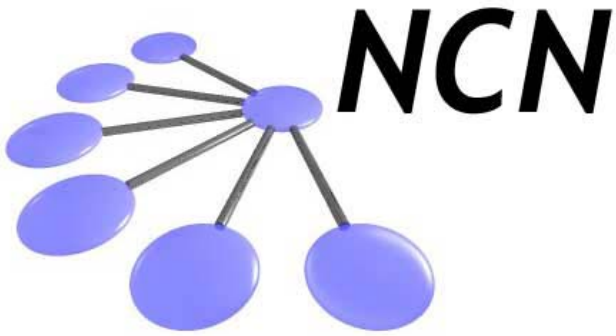
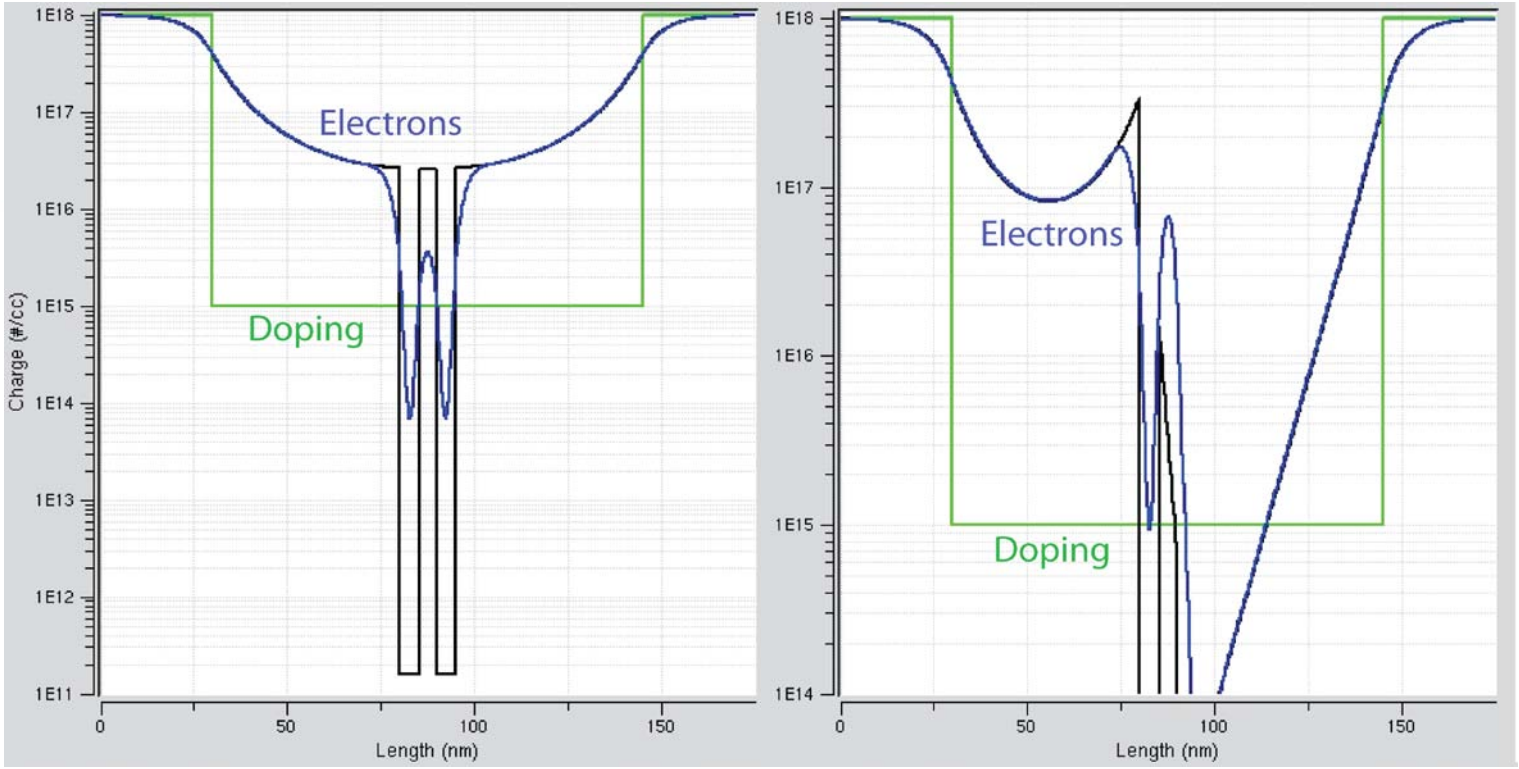
Introduction to RTDs: Quantum Charge Self-Consistency (Hartree)

