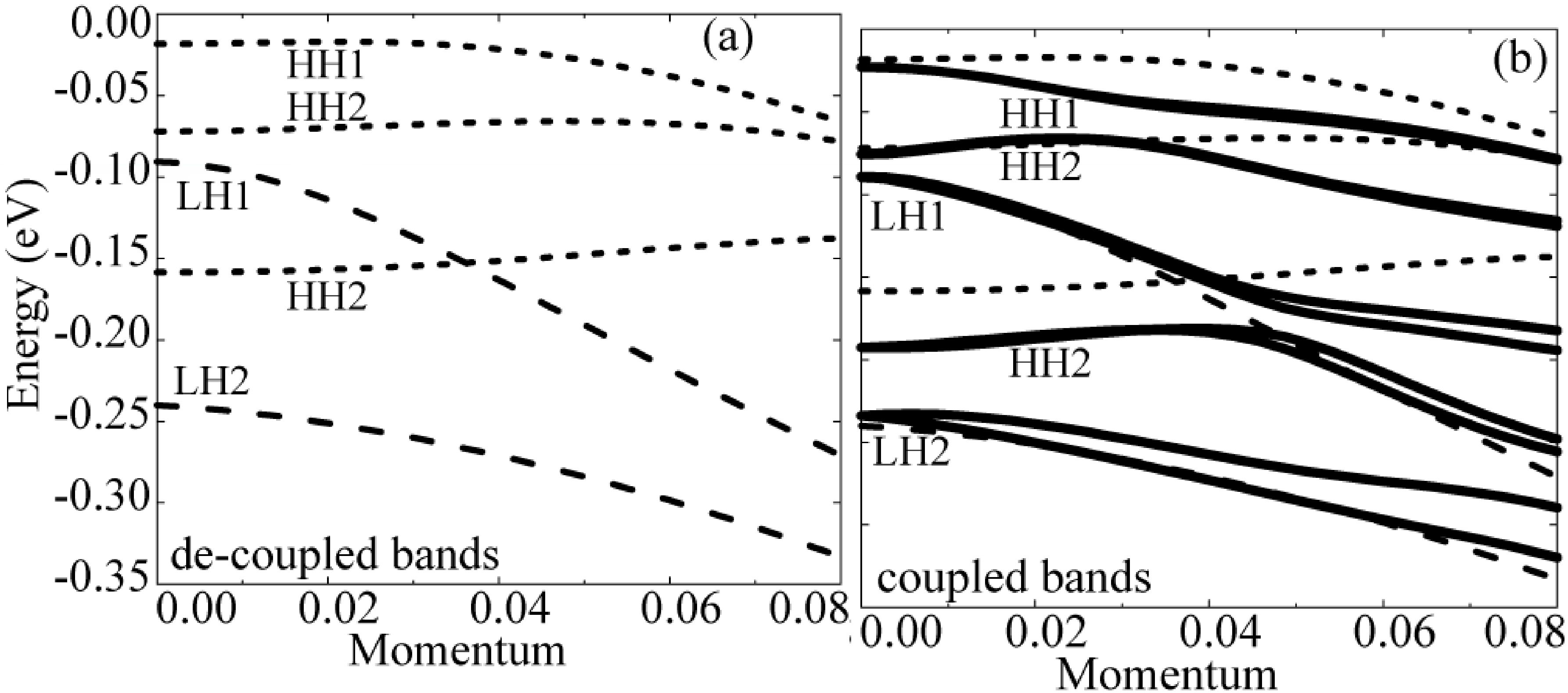
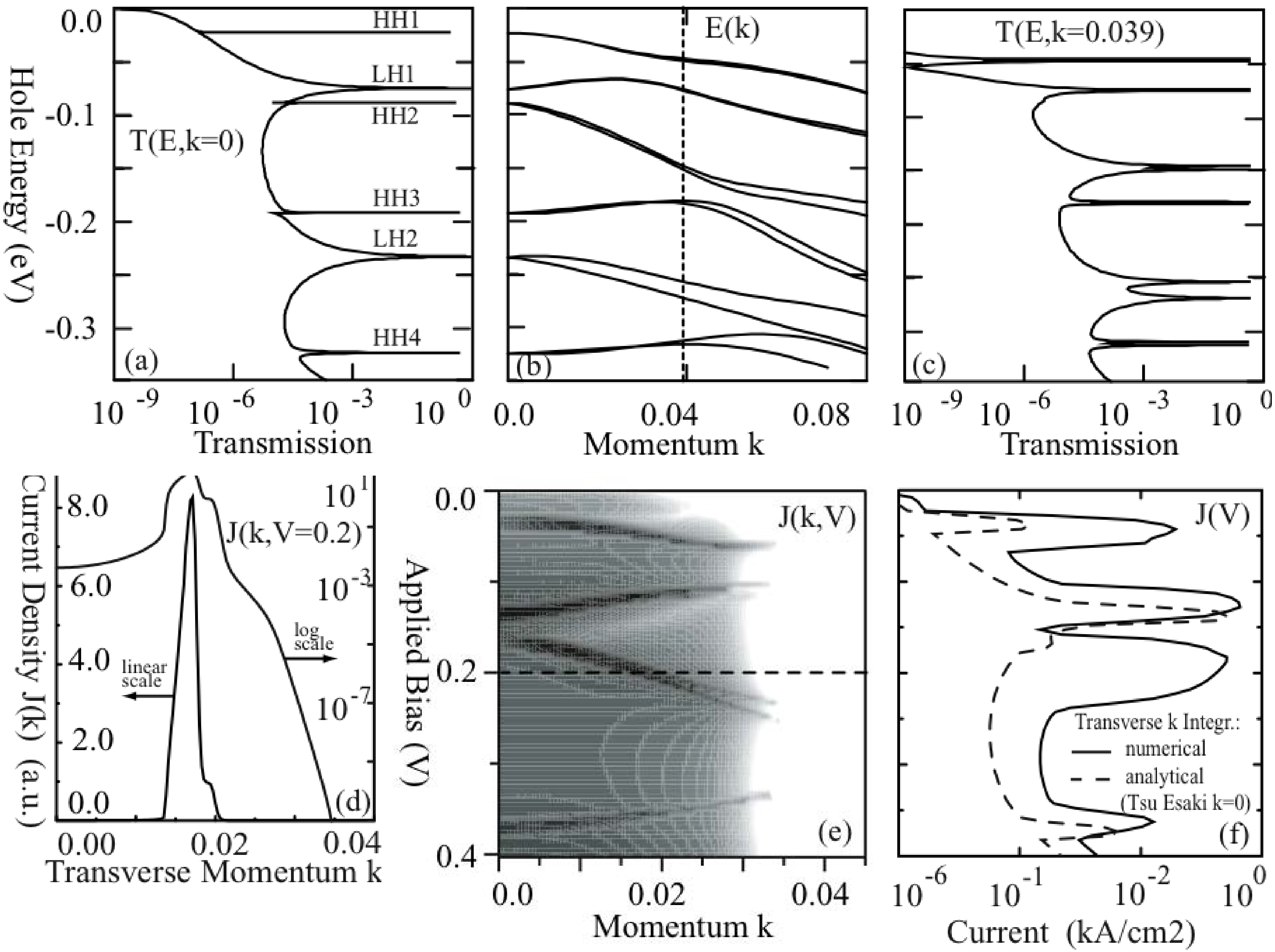
LH band strongly anisotropic
=> Electron-like

