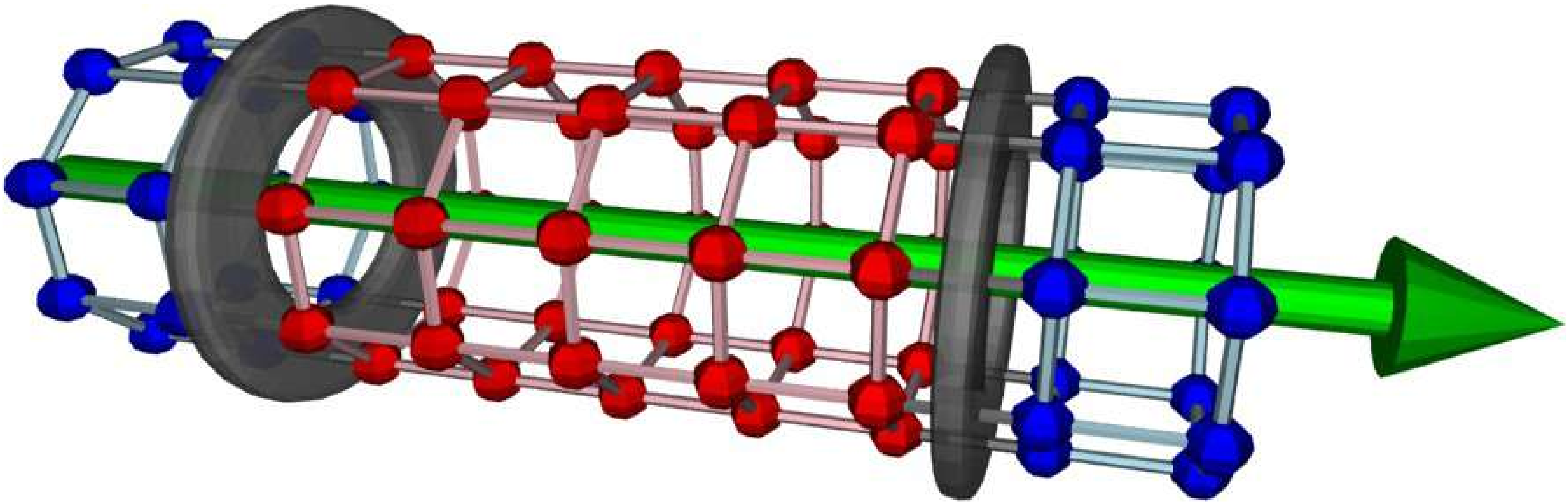
An *ab initio* study of the Little-Parks effect in ultrathin cylinders