Gerhard Klimeck

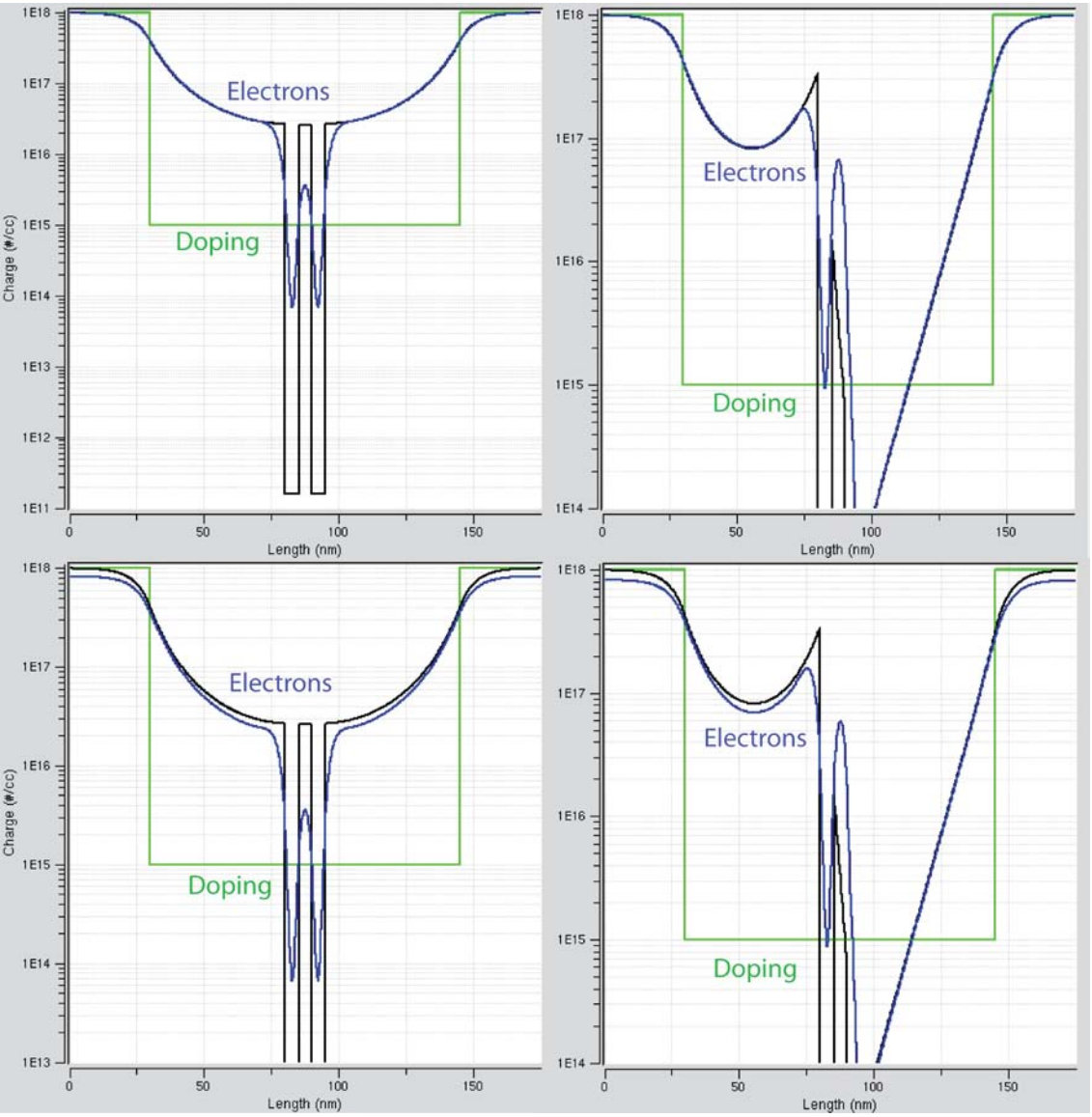


Self-consistent semi-classical charge vs. quantum mechanical charge



- So far only considered self-consistent semi-classical charge
- Use that electrostatic potential and compute the quantum charge
- Numerical quantum mechanical behavior results in smooth charge profiles in the emitter and collector, an increase charge density in the barriers, and a rounded charge profile in the central RTD.
- Under bias, quantum confined states in the triangular well shape the charge distribution to be more rounded.

Effects of relaxation *6.6meV* on the quantum charge distribution



- Quantum charge too small!

  => only about 80% of the semi-classical charge.

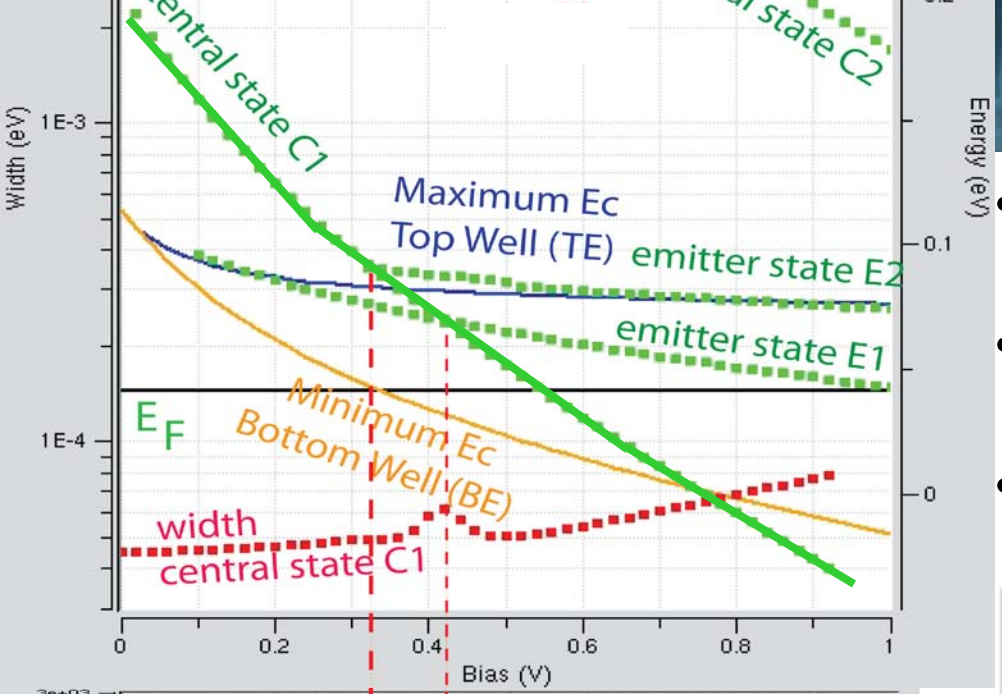
- The simple relaxation model does indeed introduce a non-conserving density of states reduction.

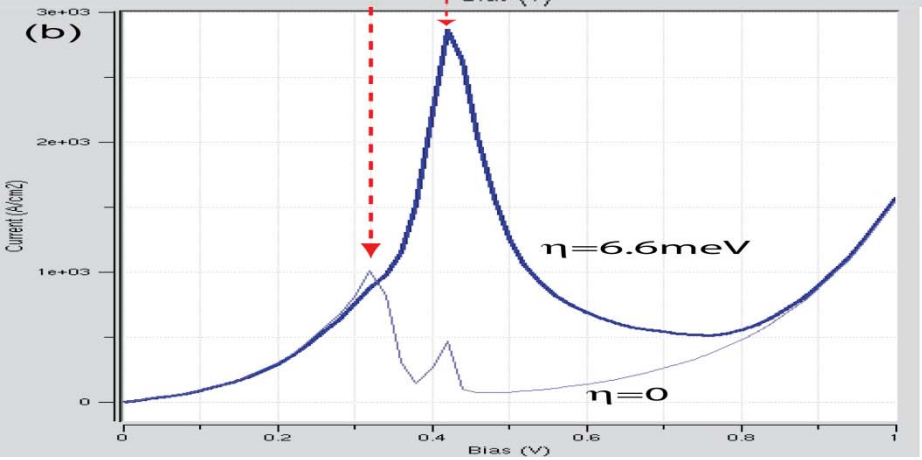
- No or negligible effect on central RTD charge!