Bulk Quantized Dispersions vs. Coupled Bands



- Plot on the left:
  - » overlay the bulk quantized HH and LH dispersions
- Plot on right:
  - » Dashed, same as left
  - » Solid, coupled bands in a RTD simulation

Bulk Quantized Dispersions vs. Coupled Bands



Transport via Transmission Coefficients

$$I \propto \int dk_x \int dk_y \int dE\, T\left(E, k_x, k_y\right)\left(f_L(E) - f_R(E)\right)$$

Cylindrical Coordinates

$$I \propto \int d\varphi \int k\, dk \int dE\, T\left(E, k, \varphi\right)\left(f_L(E) - f_R(E)\right)$$

Throw out angular dependence

$$I \propto 2\pi \int k\, dk \int dE\, T\left(E, k\right)\left(f_L(E) - f_R(E)\right)$$

Parabolic transverse subbands

$$I \propto \rho_{2D} \int T\left(E\right)\left(f_L(E) - f_R(E)\right)$$

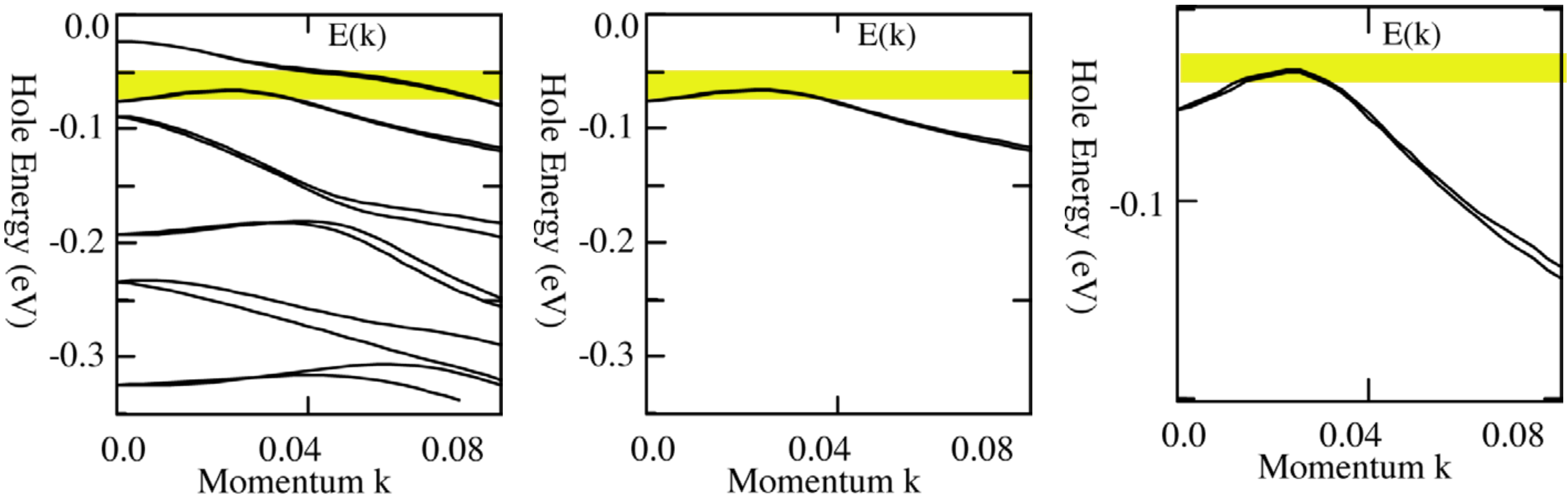
Electron-like Dispersion in second subband