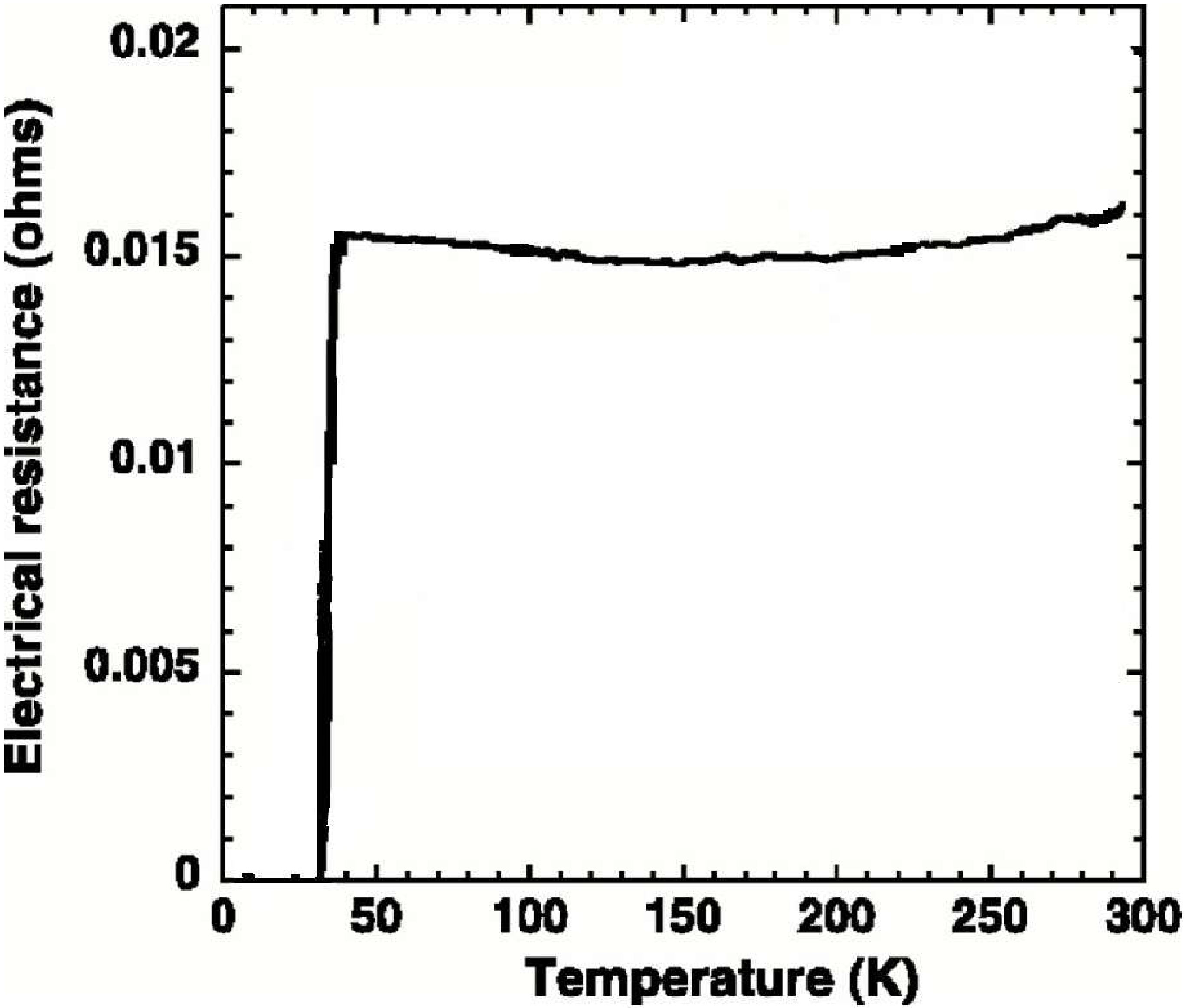


Gareth Conduit, Yigal Meir

Ben Gurion University & Weizmann Institute of Science

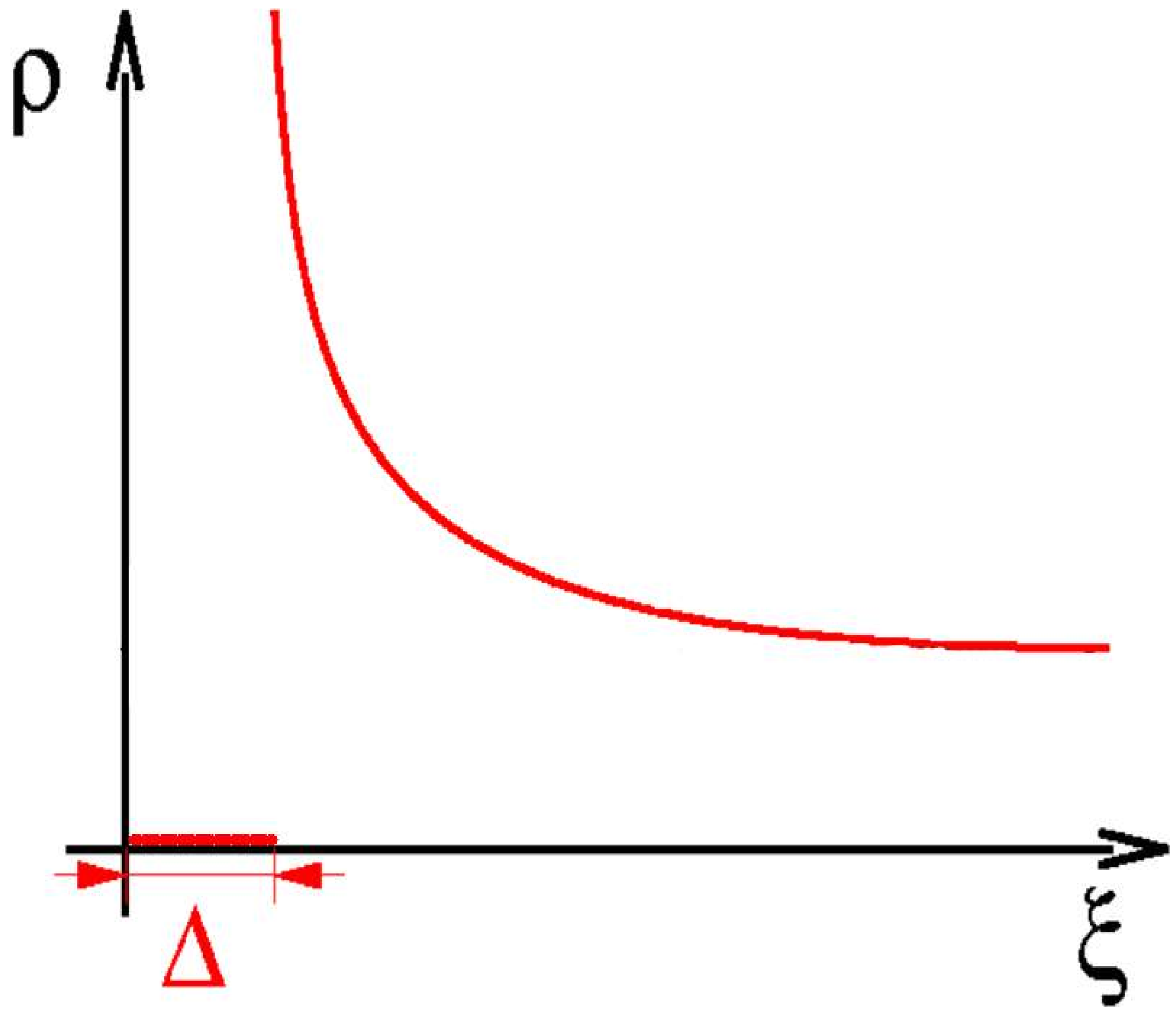
arXiv:1102.1604

BCS superconductivity in MgB_2

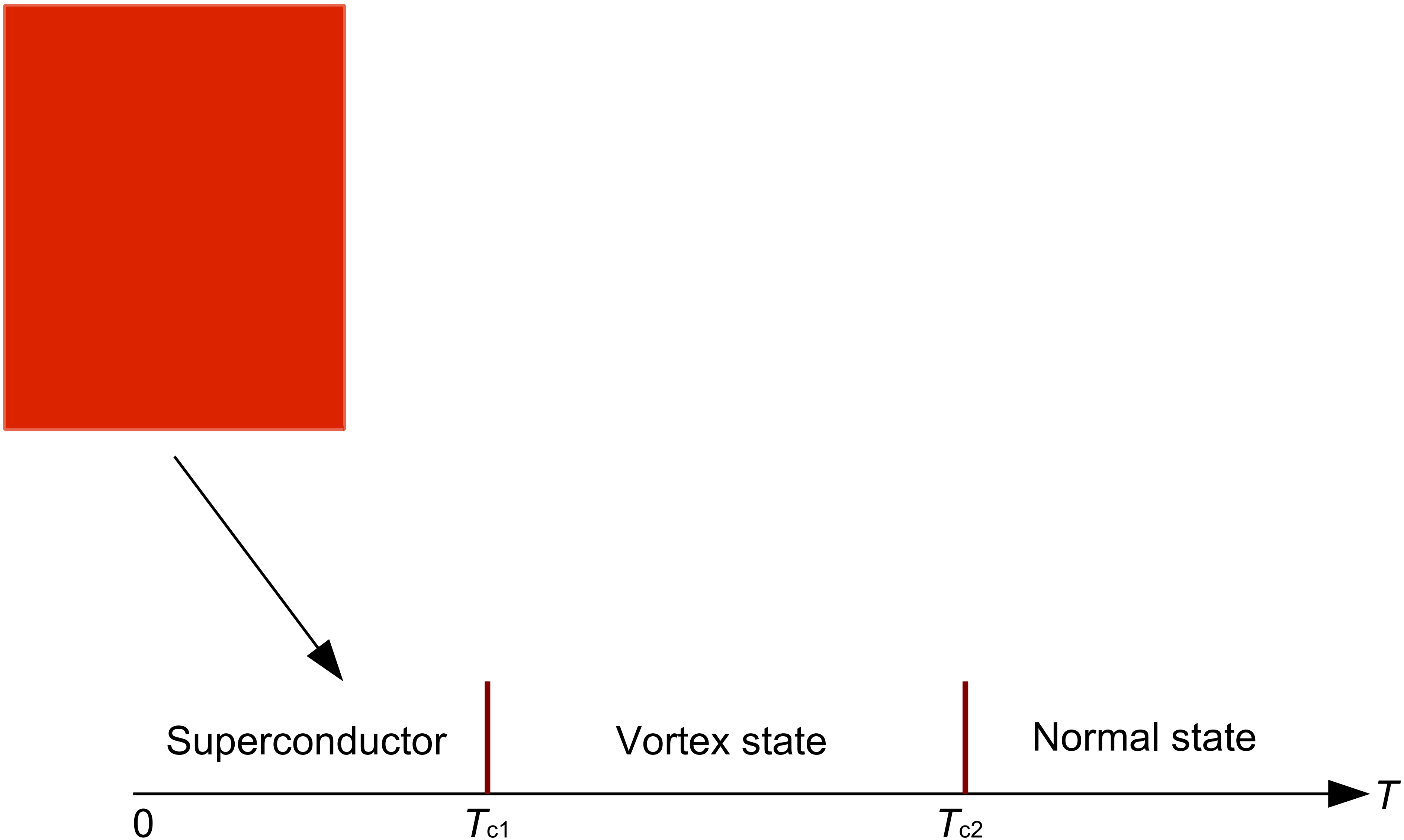


Monteverde et al., Science **292**, 75 (2001)

BCS superconductivity



Kosterlitz Thouless transition



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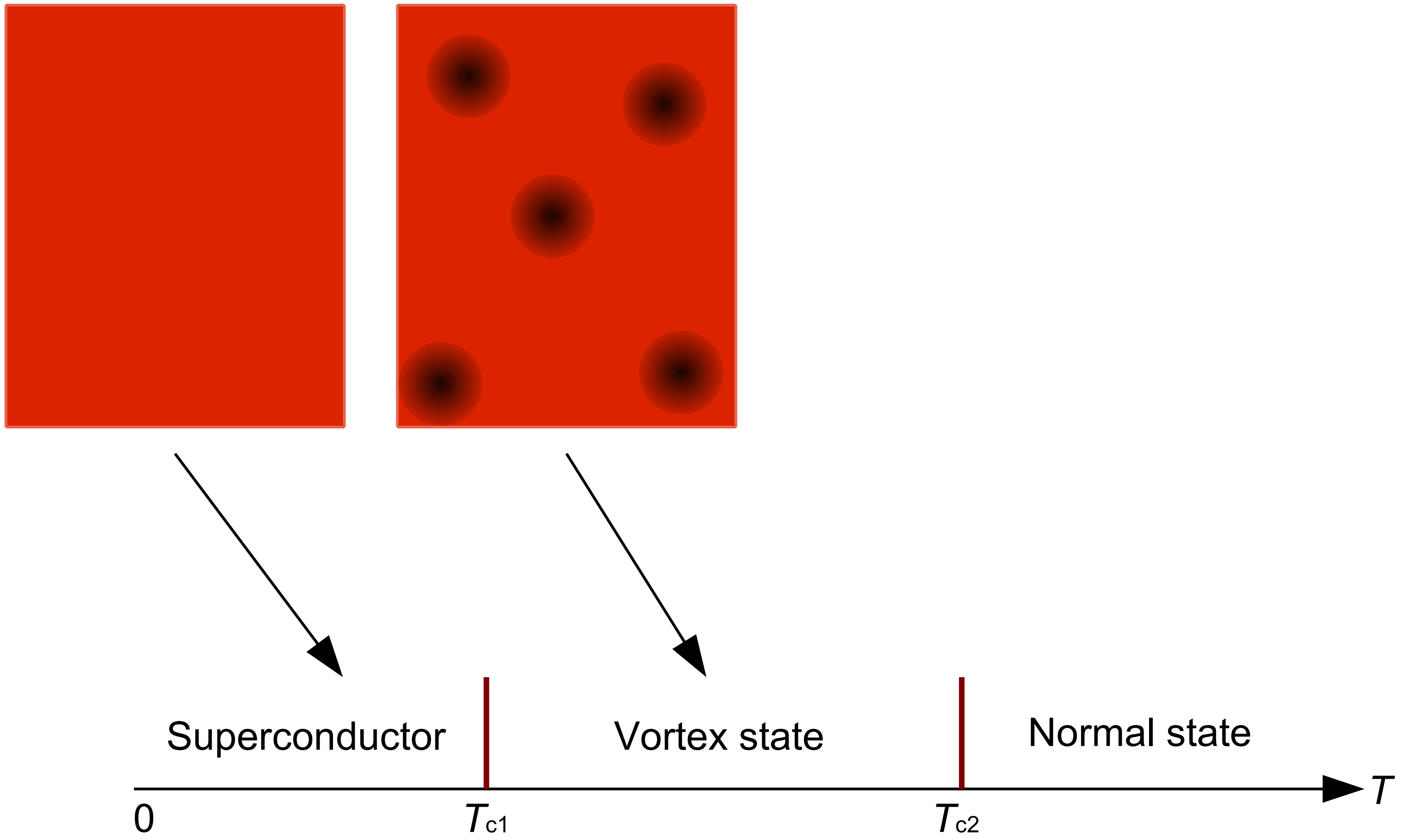
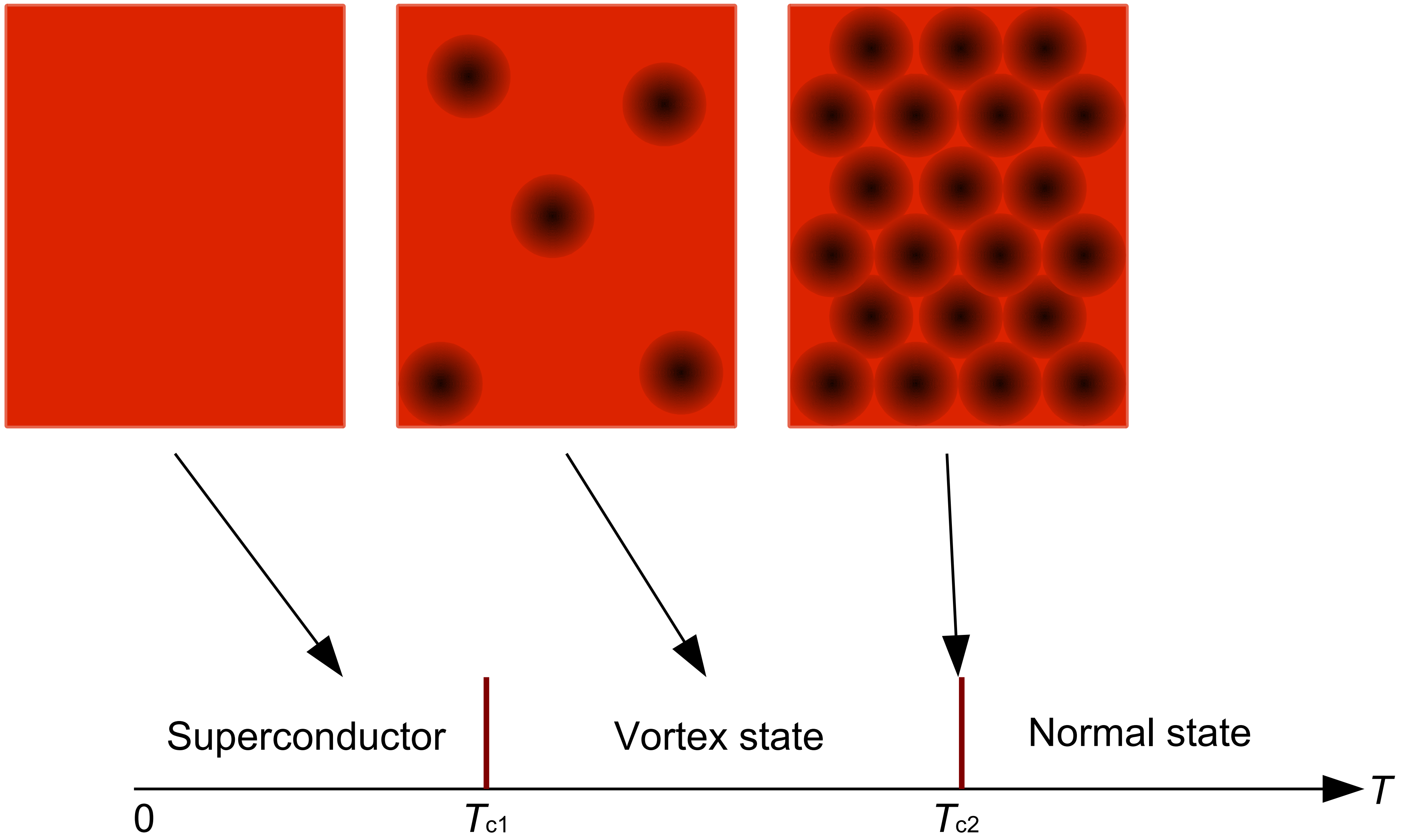