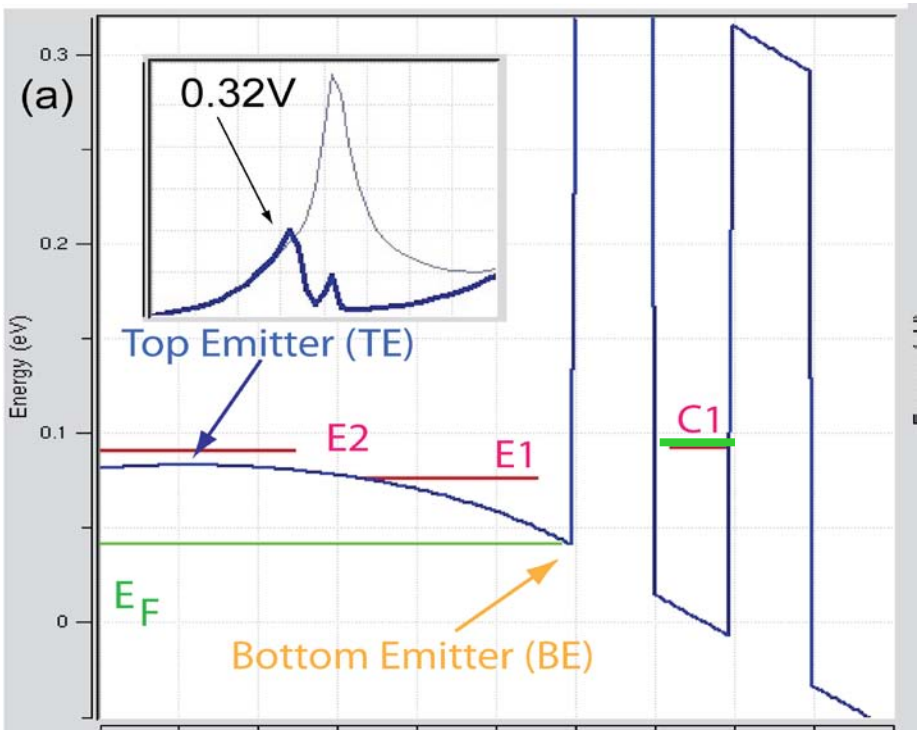
  => expected since there is no optical potential in the central region.

I-V with semi-classical charge self-consistency

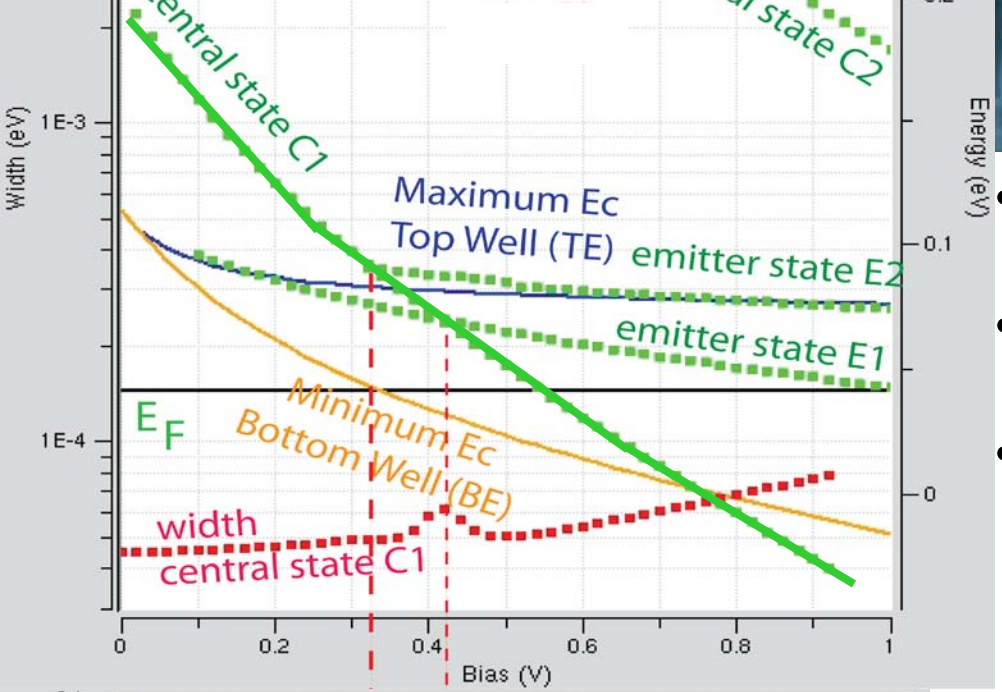
- Central resonance C1 drops almost linearly with bias
- There is current flow
  => there is charge / but no doping
- Electrostatic potential should push against charge filling







I-V with quantum charge self-consistency



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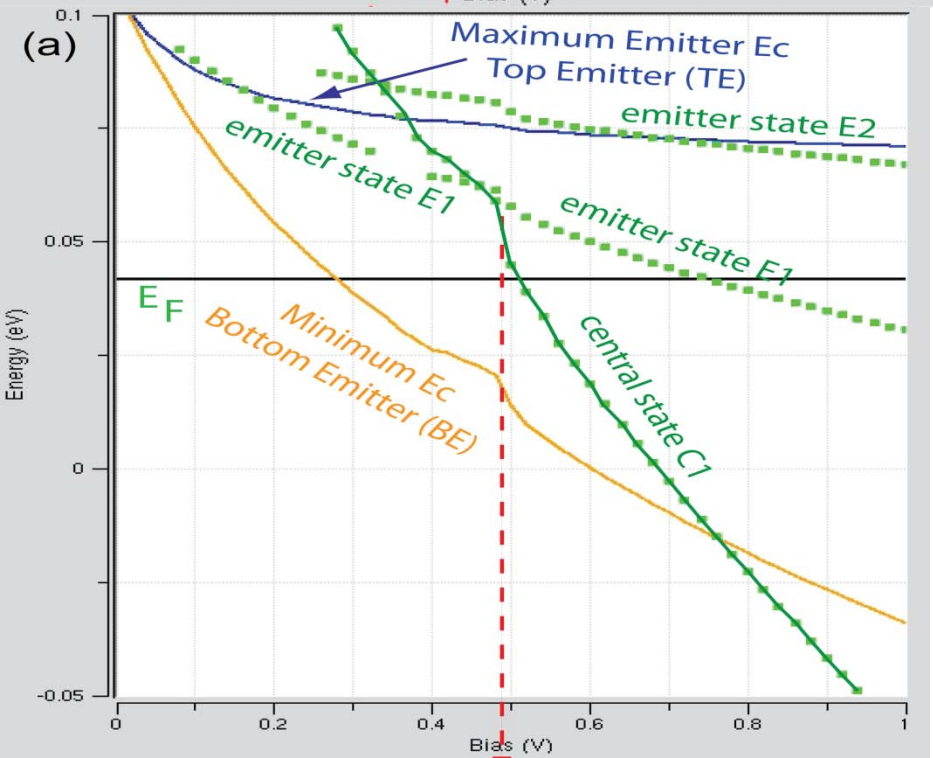