$$I \propto \int kdk \int dE\,T(E,k)\left(f_L(E) - f_R(E)\right)$$

$$I \propto \int kdk\,J(k)$$

$$J(k)$$

Non-monotonic (electron-like) dispersion can dip back into the Fermi sea



Electron-like Dispersion injected with with holes from emitter

$$I \propto \int kdk \int dE\, T(E,k)\left(f_L(E) - f_R(E)\right)$$

$$I \propto \int kdk\, J(k)$$

$J(k)$

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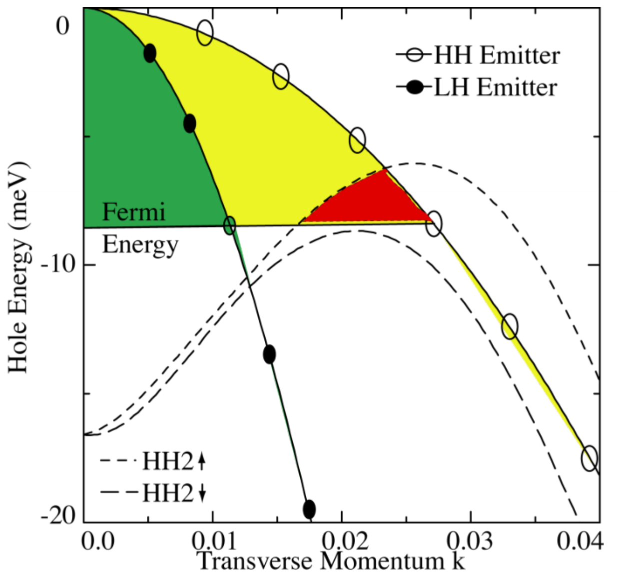
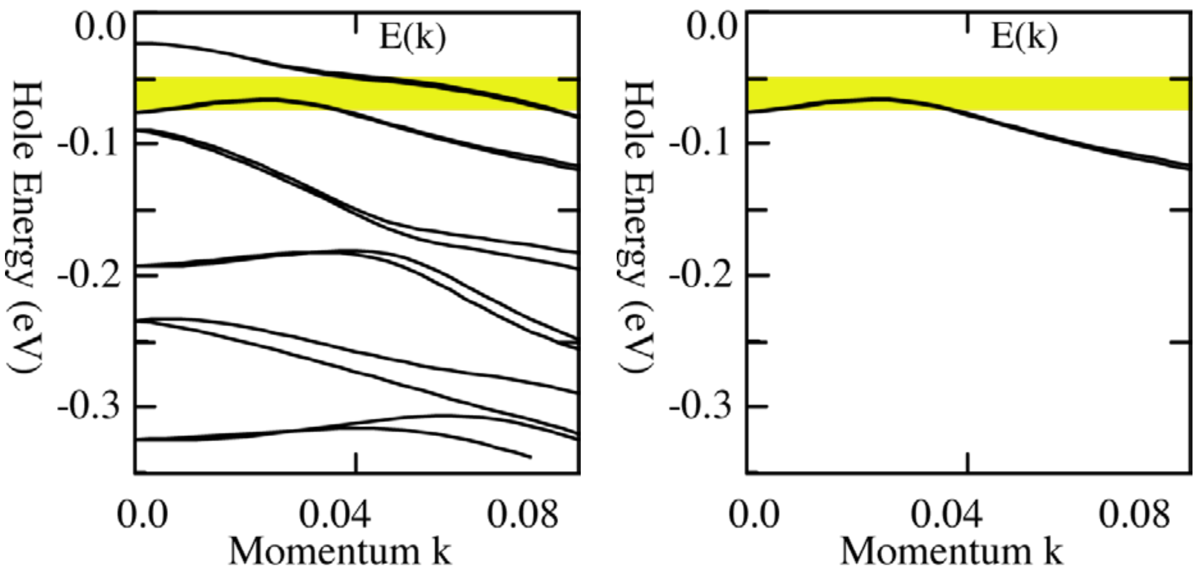
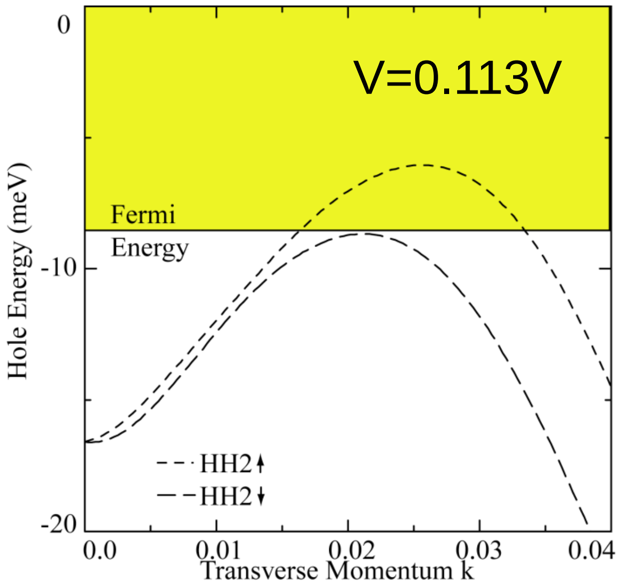