Kosterlitz Thouless transition



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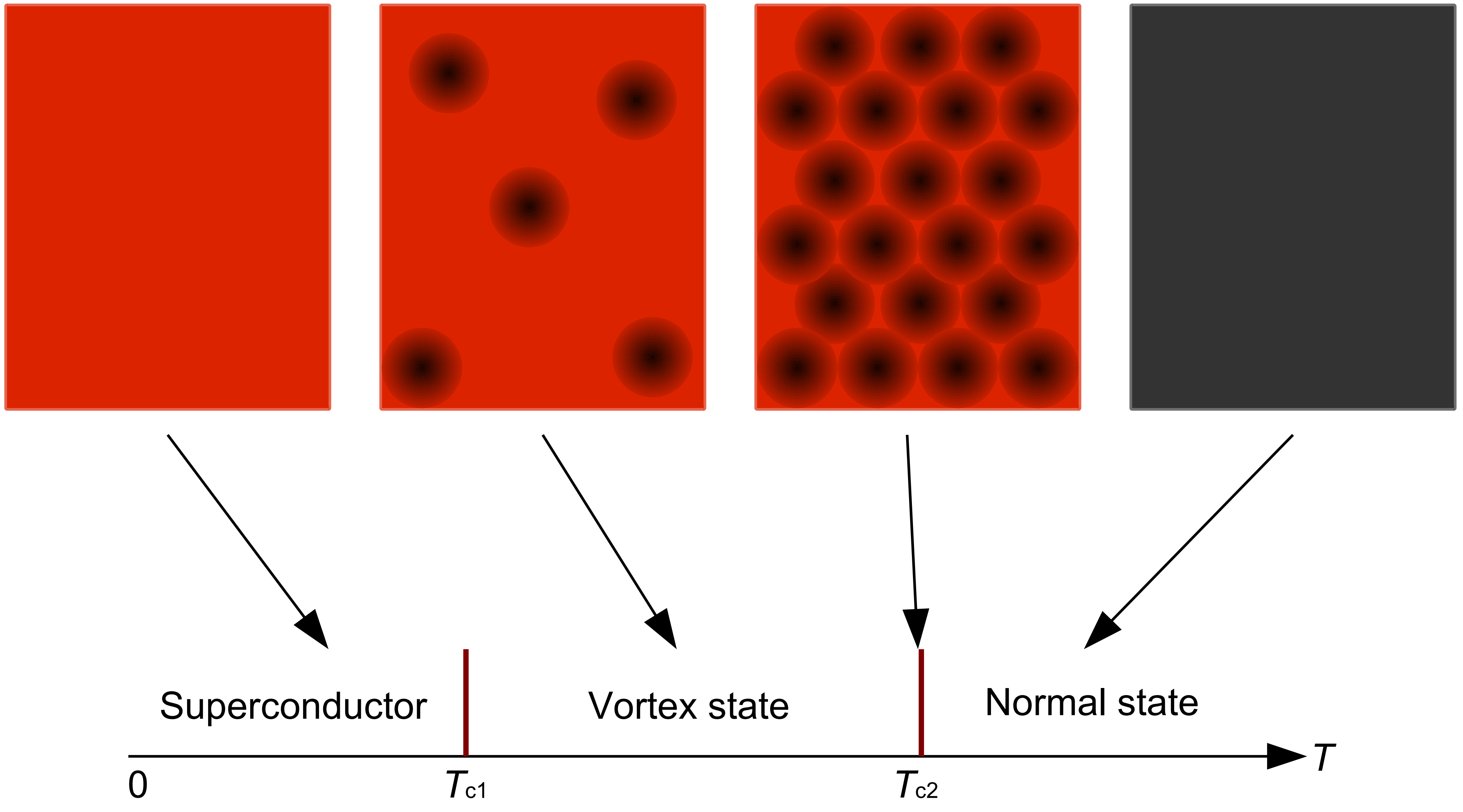
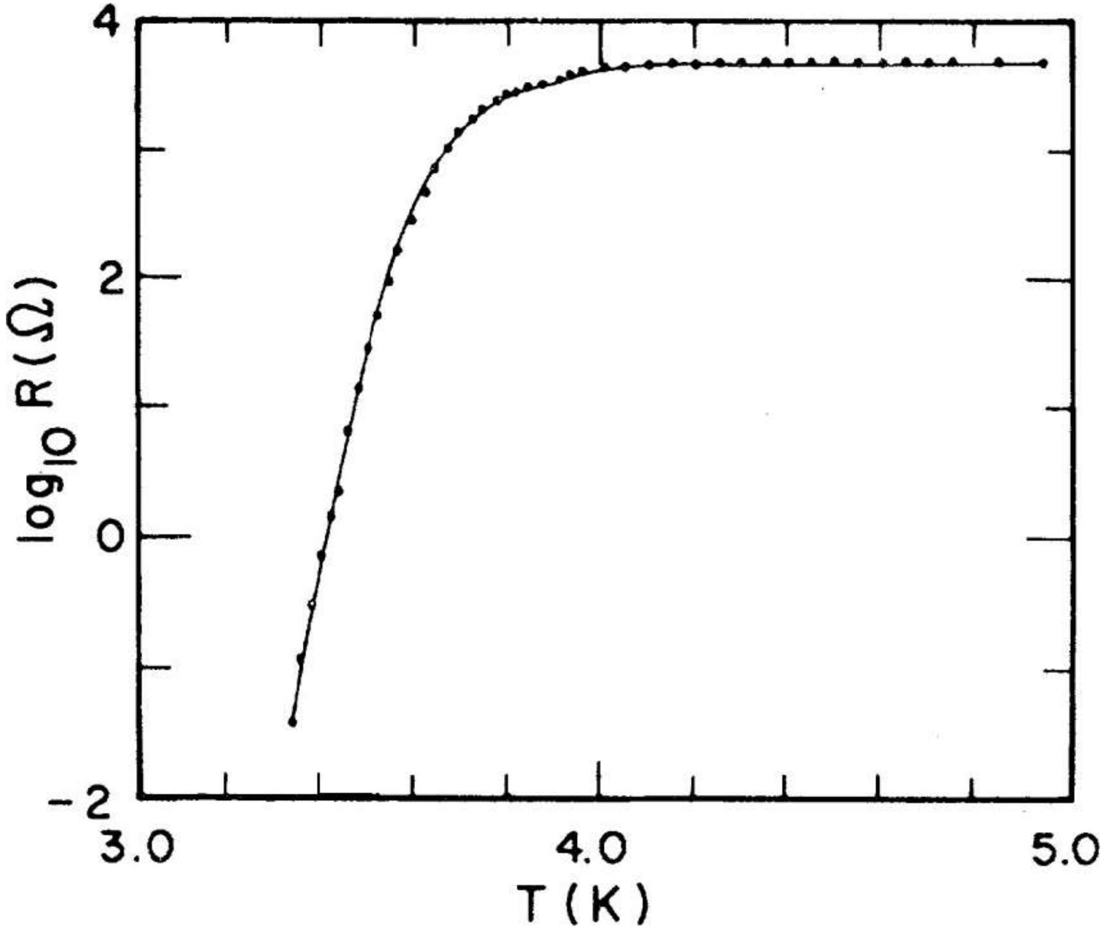
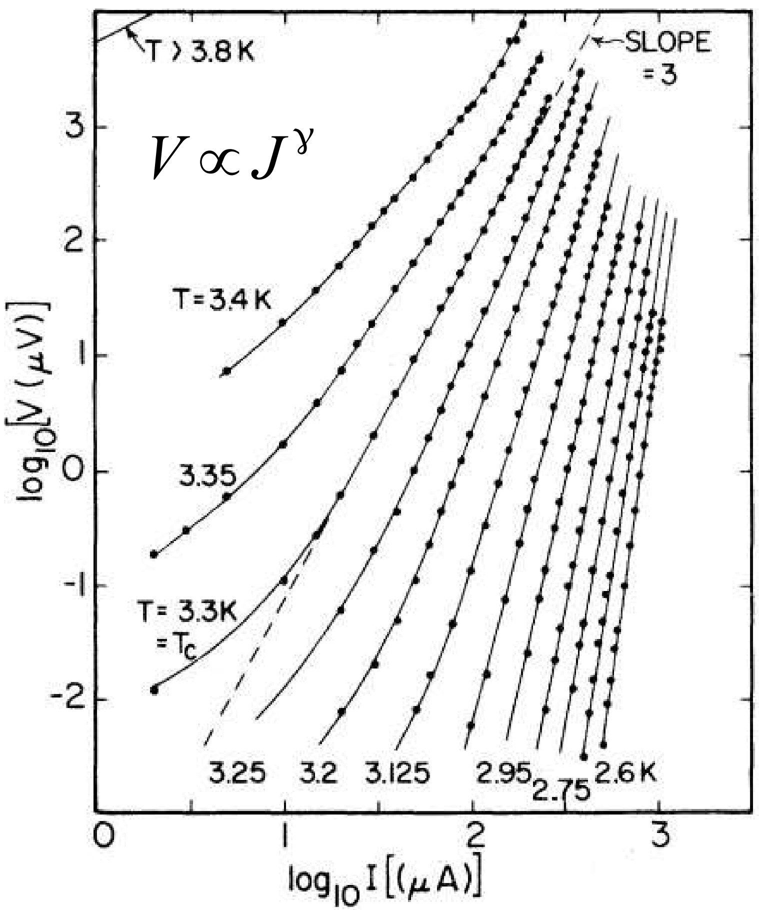
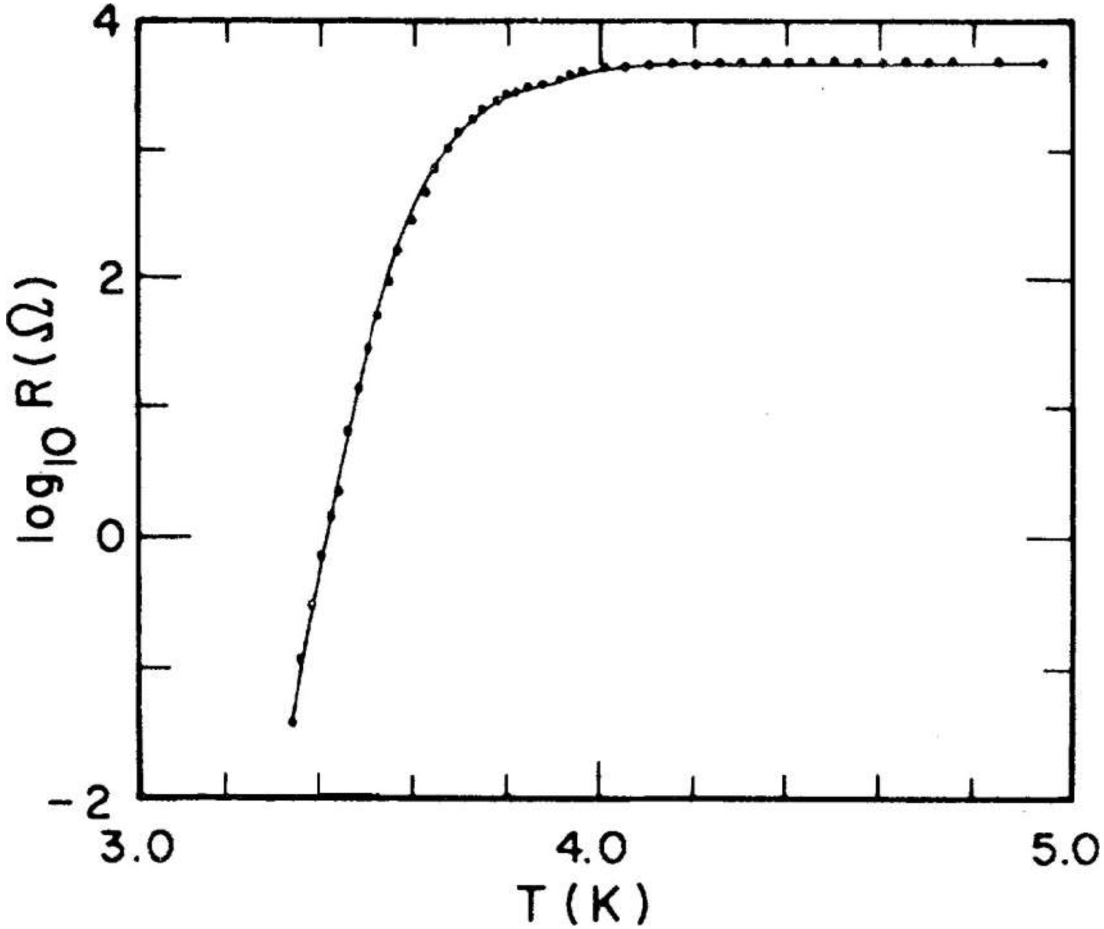


