NEMO1D: Hole Bandstructure in Quantum Wells and Hole Transport in RTDs

Gerhard Klimeck
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
  - Deep background/peak ratio: $10^{13}$
    strong confinement
    weak coupling to outside

Small effective mass: strong confinement, weak coupling to outside.

Large effective mass: small state separation, strong confinement, deep background/peak ratio.
Hole transport in RTDs: Simplified Density of States and Transmission

- Holes
  Are just upside-down????

- Not quite!
  » LH and HH are coupled
  » Highly non-parabolic dispersion
  » Highly anisotropic dispersion

- Very unintuitive transport behavior!
• 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?

<table>
<thead>
<tr>
<th>Property</th>
<th>exp.</th>
<th>GaAs sim.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_g^\Gamma$</td>
<td>1.4240</td>
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</tr>
<tr>
<td>$\Delta_{so}$</td>
<td>0.3400</td>
<td>0.3664</td>
</tr>
<tr>
<td>$m_\Gamma^*$</td>
<td>0.0670</td>
<td>0.0679</td>
</tr>
<tr>
<td>$m_{lh}[001]$</td>
<td>-0.0871</td>
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HH and LH dispersions in bulk

LH band non-parabolic

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LH band strongly anisotropic

=> Electron-like
• 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

(a) Hole Energy (eV) vs. Transmission

(b) E(k) vs. Momentum k

(c) T(E,k=0.039) vs. Transmission

(d) Current Density J(k) (a.u.) vs. Transverse Momentum k

(e) Applied Bias (V) vs. Momentum k

(f) J(V) vs. Current (kA/cm^2)

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Transport via Transmission Coefficients

\[ I \propto \int dk_x \int dk_y \int dET(E, k_x, k_y) \left( f^L(E) - f^R(E) \right) \]

\[ \text{Cylindrical Coordinates} \]

\[ I \propto \int d\varphi \int kd\varphi \int dET(E, k, \varphi) \left( f^L(E) - f^R(E) \right) \]

\[ \text{Throw out angular dependence} \]

\[ I \propto 2\pi \int kd\varphi \int dET(E, k) \left( f^L(E) - f^R(E) \right) \]

\[ \text{Parabolic transverse subbands} \]

\[ I \propto \rho_{2D} \int T(E) \left( f^L(E) - f^R(E) \right) \]
Electron-like Dispersion in second subband

\[ I \propto \int kdk \int dET(E,k) \left( f_L(E) - f_R(E) \right) \]

\[ I \propto \int kdk J(k) \]

Non-monotonic (electron-like) dispersion can dip back into the Fermi sea.
Electron-like Dispersion injected with holes from emitter

\[ I \propto \int kdkdET(E,k)\left(f_L(E) - f_R(E)\right) \]

\[ I \propto \int kdkJ(k) \]

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

\[ J(k) \]

\[ V=0.113V \]
Electron-like Dispersion results in off-zone center flow

\[ I \propto \int kdk \int dET(E,k) \left( f_L(E) - f_R(E) \right) \]

\[ I \propto \int kdk J(k) \]

\[ J(k) \]

- \( J(k) \) can be sharply peaked away from \( k=0 \)
- \( \Rightarrow \) off-zone center current

- More electrons flow through an angle than straight through
• HH1 is mixture of the bulk HH and LH bands
• $m^*_{HH1} < m^*_{HH}$
• Surprising energy crossings
• HH1 is mixture of the bulk HH and LH bands
• $m^*_{HH1} < m^*_HH$
• Surprising energy crossings

• Current flow peaked at $k>0$
• Background provided by HH2

$J(k)$
Off-zone-center current: Resonance Width Modulation
anti-crossing modulates resonance width
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anti-crossing modulates resonance width

\[ J(k) \]

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

=> off-zone center current
Off-zone Center Current Flow in Hole RTDs
Must have full band integration!
Quantum Transport in non-parabolic, strained, and coupled bands

Electron:
- Dispersion looks parabolic, but is NOT
- Transmission looks replicated, but is NOT

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

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

Tight Binding Handles Coupling Between Bands
Strain, Non-Parabolicity
• 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
Hole Transport

- 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
- 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