- Emitter potential floats up
  => resists further charge filling
  => emitter resonances float up
- Central resonance fills with charge
  => central potential floats up
  => resists further charge filling
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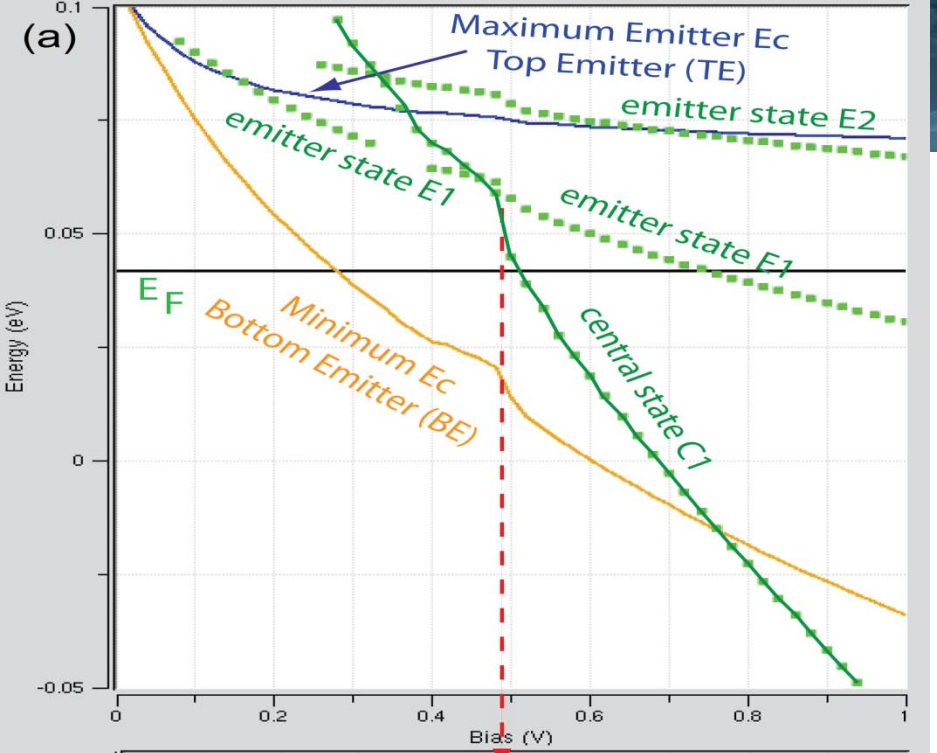
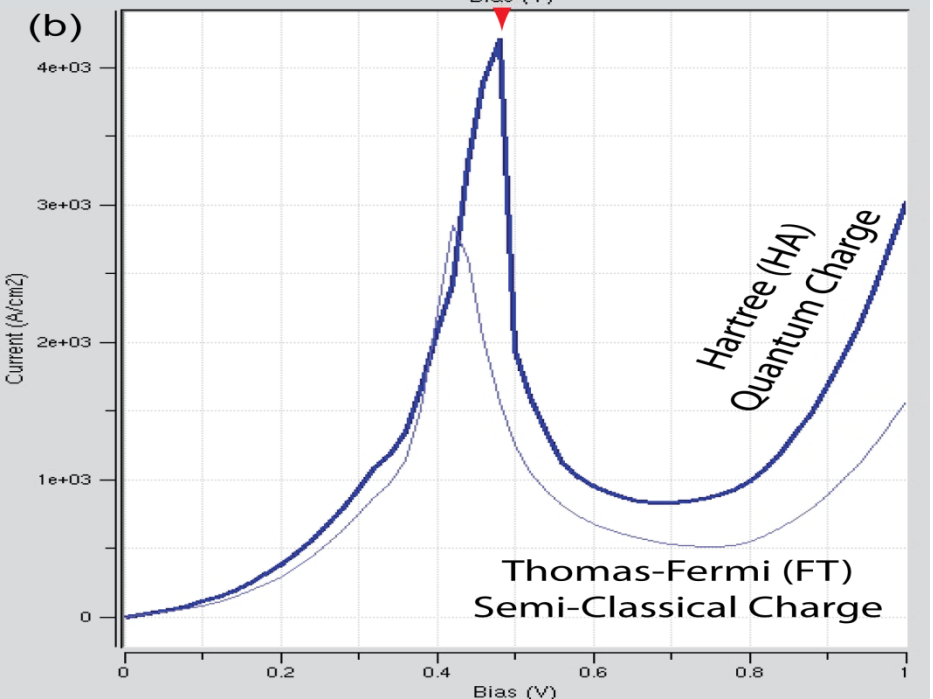
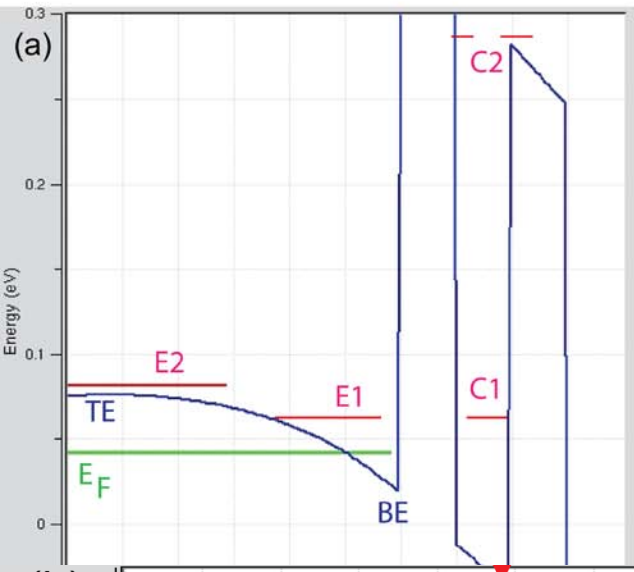
I-V with quantum charge self-consistency