KT transition conductivity



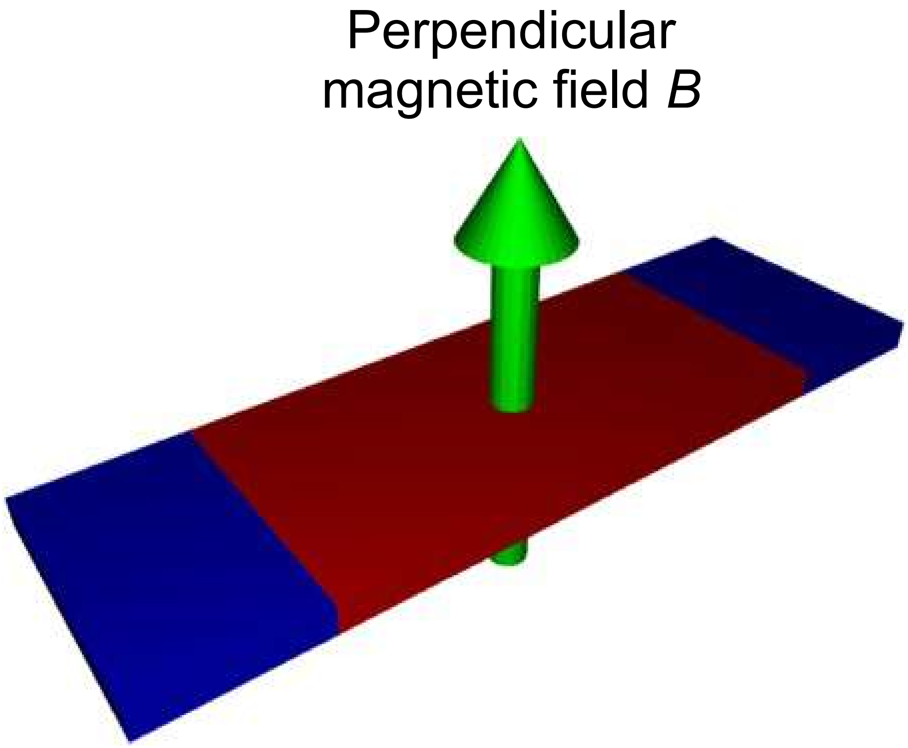
KT transition conductivity

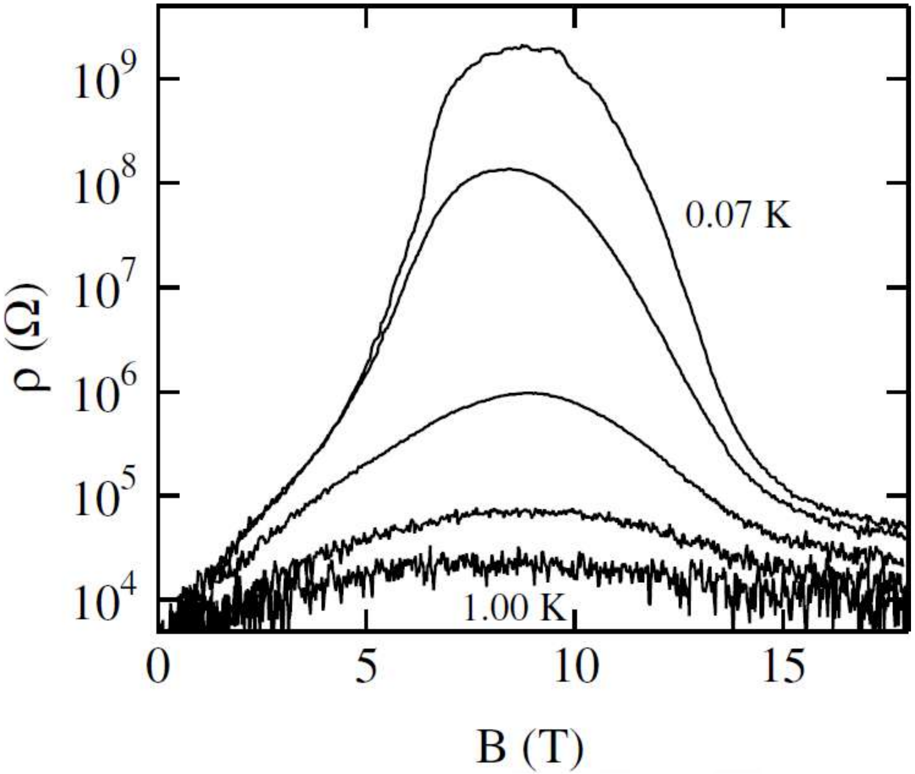




Transition in highly disordered systems

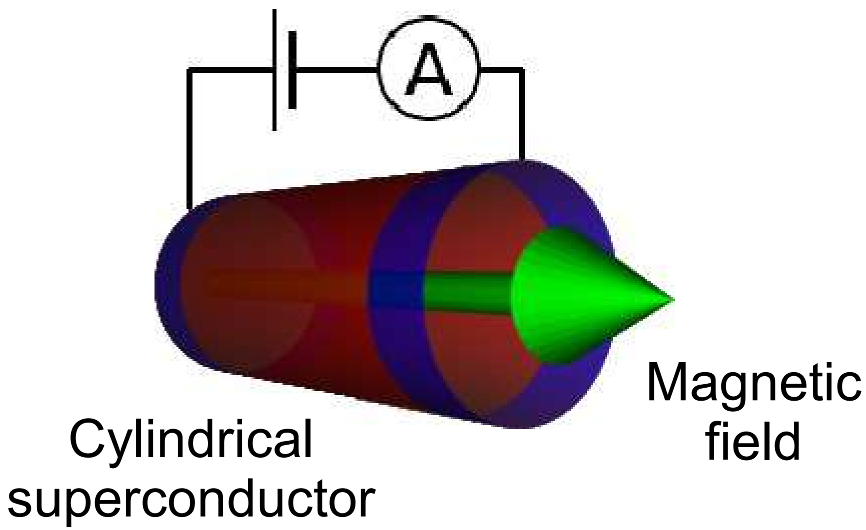
- Magnetoresistance peak [Sambandamurthy 04]

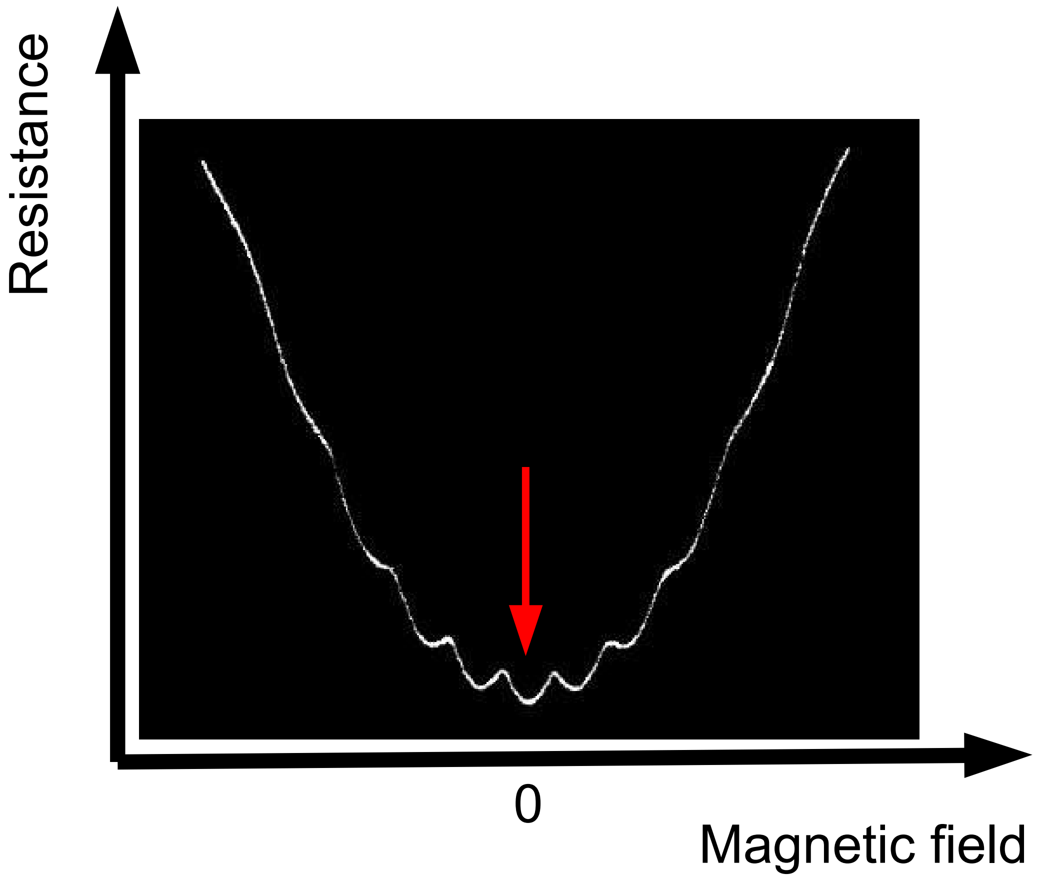




Little-Parks in a large diameter cylinder

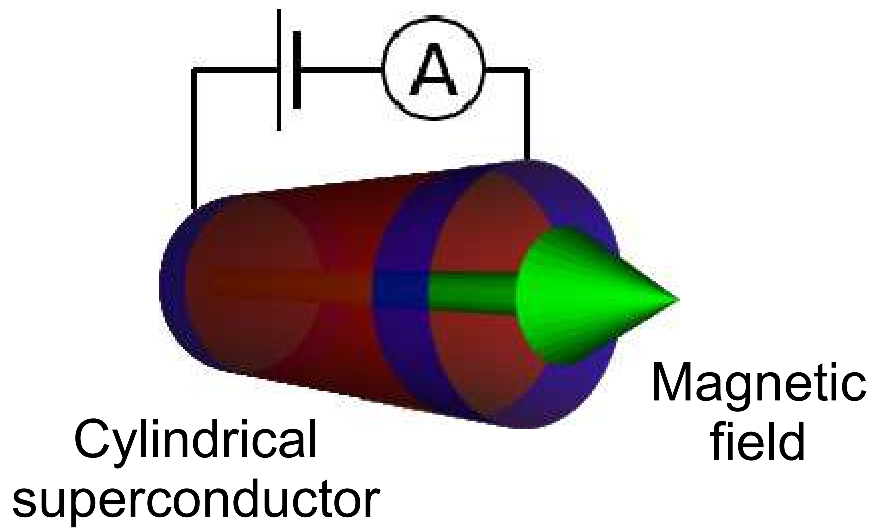
- Cylindrical superconductor held at transition temperature and zero threading flux [Little & Parks, PRL 1962]

