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Non-Ohmic Hopping Transport in 1D Conductors
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Systems of interest

1D
- carbon nanotubes
- quantum and nano-wires

Quasi-1D
- organic conductors
- chain-like compounds

K$_2$NiF$_4$
TMTSF
Why study 1D and quasi-1D systems?

1. Unusual physics:
   - dominance of quantum effects
   - strong correlations
   - strong effects of disorder

2. Intellectual challenge
   - non-perturbative theory
   - understanding real experiments

3. Promising applications
   - new materials: nanotubes, composites, organic-inorganic hybrids
   - new electronics: plastic & molecular
   - new devices: nano-sensors, flat-panel displays, etc.
Disorder-induced localized states

1D nanostructures are often have lots of defects

Wavefunction decays exponentially:

\[ e^{-|x|/a} \]

\( a \) = localization length

Materials with localized electrons states are insulators
Variable-Range Hopping = Transport Mechanism in Insulators

Hopping rate \( \sim \exp \left( -\frac{2\Delta x}{a} - \frac{\varepsilon_2 - \varepsilon_1}{T} \right) \)

Conductivity of the entire system is determined by the optimal network of hopping sites. Typical hopping distance varies (decreases) with temperature; hence, Variable Range Hopping.

Mott (1960's)
Non-Ohmic hopping transport

- Recent experiments: 1D VRH transport is easily made non-Ohmic
  - McInnes, Butcher, and Triberis (1990)

- Surprisingly little theoretical work on the non-Ohmic VRH in 1D
  - McInnes, Butcher, and Triberis (1990)

- VRH in higher dimensions is essentially different

Polydiacetylene:
Aleshin et al. (2004)

Nanotube arrays:
Tang et al. (2000);
Tzolov et al. (2004)

Also individual nanotubes:
Cumings and Zettl (2004)
Basic ingredients of the model

- **Hopping rate from** $i$ **to** $j$

  $$\Gamma_{ji} = \exp \left[ -\frac{2\Delta x}{a} - \max \left( \frac{E_j - E_i}{T}, 0 \right) \right] f_i(1 - f_j)$$

- **Net current from** $i$ **to** $j$

  $$I_{ji} = \Gamma_{ji} - \Gamma_{ij}$$

- **Occupation factor**

  $$f_i = \frac{1}{\exp[(\epsilon_i - \mu_i)/T] + 1}$$

- **Local chemical potential**

  $$\mu_i$$

- **Equation to solve**

  $$\sum_i I_{ji} = 0$$

- **$F$ is the electric field**

  $$E_i = \epsilon_i - Fx_i$$
Ohmic VRH. Equivalence to Resistor Network

\[ I_{ji} = \frac{T}{R_{ji}} \sinh \left( \frac{\xi_i - \xi_j}{T} \right) \quad \text{Net current from } i \text{ to } j \]

\[ \xi_i = \mu_i - Fx_i \quad \text{is the local electro-chemical potential} \]

\[ R_{ji} = \exp \left( \frac{2}{a} \Delta x_{ij} + \frac{|\epsilon_i - \mu_i| + |\epsilon_j - \mu_j| + |\epsilon_i - \epsilon_j|}{2T} \right) \]

At small electric fields \[ I_{ji} \approx \frac{\xi_i - \xi_j}{R_{ji}} \]

Resistor network:
Problem of finding the optimal current path

Conventional argument:

- $x_M$: typical length of the links
- $\epsilon_M$: typical energy change across each link
- $\epsilon_M \geq 1 / g x_M$
- $g$ is the density of states

Minimize the typical resistance

$$ R \sim \exp \left( \frac{2x_M}{a} + \frac{\epsilon_M}{T} \right) $$

$$ x_M \sim a \sqrt{\frac{T_0}{T}}, \quad \epsilon_M \sim \sqrt{T_0 T}, \quad \ln R \sim \sqrt{\frac{T_0}{T}} \quad \text{1D analog of Mott's formula} $$

$$ T_0 \equiv 1 / g a \quad \text{energy level spacing within a localization volume} $$

This argument and the result for the resistance are **WRONG** in 1D!
"Breaks" on the current path

\[ P \sim \exp \left( -g A \right) = \exp \left( -\frac{T}{2T_0} u^2 \right) \]

\[ A = (au)(Tu)/2 \quad \text{area of the break} \]

Resistance of the break:

\[ R \sim \exp(u) \]

Breaks dominate over typical resistors:

\[ R \sim \exp \left( \frac{T_0}{2T} \right) \gg \exp \sqrt{\frac{T_0}{T}} \]

1D Mott's law is incorrect!
Statistical distribution of the conductance

The conductance of a finite-length wire is random and depends on what configuration of breaks is realized.