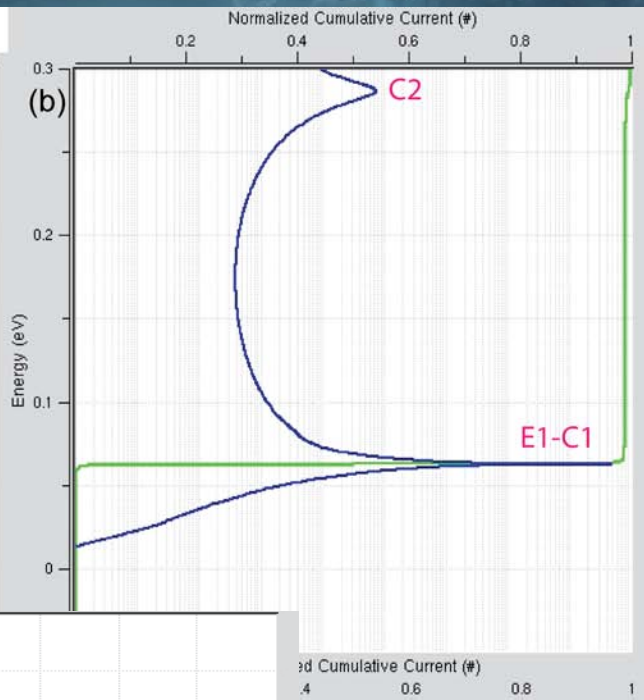


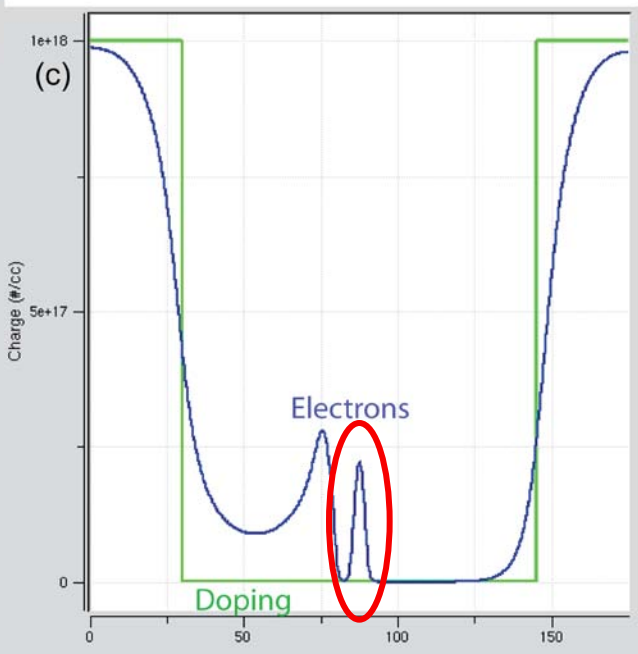


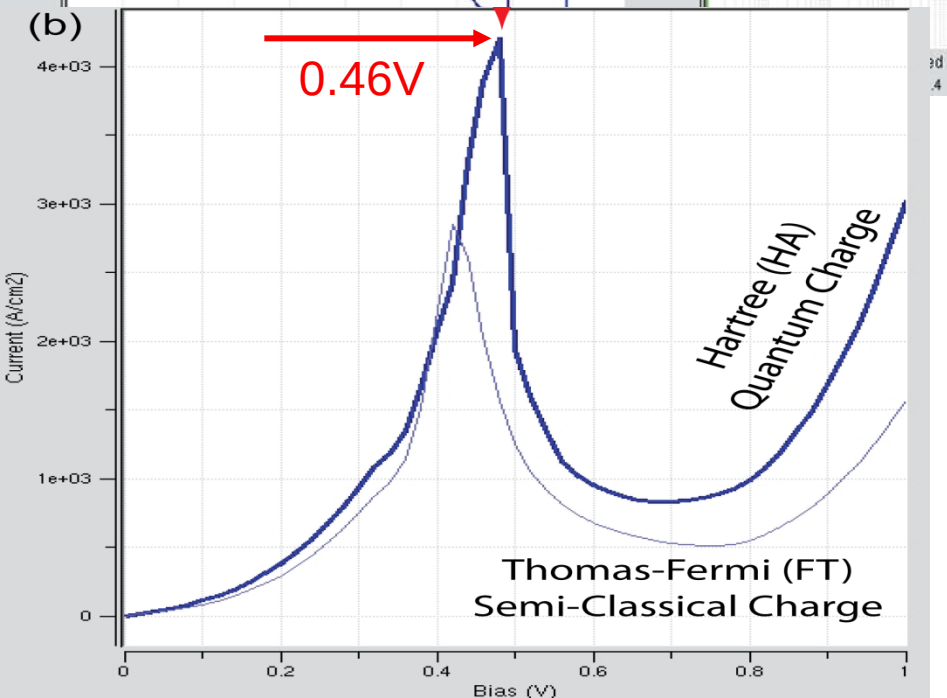
- Emitter potential floats up
  => resists further charge filling
  => emitter resonances float up
- Central resonance fills with charge
  => central potential floats up
  => resists further charge filling
  => central resonance floats up
- It requires a higher voltage to pull the resonance down
- I-V is linearized
- Peak occurs at higher voltage