Electron-like Dispersion results in off-zone center flow

$$I \propto \int k\,dk \int dE\,T(E,k)\left(f_L(E) - f_R(E)\right)$$

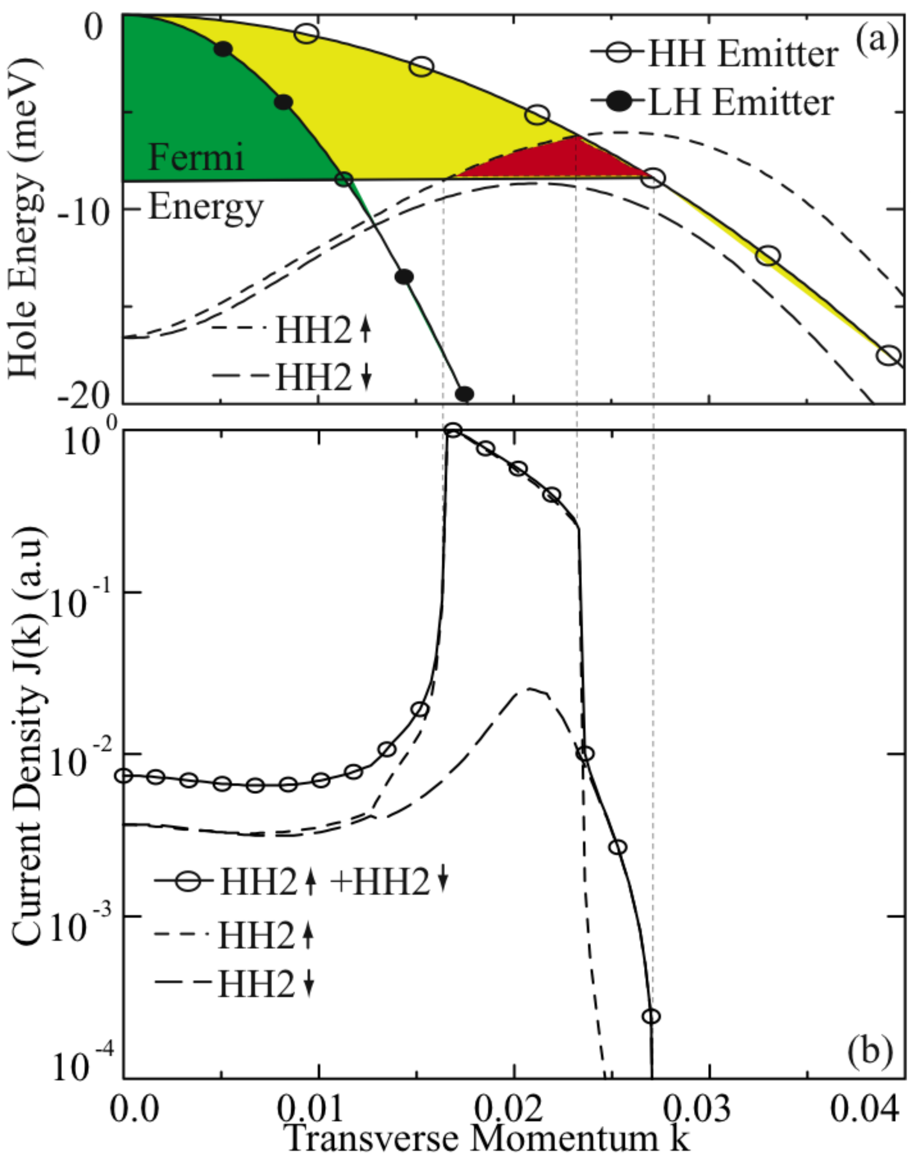
$$I \propto \int k\,dk\,J(k)$$

$J(k)$

- J(k) can be sharply peaked away from k=0

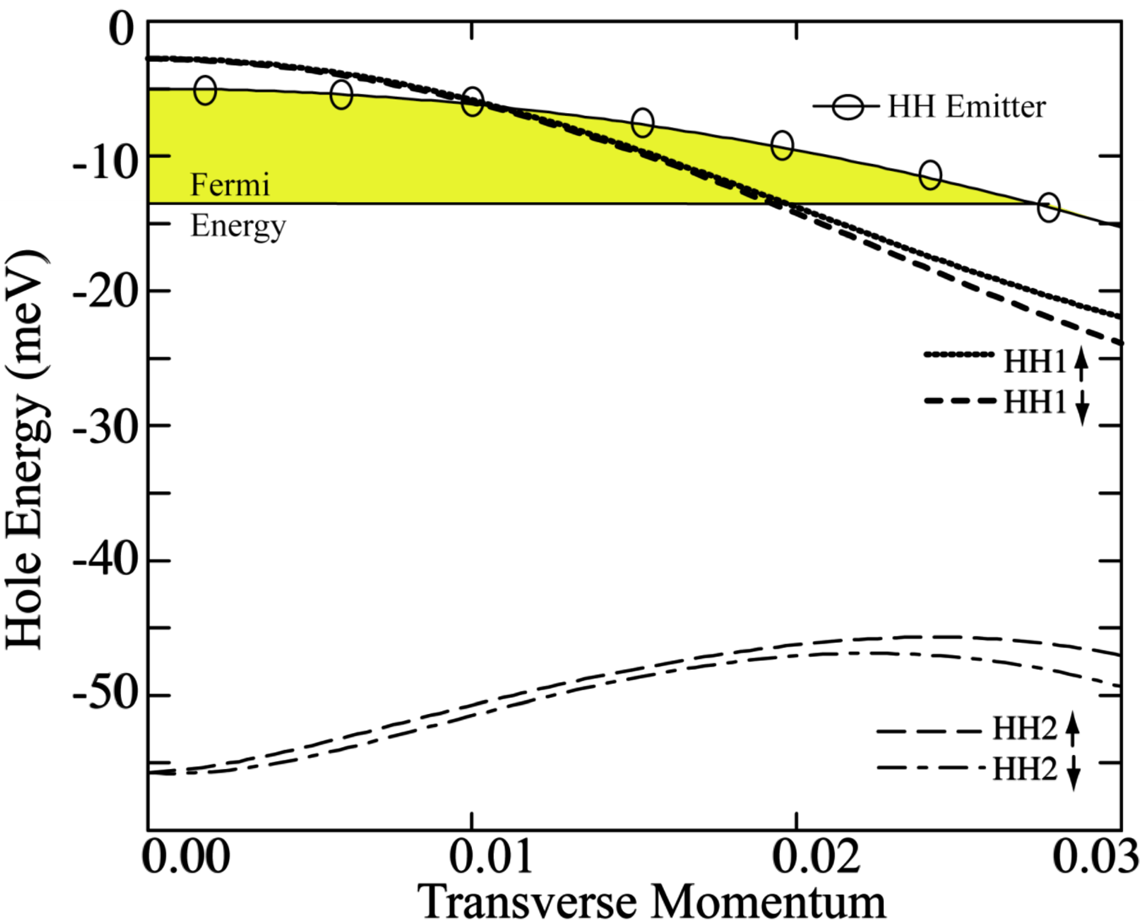
=> off-zone center current

- More electrons flow through an angle than straight through



Off-zone-center current: different $m^*_{emitter} > m^*_{RTD}$

- HH1 is mixture of the bulk HH and LH bands
- $m^*_{HH1} < m^*_{HH}$
- Surprising energy crossings