Bar plot:

Distribution function of conductance through a $1.8 \times 0.2$ μm GaAs device
Hughes et al. (1996)

Solid curves:

The best fit to the theory
Raikh and Ruzin (1989)
New questions addressed in this work

- What is the highest electric field $F$ at which the VRH is still Ohmic?
- Do “breaks” continue to play a role at larger fields?
- How does the resistivity depend on $F$ at such fields?
Early “break”-down of the Ohmic transport

Voltage drop per optimal break: \[ \Delta \xi \sim F L \]

Current through the break: \[ I = \frac{T}{R_{br}} \sinh \left( \frac{\Delta \xi}{T} \right) \]

Ohmic regime is valid if \[ \Delta \xi \ll T \]

\[ F \ll \exp \left( -\frac{T_0}{2T} \right) \]
Non-Ohmic transport. Intermediate fields

- Breaks are still relevant
- Electrochemical potential (voltage) drops mainly on the breaks, in a cascade fashion
- Hardest breaks are progressively circumnavigated as the current (electric field) increases
Chemical and electrochemical potentials

Chemical potential adjusts itself to the existing distribution of breaks.
Calculational strategy

- Assume a given fixed current $I$
- Each link of the optimal path is a “voltage generator”

\[ V_i(I) \text{ is determined by inverting } I = \frac{T}{R_{i, i+1}} \sinh \left( \frac{V_i}{T} \right) = \text{const} \]

- Most effective generators operate in the non-linear regime
- Need to determine their geometry and distribution function
- Averaging over this distribution we obtain the electric field needed to sustain the given current

Similar approach was used by Shklovskii (1976) in 3D
Intermediate current (field) regime is defined by:
\[
\sqrt{\frac{T_0}{T}} \ll u_i \equiv \ln \left( \frac{I_0}{I} \right) \ll \frac{T_0}{T}
\]

Breaks still control the transport. Optimal breaks are shaped as hexagons. They have average linear density

\[
P \sim \exp(-gA) = \exp \left( -\frac{T}{2T_0}u_i^2 - \frac{V_i}{2T_0}u_i \right)
\]

Field needed to sustain this current is

\[
F \sim \frac{V_i}{L} \sim V_iP \sim \exp \left( -\frac{T}{2T_0}u_i^2 \right) \quad \Rightarrow \quad \ln \rho \sim \sqrt{\frac{2T_0}{T} \ln \left( \frac{k_B T}{Fa} \right)}
\]

1D Mott's law is recovered at \( F \sim k_B T / a \)
Non-Ohmic transport. Strong fields

- Breaks are no longer relevant
- Electron distribution function is driven far from equilibrium
- Only forward hops are important
Calculational strategy: directed percolation

\[ I = f_i (1 - f_{i+1}) \exp \left( -\frac{2}{a} |x_i - x_{i+1}| \right) \]

\[ |x_i - x_{i+1}| \leq \frac{a}{2} u_I \]

\[ \rho = \exp \left( C \frac{k_B T}{F a} \right)^{1/2} \]

Like the 1D Mott’s law with an effective temperature

\[ k_B T_{\text{eff}} \sim F a \]

The real temperature plays no role

Previous work: the exponential differs by a large log
Predictions for experiments

- In an ensemble of finite-length wires, there are enormous resistance variations
- The distribution (or, simply, the mean) of log-resistance should be studied instead
- Temperature should be low enough; otherwise, one has Nearest-Neighbor-Hopping instead of the Variable-Range-Hopping
- Three types of behavior are predicted for the log-averaged resistivity:

\[
\langle \ln \rho \rangle \sim -eV / 2k_B T, \quad k_B T << eV << k_B \sqrt{T T_0 / \ln L} \quad \text{("weak")}
\]

\[
\langle \ln \rho \rangle \sim \sqrt{\frac{2T_0}{T} \ln \left( \frac{k_B T}{F a} \right)}, \quad F << \frac{k_B T}{a} \quad \text{(intermediate)}
\]

\[
\langle \ln \rho \rangle = \sqrt{8 \frac{k_B T}{F a}}, \quad F >> k_B T / a \quad \text{(strong)}
\]
Conclusions and future challenges

- Constructed the theory of a 1D Variable-Range Hopping in finite electric fields with a due account of rare events specific for the 1D geometry.

- The dependence of the resistivity on the field shows a rich structure with three different functional laws in weak, intermediate, and strong electric fields.

- Need to compute the statistical distribution of the resistivity in finite-length wires.

- Need to account for small transverse hopping in quasi-1D systems.

- Need to include Coulomb interaction effects.