Charge Accumulation on Resonance Alignment of E1 and C1



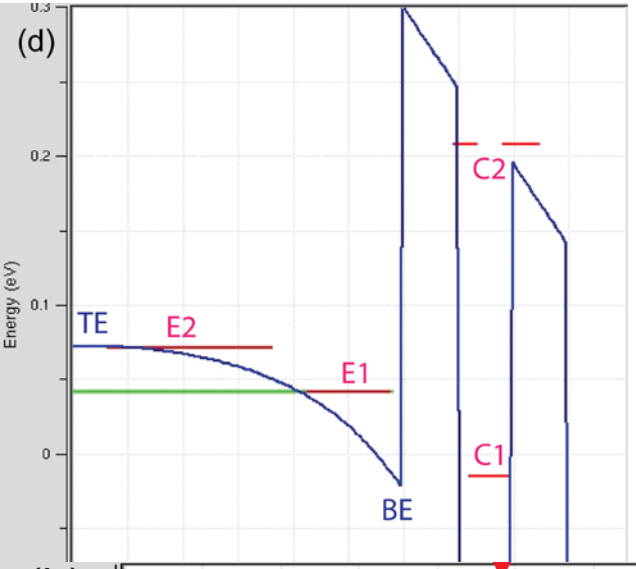


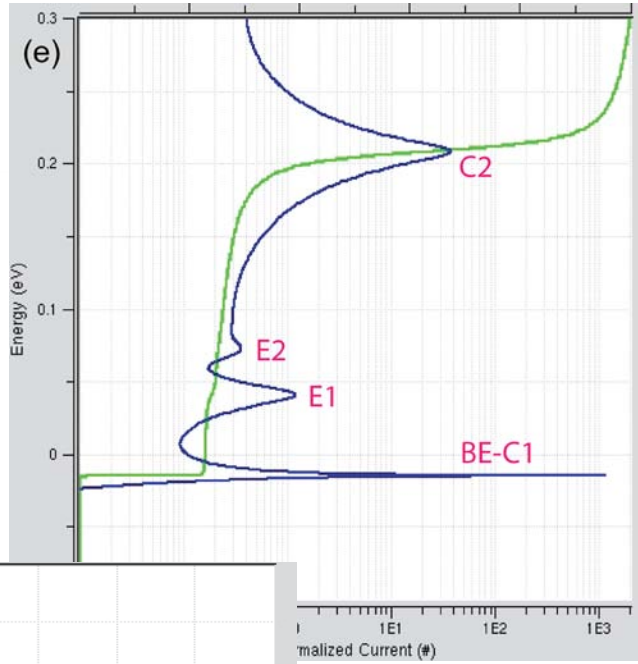


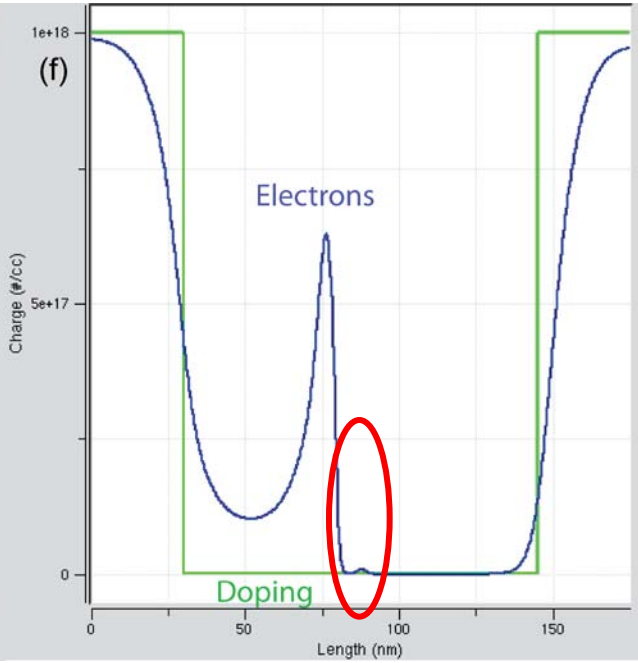


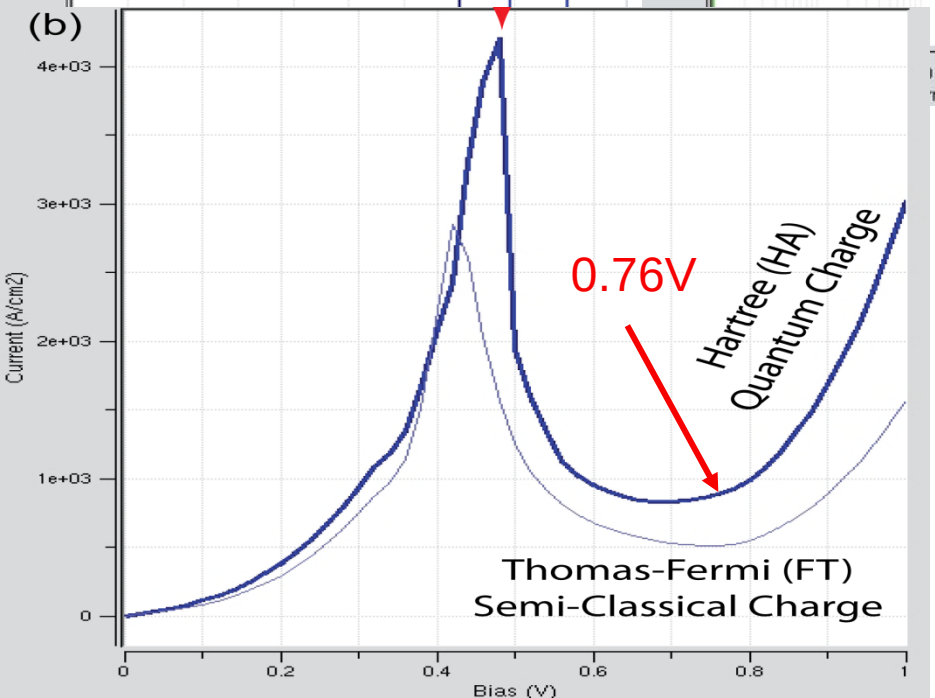
- At a bias of 0.46V.
- current carried in ground state C1.
- Significant charge accumulation
- Charge is highly out of equilibrium!
- Note that the RTD is nominally symmetric and collector barrier is smaller due to bias!
  => C1 should empty out faster than it fills, but still charge accumulation!