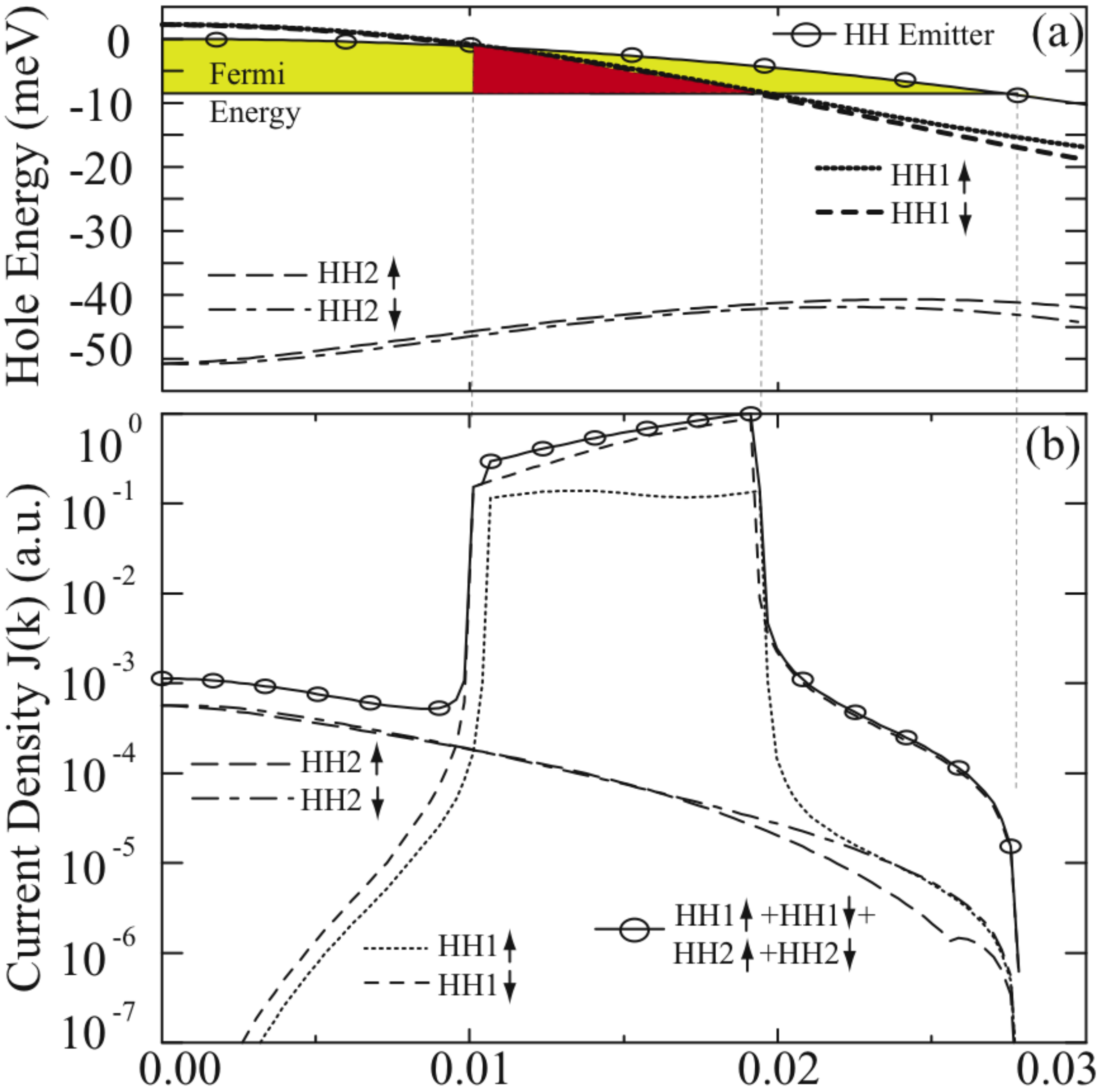


Off-zone-center current: different $m^*_{emitter} > m^*_{RTD}$

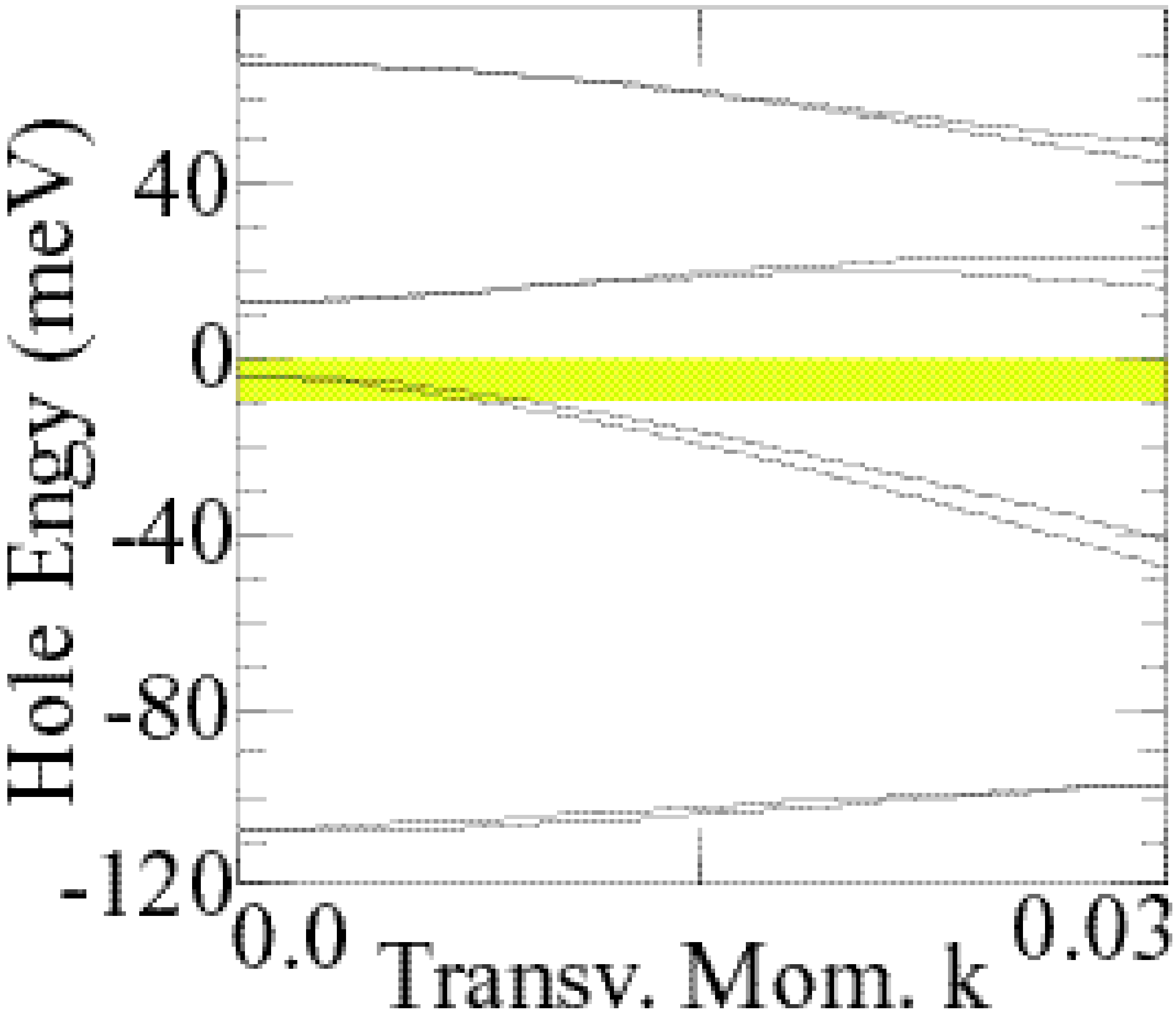
- HH1 is mixture of the bulk HH and LH bands
- $m^*_{HH1} < m^*_{HH}$
- Surprising energy crossings

- Current flow peaked at k>0
- Back ground provided by HH2

$J(k)$

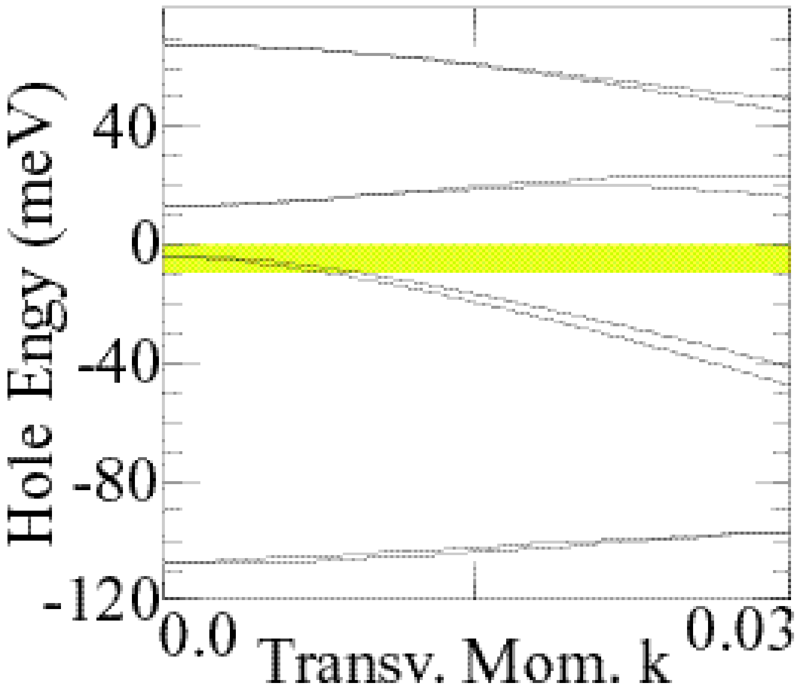


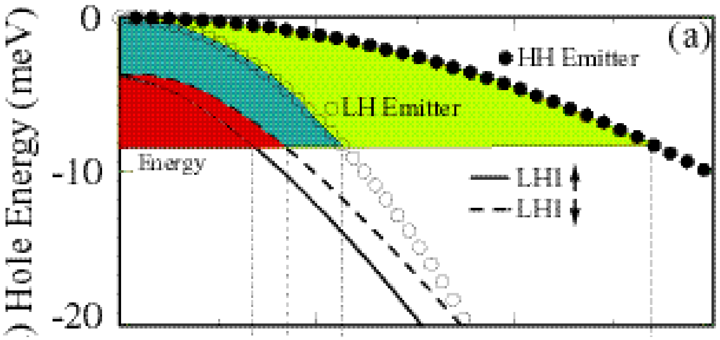
Off-zone-center current: Resonance Width Modulation