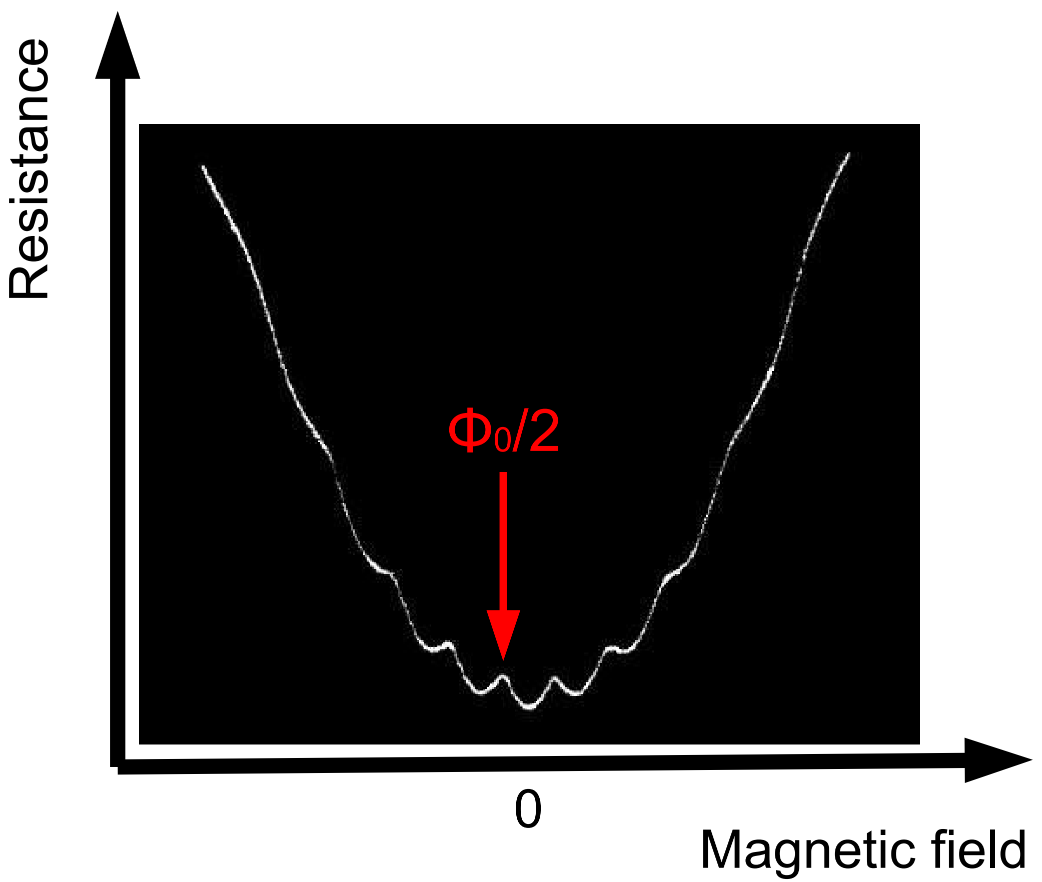




Little-Parks in a large diameter cylinder

- Cylindrical superconductor held at transition temperature and threading flux is increased [Little & Parks, PRL 1962]





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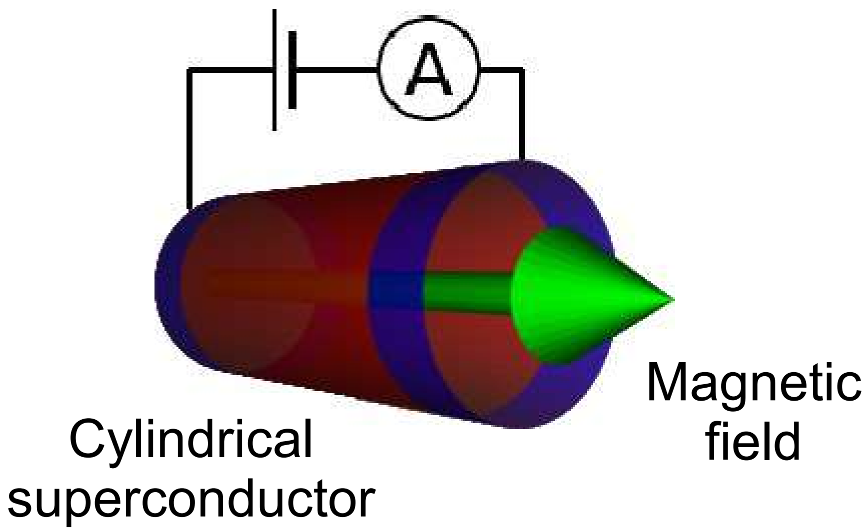
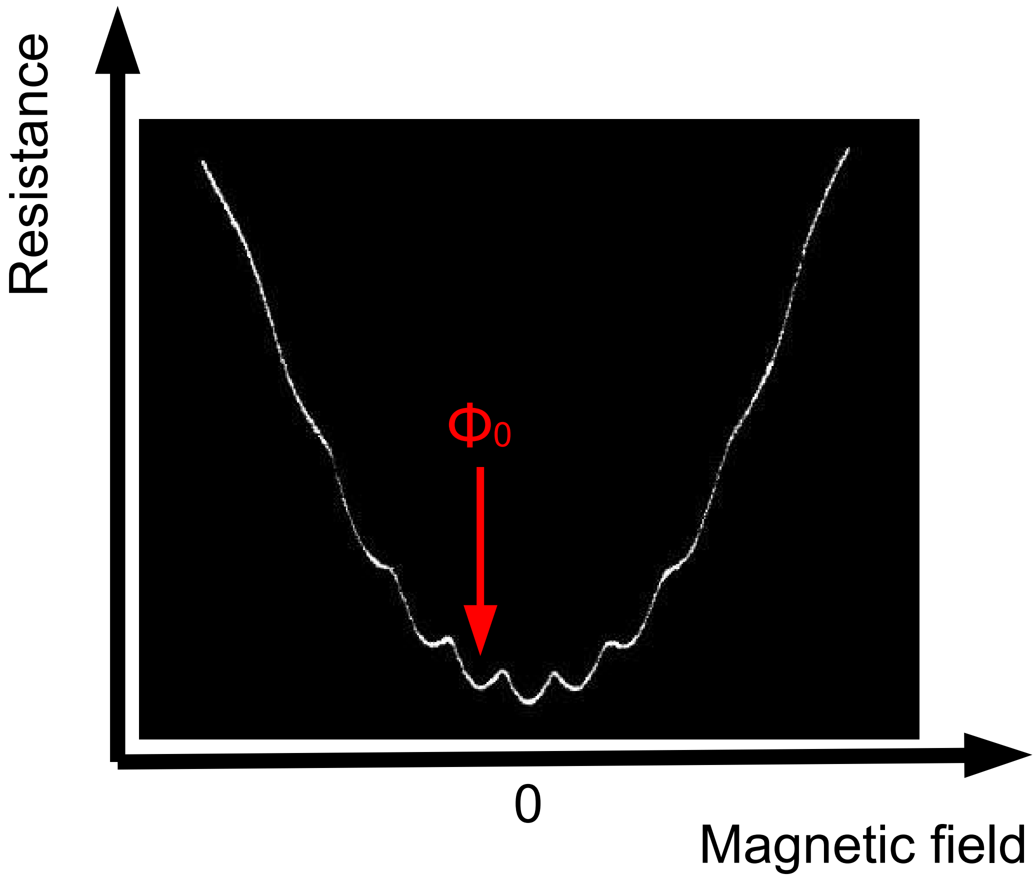
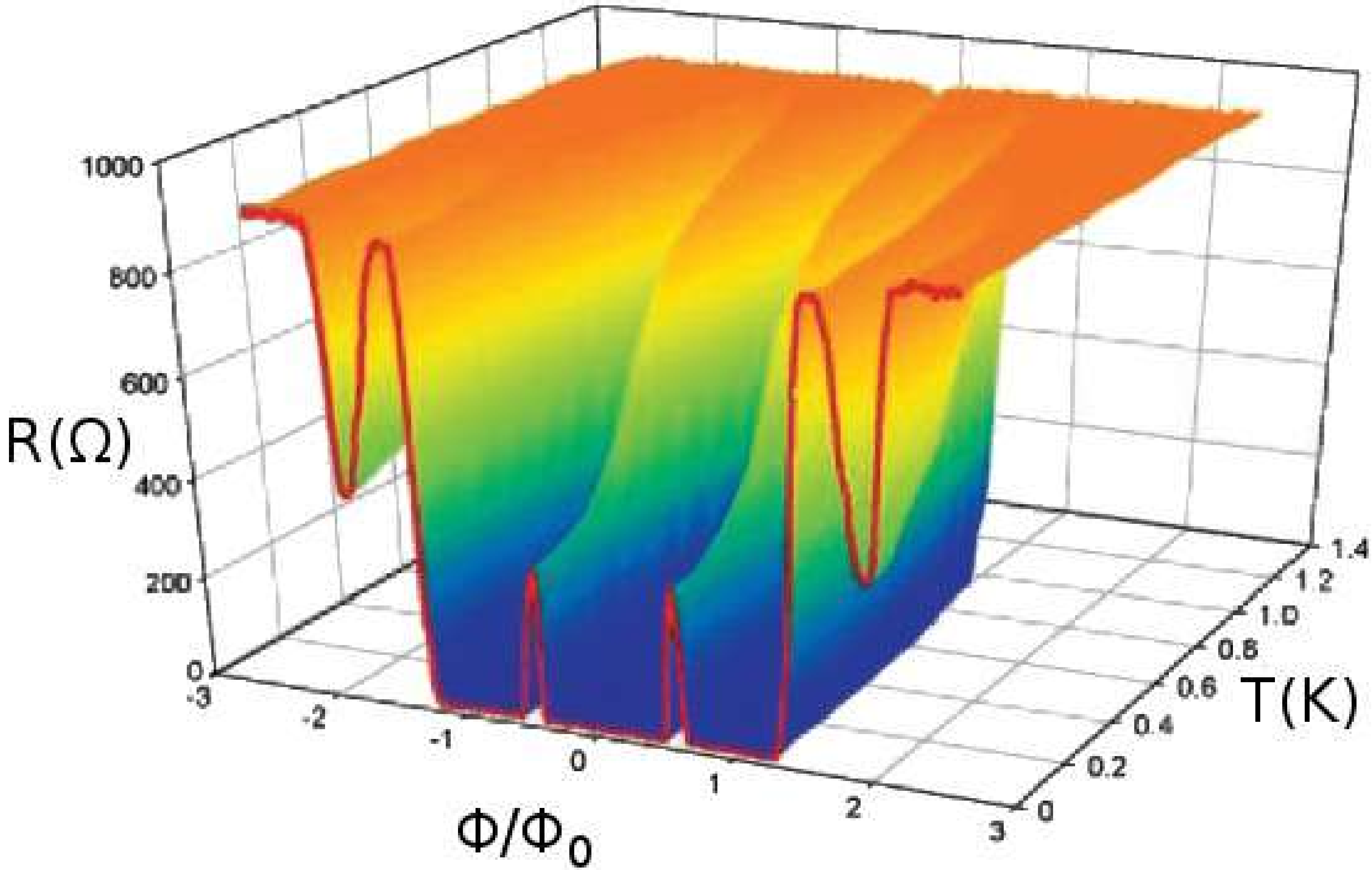




Little-Parks in a small diameter cylinder

- Reduce cylinder diameter to superconducting correlation length [Liu *et al*., Science 2001; Wang *et al*., PRL 2005]