Valley Current
Alignment of BE and C1

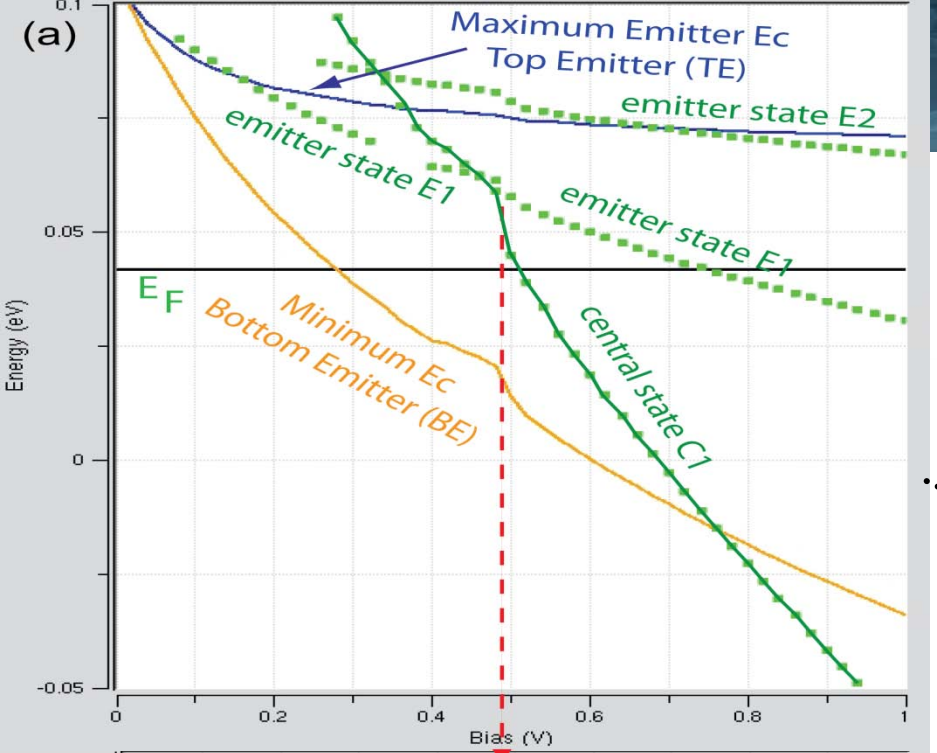


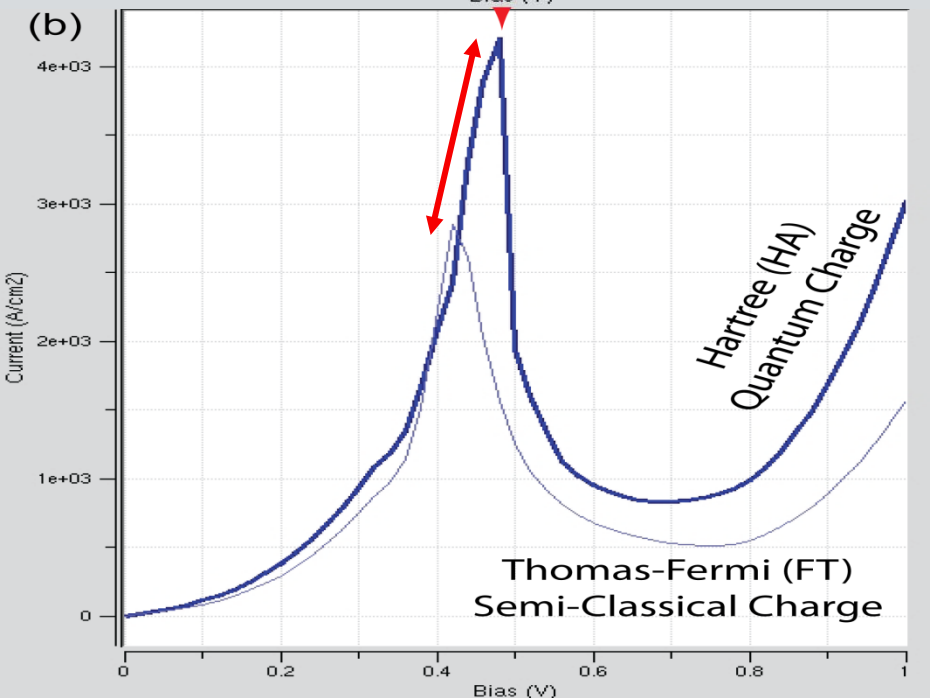






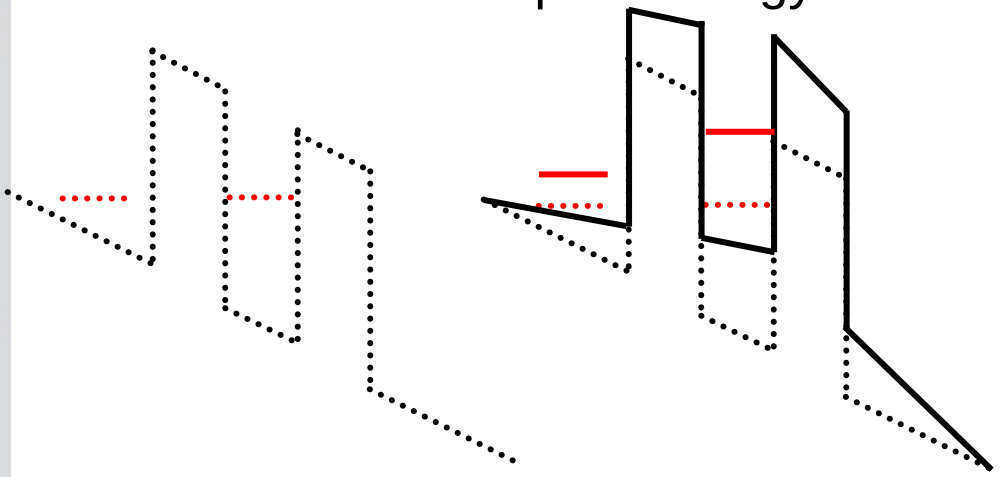
- At a bias of 0.76V.
- C1 is aligned with BE
- Supply of charge from emitter is diminished
- Little charge in the well – resonance emptied out
- 25% of current still goes through C1 due to relaxation





Why is the Peak Current Increasing?