Off-zone-center current: Resonance Width Modulation

anti-crossing modulates resonance width





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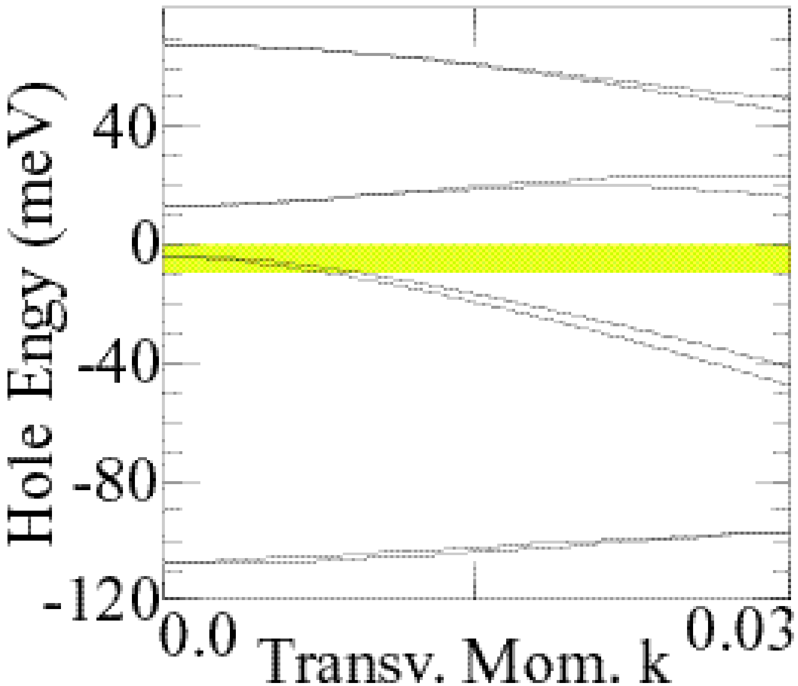
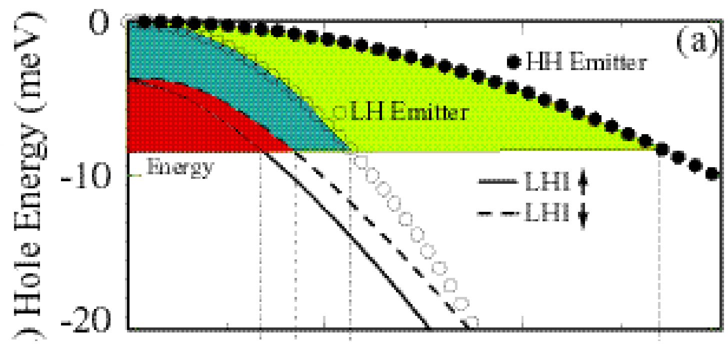
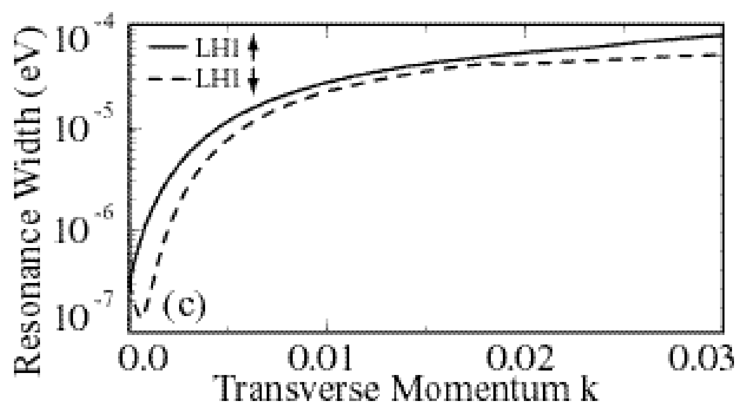
anti-crossing modulates resonance width







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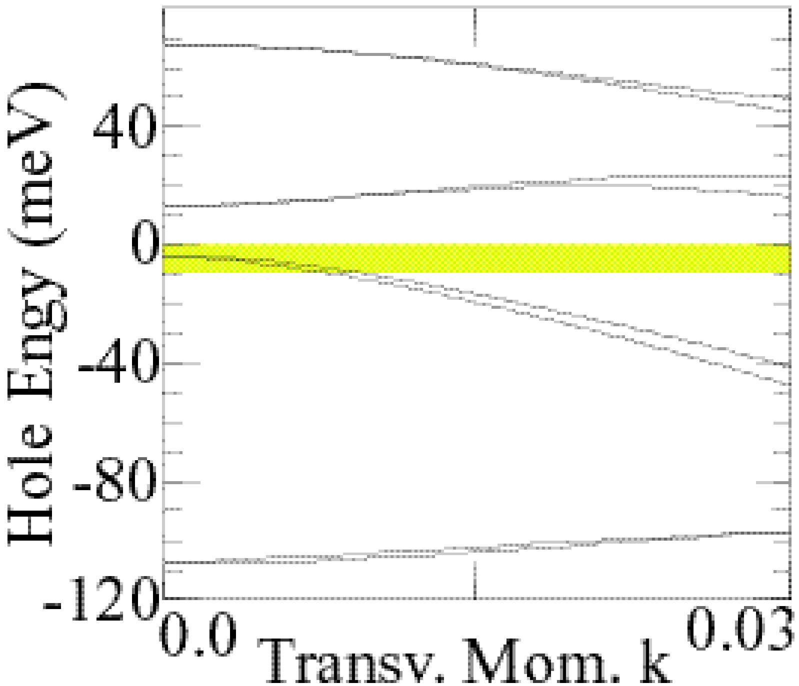