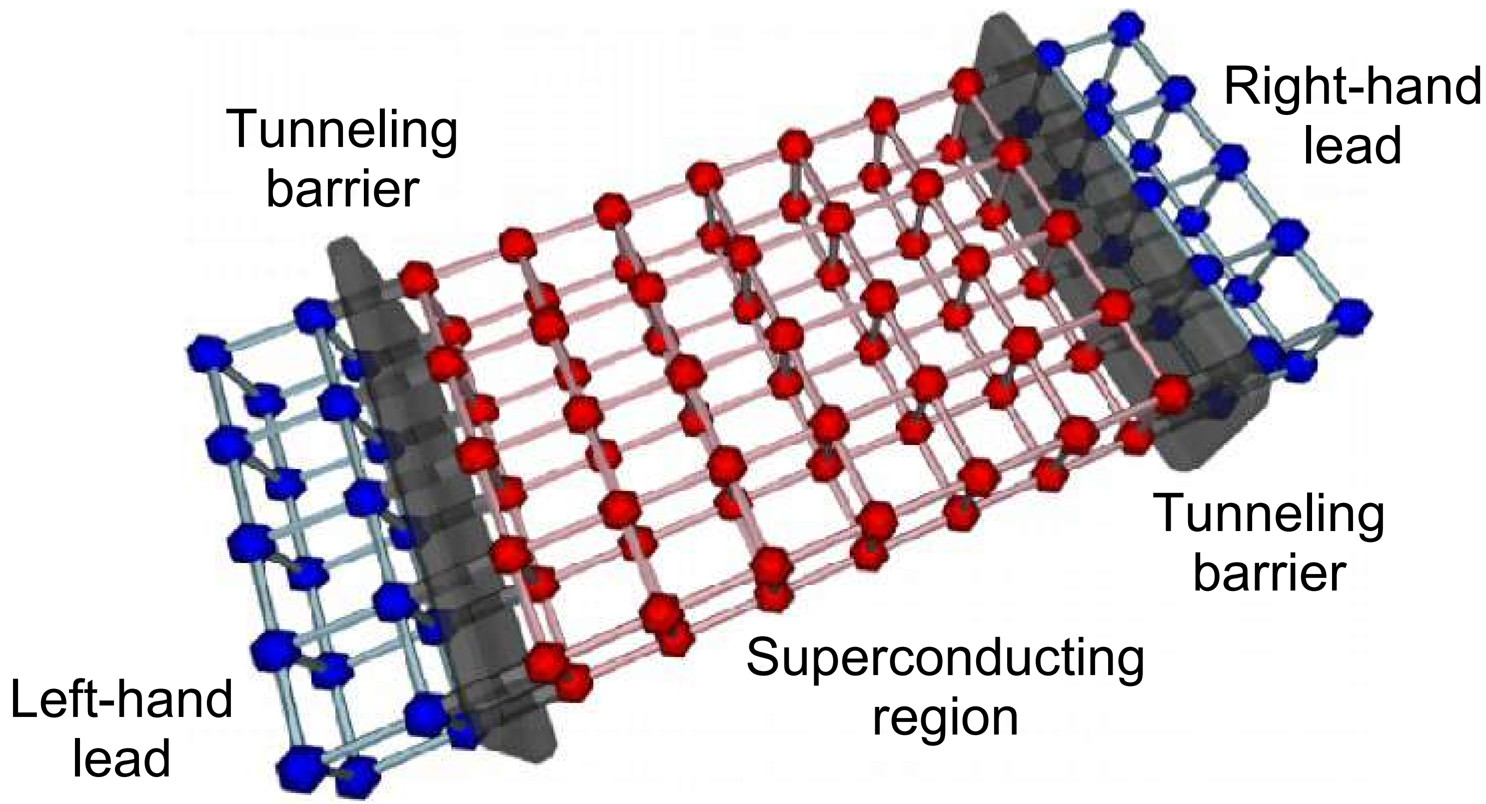
Strategy to study superconductors

- Develop new formalism to:
  - Calculate exact net current flow
  - Extract the microscopic current flow
  - Account for phase and amplitude fluctuations
  - Develop algorithm that permits access to large systems
- Test the formalism against a series of well-established results
- Study the Little Parks effect and magnetoresistance peak

How to calculate the current

- General expression for the current [Meir & Wingreen, PRL 1992]

$$J = \frac{\mathrm{i}e}{2h} \int \mathrm{d}\epsilon \Big[\mathrm{Tr}\left\{ \left(f_{\mathrm{L}}(\epsilon)\Gamma^{\mathrm{L}} - f_{\mathrm{R}}(\epsilon)\Gamma^{\mathrm{R}} \right) \left(G^{\mathrm{r}}_{\mathrm{e}\sigma} - G^{\mathrm{a}\sigma}_{\mathrm{e}} \right) \right\} + \mathrm{Tr}\left\{ (\Gamma^{\mathrm{L}} - \Gamma^{\mathrm{R}}) G^{<}_{\mathrm{e}\sigma} \right\} \Big]$$



Decoupling the interactions

- Negative *U* Hubbard model

$$\hat{H}_{\rm Hubbard} = \sum_{i,\sigma} \epsilon_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} - \sum_i U_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} c_{i\uparrow}$$

$$- \sum_{\langle i,j \rangle,\sigma} \left(t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + t^*_{ij} c^\dagger_{j\sigma} c_{i\sigma} \right)$$

- Decouple in density and Cooper pair channels

$$\rho_{i\sigma} = -|U_i| c^\dagger_{i\sigma} c_{i\sigma} \qquad \Delta_i = |U_i| \; c_{i\downarrow} c_{i\uparrow}$$

- Hamiltonian now contains single-body operators

$$\hat{\mathcal{H}}_{\rm BdG} = \sum_{i,\sigma} (\epsilon_i + \rho_i) c^\dagger_{i\sigma} c_{i\sigma} - \sum_{\langle i,j \rangle,\sigma} \left(t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + t^*_{ij} c^\dagger_{j\sigma} c_{i\sigma} \right)$$

$$+ \sum_i \left(\Delta_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} + \bar{\Delta}_i c_{i\downarrow} c_{i\uparrow} \right) + \sum_i \frac{|\Delta_i|^2 + \rho_i^2}{U_i}$$

Diagonalizing the Hamiltonian

- Hamiltonian now contains single-body operators

$$\hat{\mathcal{H}}_{\mathrm{BdG}} = \sum_{i,\sigma}(\epsilon_i + \rho_i)c^\dagger_{i\sigma}c_{i\sigma} - \sum_{\langle i,j\rangle,\sigma}\left(t_{ij}c^\dagger_{i\sigma}c_{j\sigma} + t^*_{ij}c^\dagger_{j\sigma}c_{i\sigma}\right)$$

$$+ \sum_i \left(\Delta_i c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} + \bar{\Delta}_i c_{i\downarrow}c_{i\uparrow}\right) + \sum_i \frac{|\Delta_i|^2 + \rho_i^2}{U_i}$$

- Energy eigenstates can be found from diagonalization of

$$\hat{\mathcal{H}}_{\mathrm{BgG}} = \frac{|\Delta|^2 + \rho^2}{U} + \begin{pmatrix} c^\dagger_\uparrow & c_\downarrow \end{pmatrix} \begin{pmatrix} \epsilon + \rho & \Delta \\ \bar{\Delta} & -(\epsilon + \rho) \end{pmatrix} \begin{pmatrix} c_\uparrow \\ c^\dagger_\downarrow \end{pmatrix} + \epsilon + \rho$$

Accelerated Metropolis sampling

- To perform thermal sum calculate

  $$\langle J \rangle = \sum_{\Delta,\rho} J[\Delta,\rho] e^{-\beta(E[\Delta,\rho]-E_0)}$$

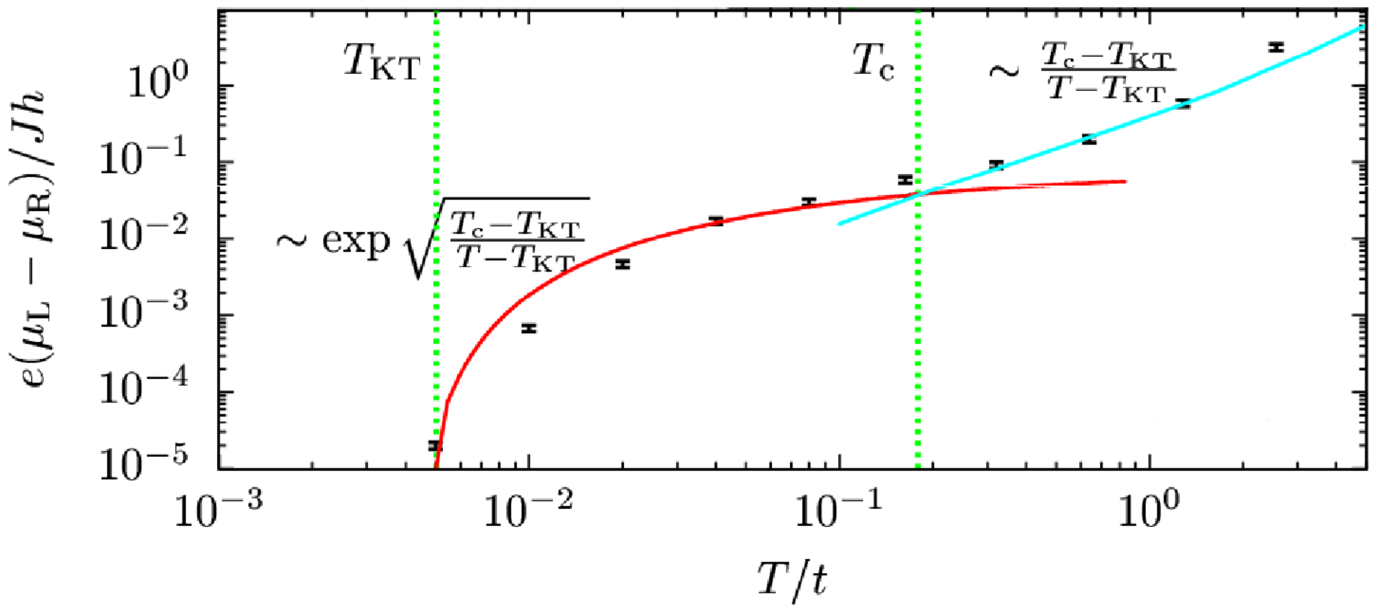
- Propose new configuration of Δ and ρ, accept with probability

  $$\exp(\beta E[\Delta_{\mathrm{old}},\rho_{\mathrm{old}}]-\beta E[\Delta_{\mathrm{new}},\rho_{\mathrm{new}}])$$

- Calculating $E[\Delta,\rho]$ costs $O(N^3)$, where N is the number of sites
- New method calculates $E[\Delta,\rho]-E[\Delta+\delta\Delta,\rho+\delta\rho]$ using a order M Chebyshev expansion [Weisse 09] in $O(N^{0.9} M^{2/3})$ time

Verification

- Resistivity at the Kosterlitz-Thouless transition
- Nonlinear *IV* characteristics
- Length dependence of conductivity
- Andreev reflection
- Josephson junction
- Little-Parks effect in large diameter cylinder



Halperin & Nelson, J. Low Temp. Phys 1979

Ambegaokar *et al.*, PRB 1980

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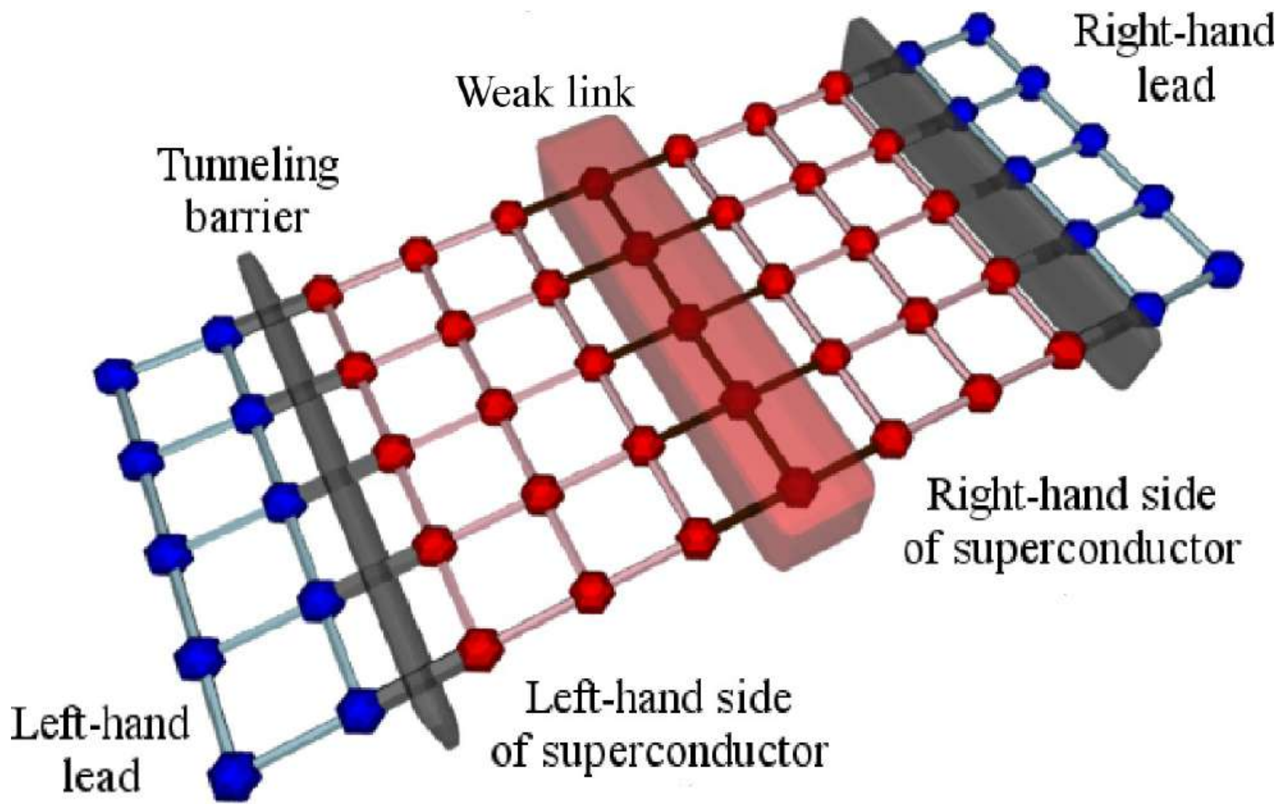