- Charge filling of C1 and E1 causes a “float-up” in energy



⇒more potential drops over collector barrier

⇒C1 feels a smaller collector barrier

⇒Resonance C1 should become broader

⇒More current should flow

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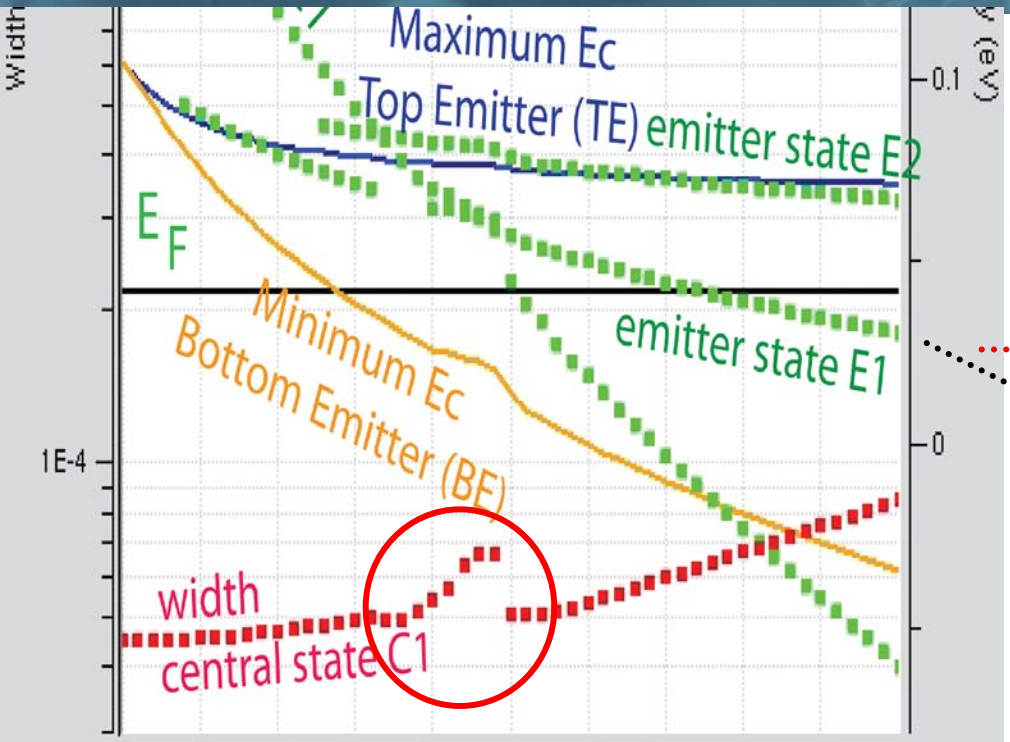

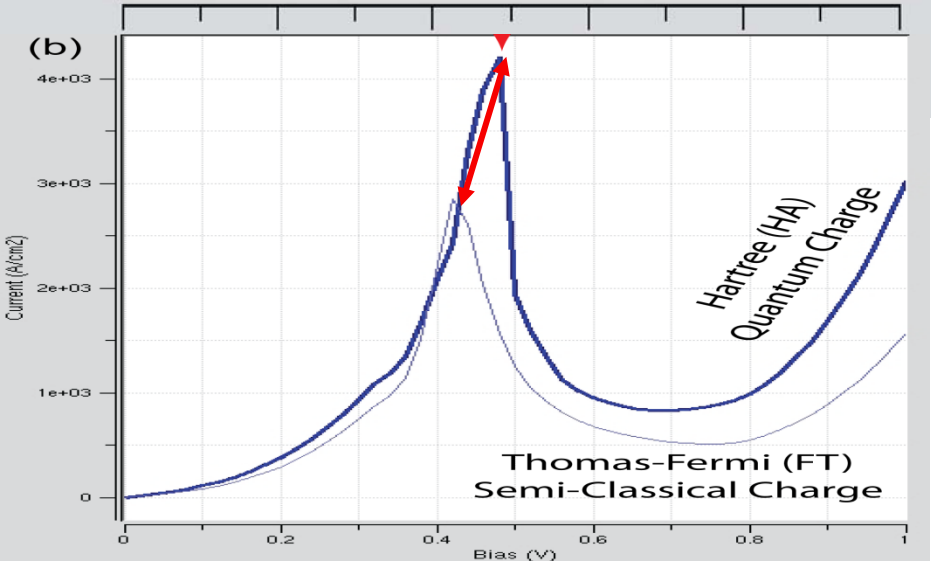

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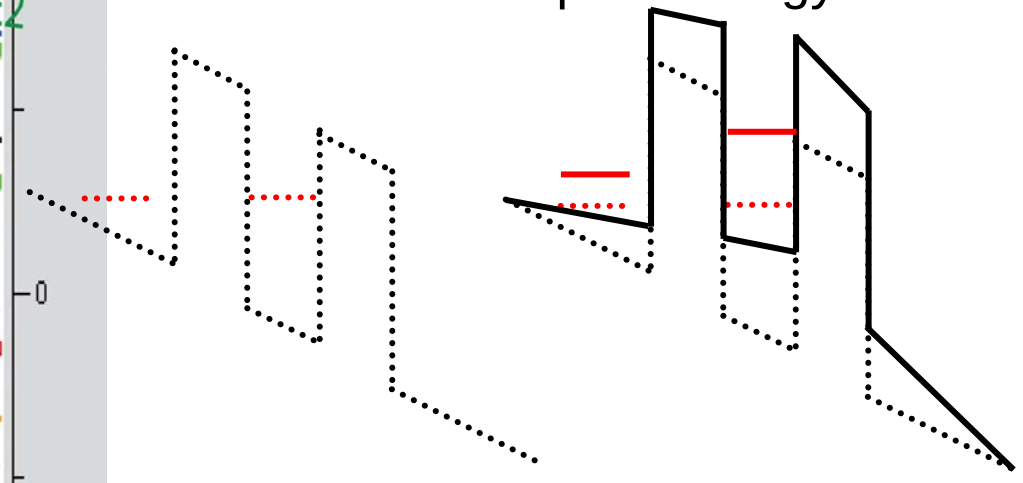

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Conclusions
Quantum Charge Self-Consistency

- Semi-classical charge and quantum charge differ significantly at the interfaces and inside the RTD.
- The electrostatic potential based on a semi-classical charge is a much better approximation to the Hartree-self-consistent charge, compared to the linear potential drop assumption.
- Resonance energies are no longer simple linear functions of bias => non-linear
- Hartree charge self-consistent calculations stretch out the voltage axis at the current peak and linearize the I-V curve.
- The current peak is increased.
- Even symmetric RTDs show a significant charge accumulation at the current peak which is highly out-of equilibrium.