$J(k)$

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away from k=0

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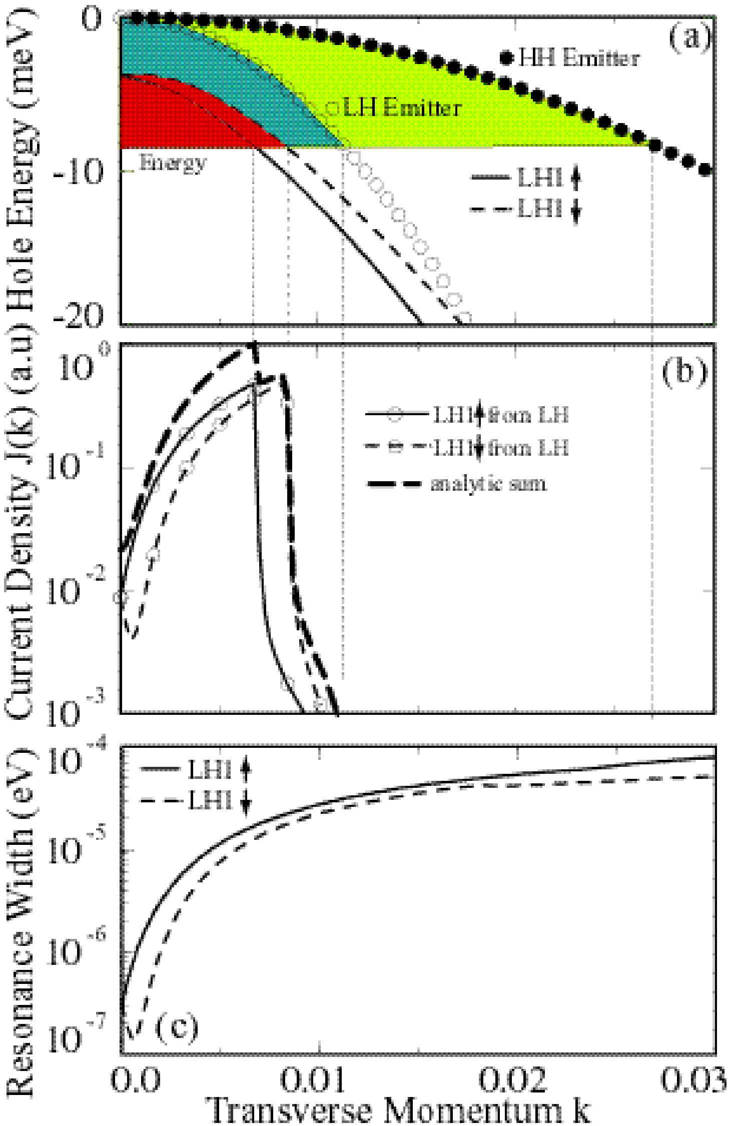
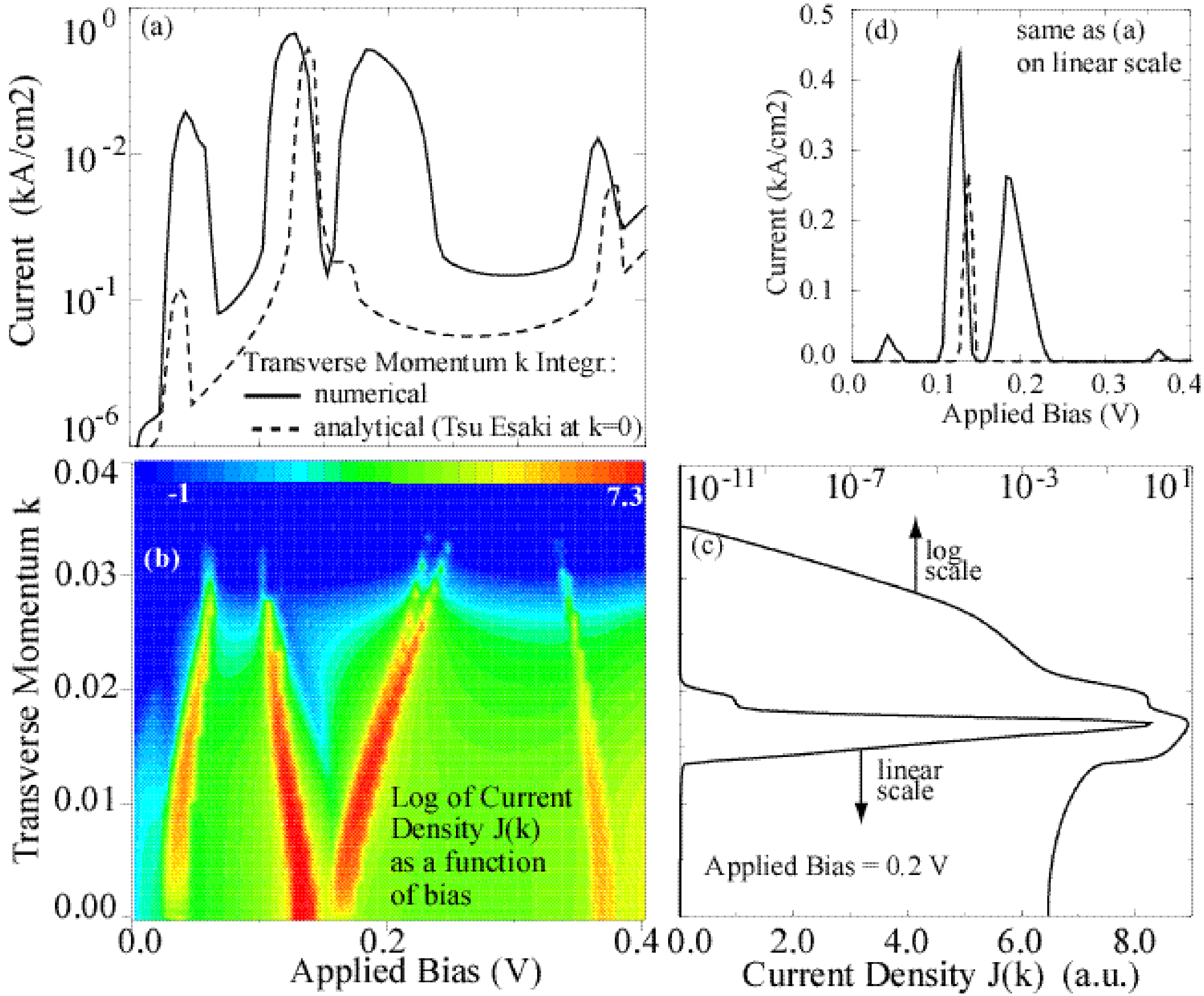
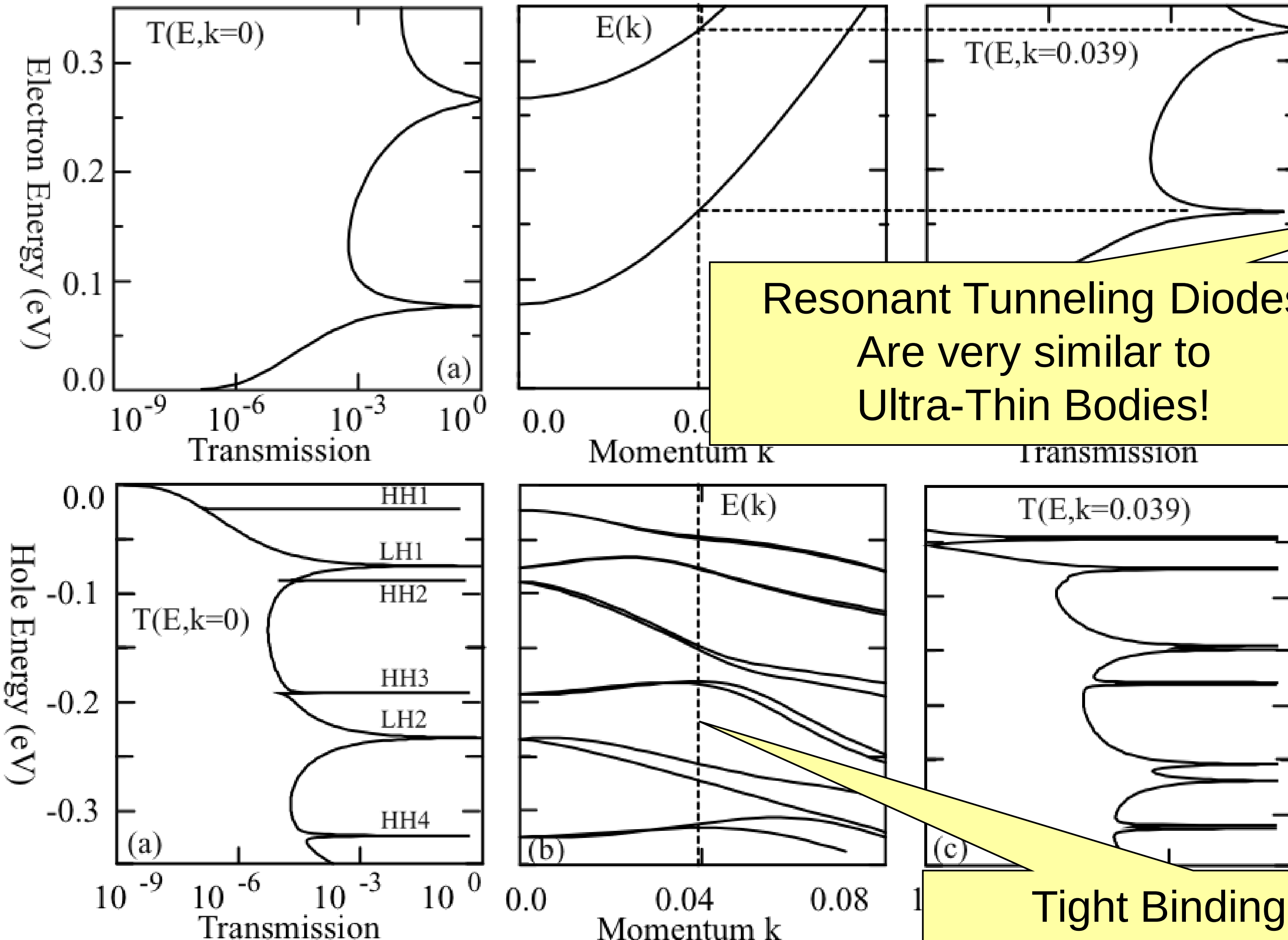
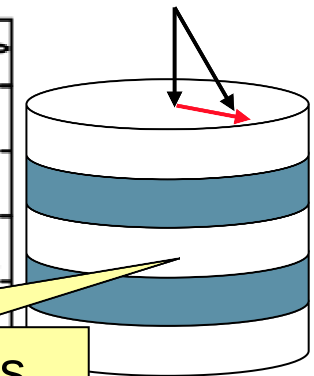