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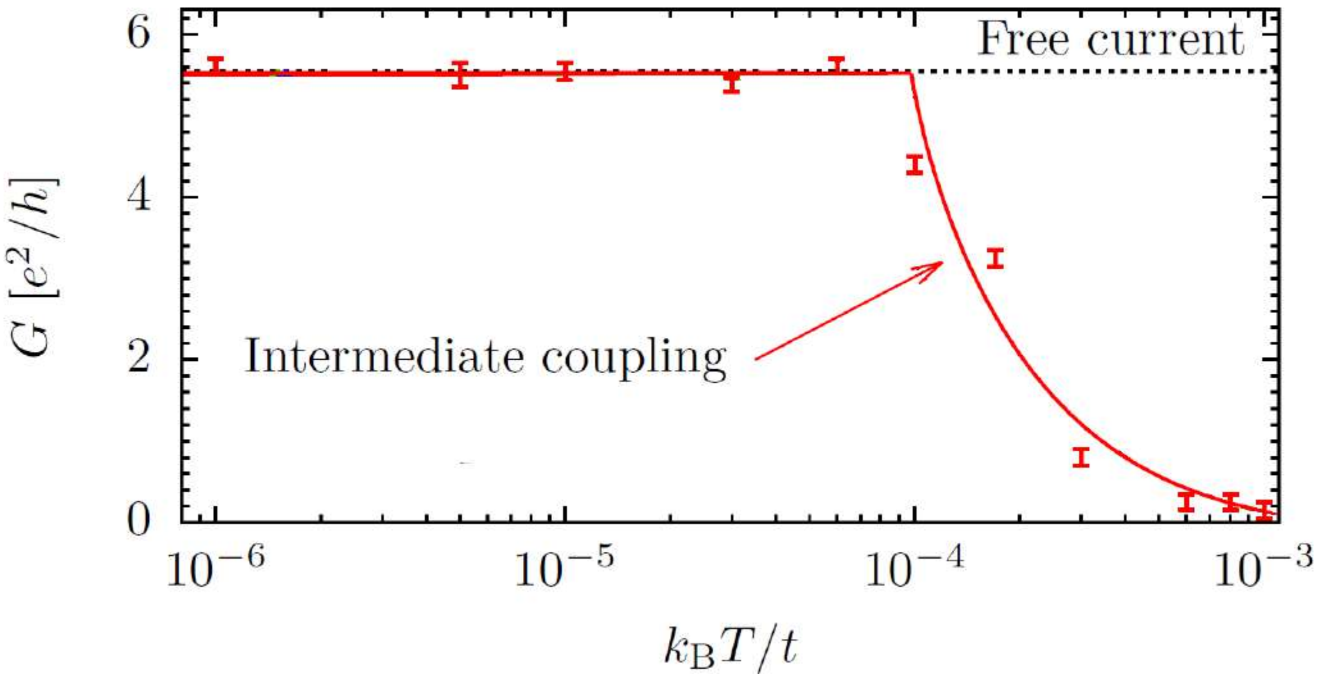

Ambegaokar & Baratoff, PRL **10**, 486 (1963)

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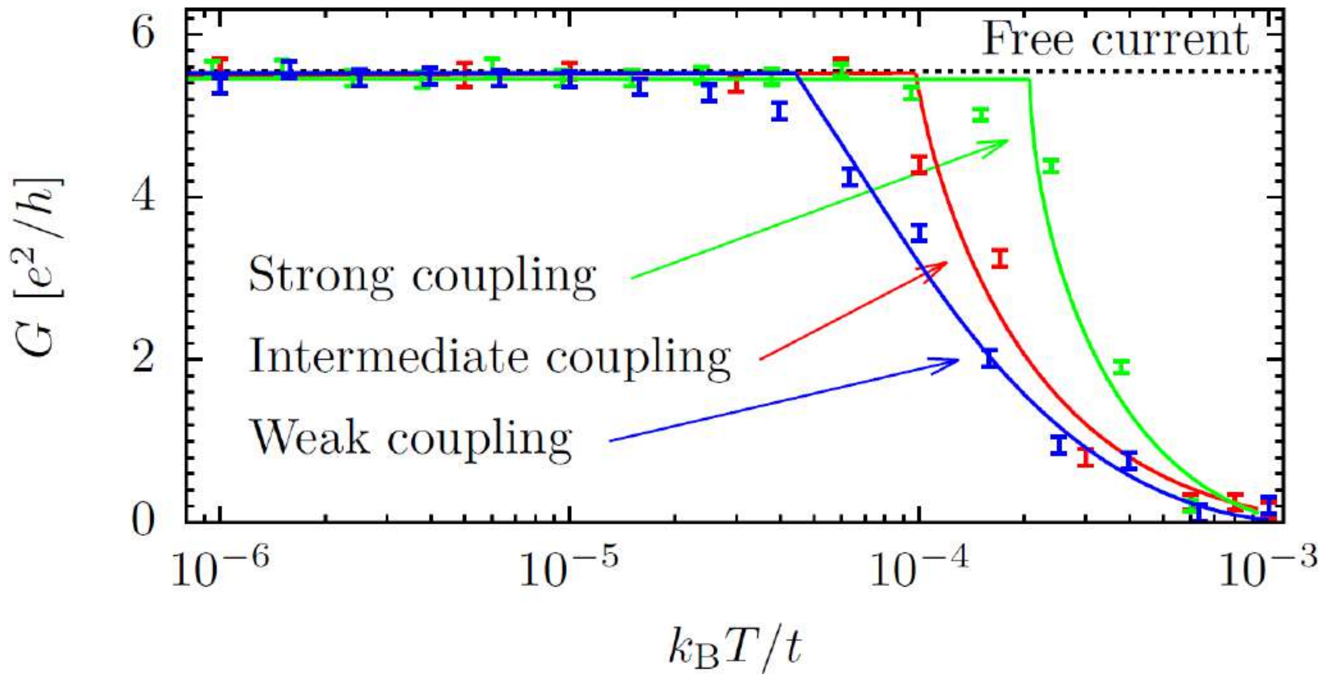

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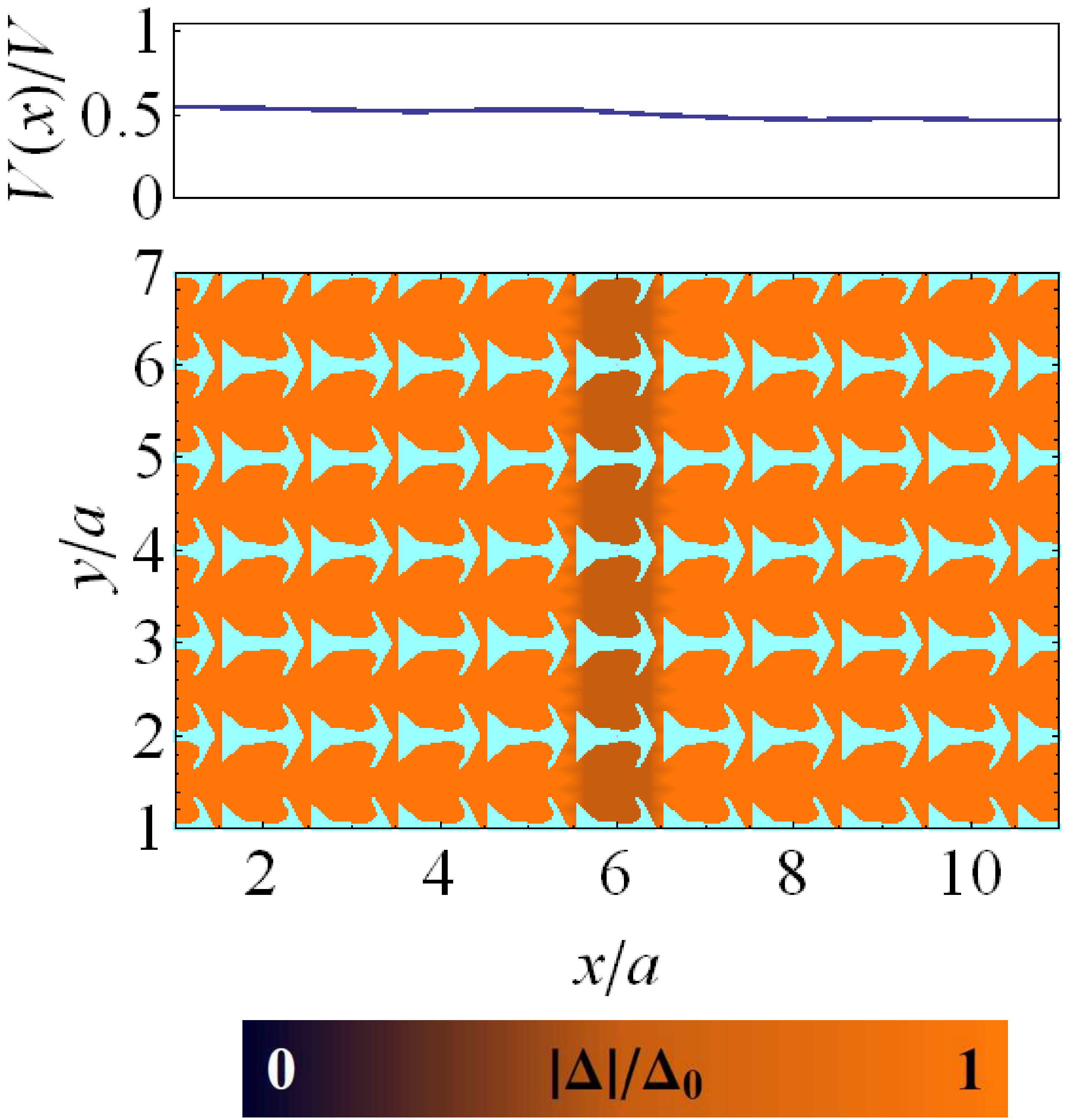