Off-zone Center Current Flow in Hole RTDs
Must have full band integration!



Quantum Transport in non-parabolic, strained, and coupled bands





Resonant Tunneling Diodes
Are very similar to
Ultra-Thin Bodies!

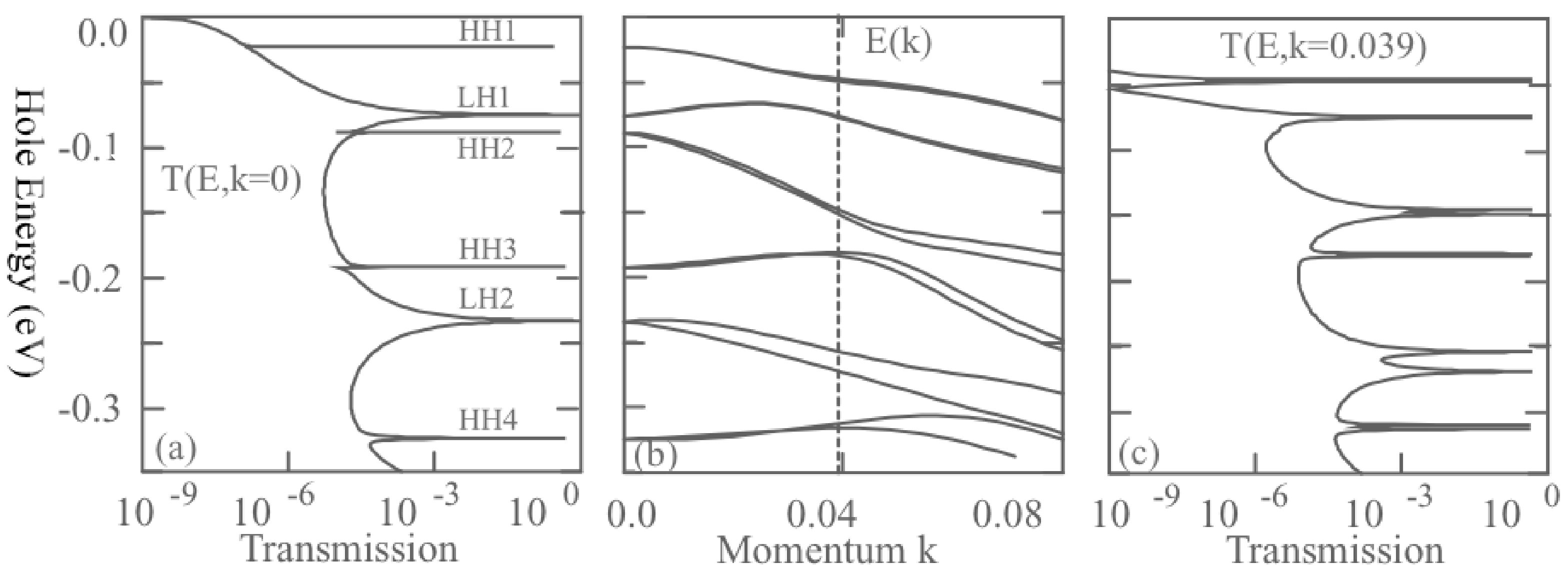
ctron:
spersion
oks parabolic,
but is NOT
- Transmission looks replicated, but is NOT

Holes:
- LH, HH, SO coupled
- Dispersion “complicated”
- Transmission dramatically

Tight Binding Handles
Coupling Between Bands
Strain, Non-Parabolicity

State-of-the-art RTD Modeling and Simulation Knowledge 1998 / 2000

- Bandstructure – atomistic device resolution
  - » Critical for understanding high temperature, high performance devices
  - » Effective mass leads to non-predictive and wrong conclusions
  - » Tight binding can handle electrons, holes, strain, band-coupling/mixing
  - » Ultra-Thin bodies, nanowires, and quantum dots will look similar to RTD



Conclusion Hole Transport

Hole Tranport

- Highly non-parabolic behavior in dispersion
- Bands are strongly coupled
- Carriers can travel in various k directions

Bandstructure – atomistic device resolution

- Critical for understanding high temperature, high performance devices
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