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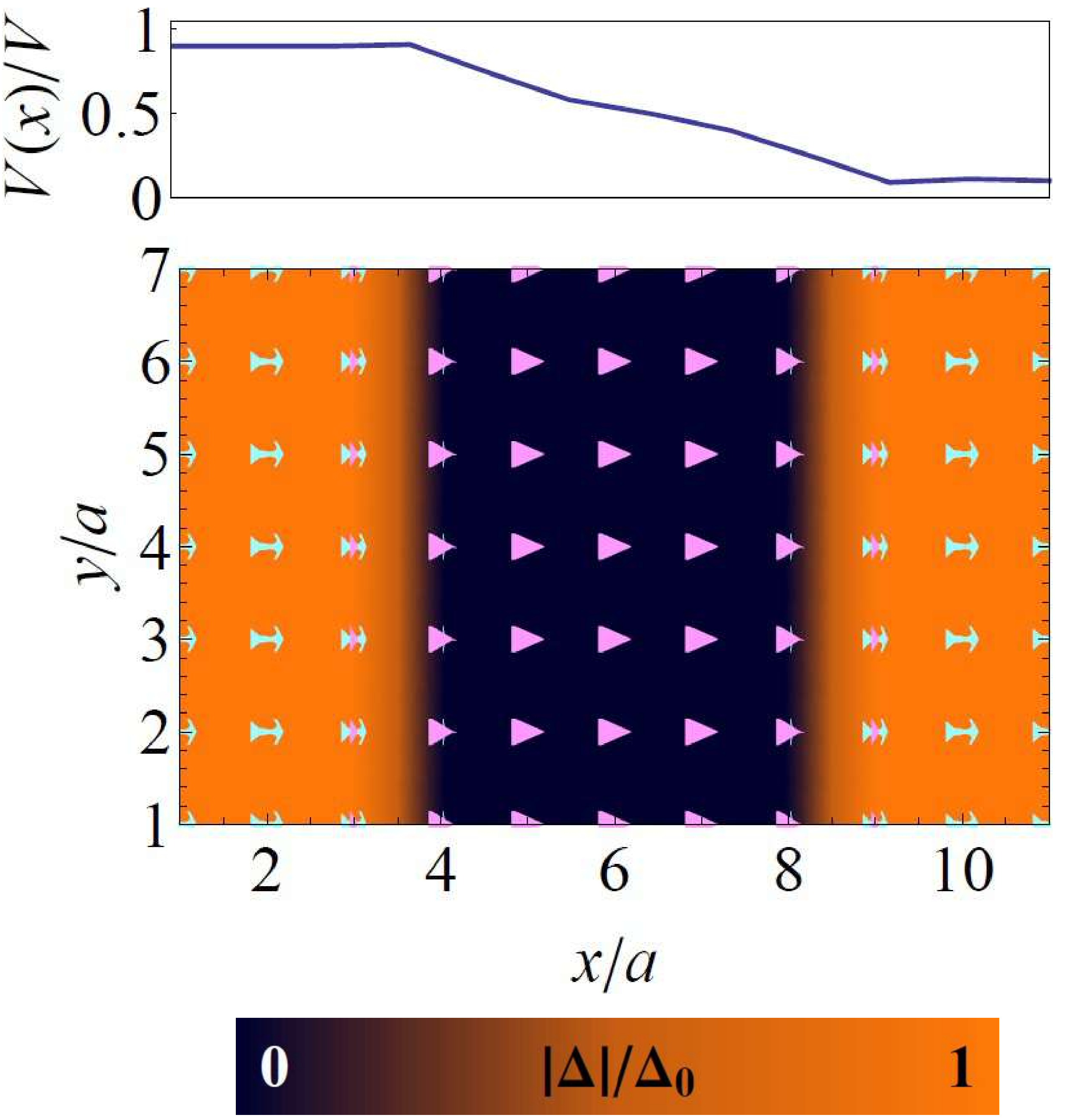

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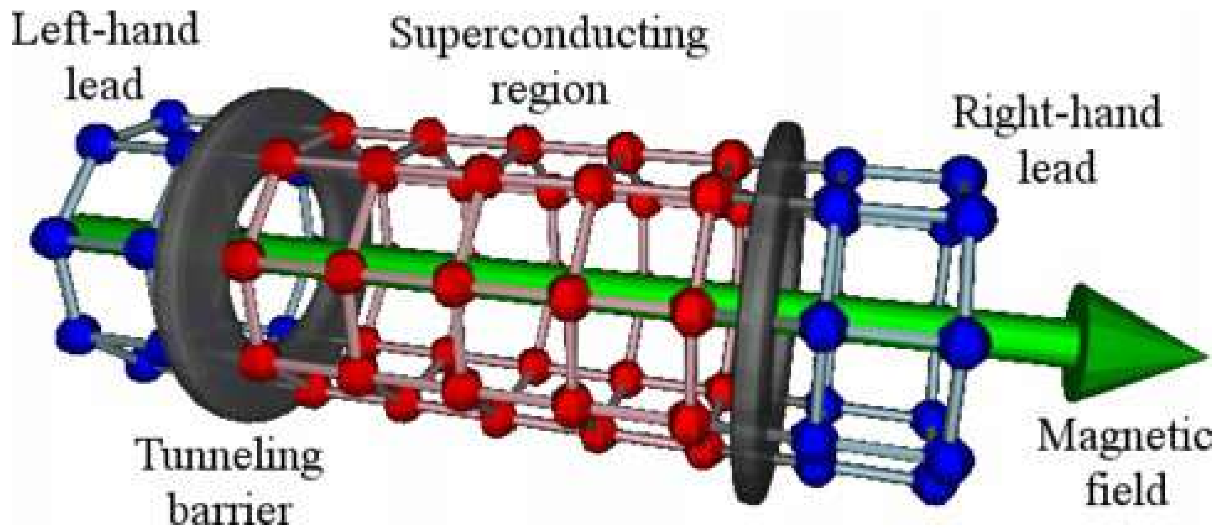
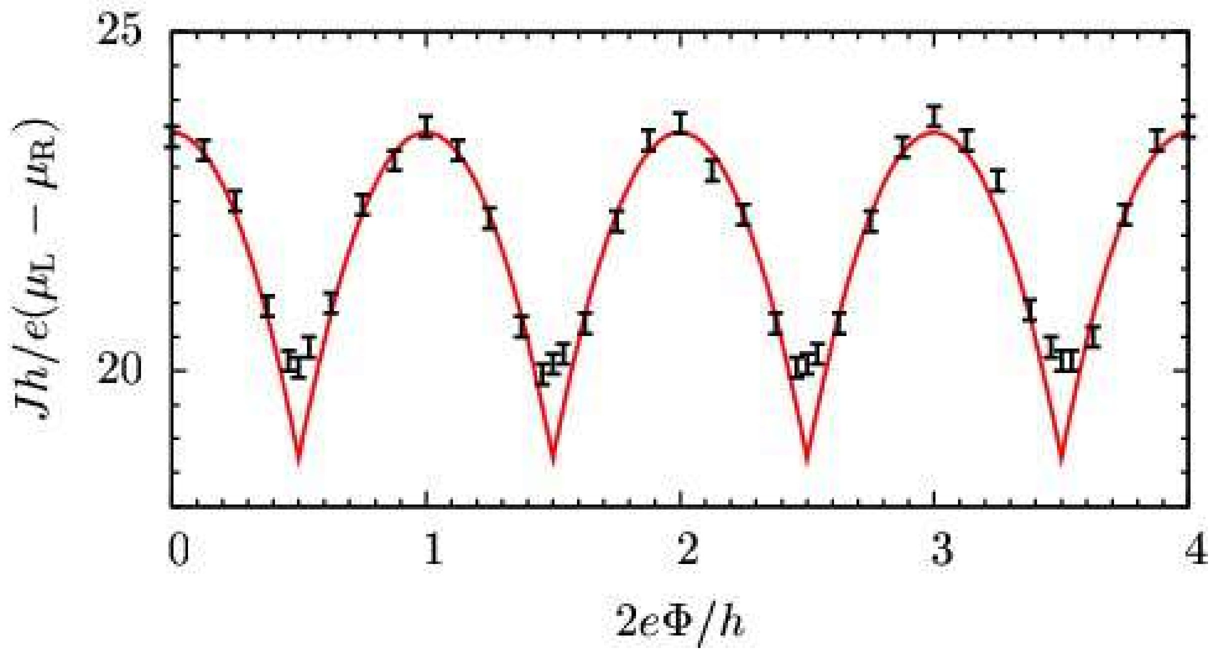
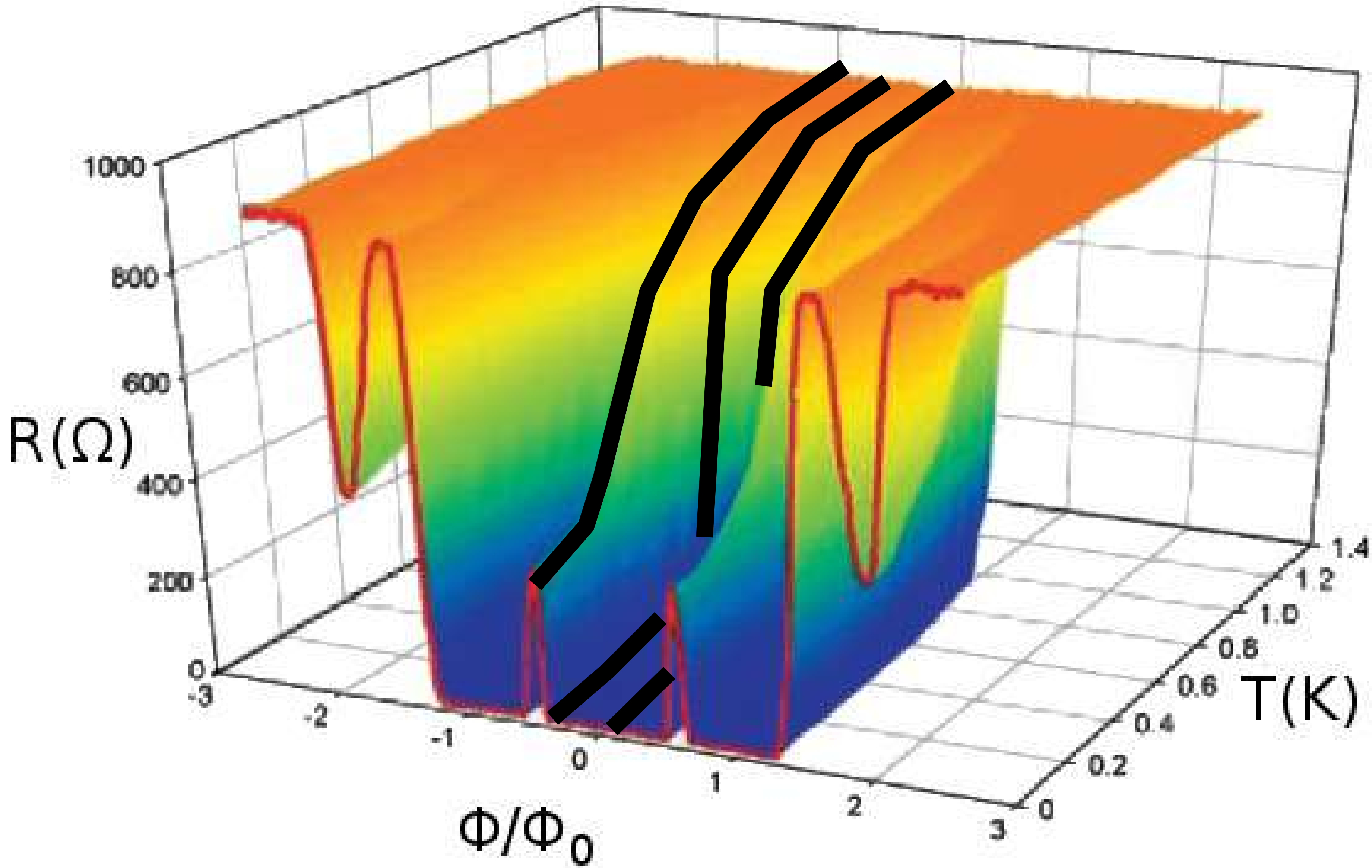
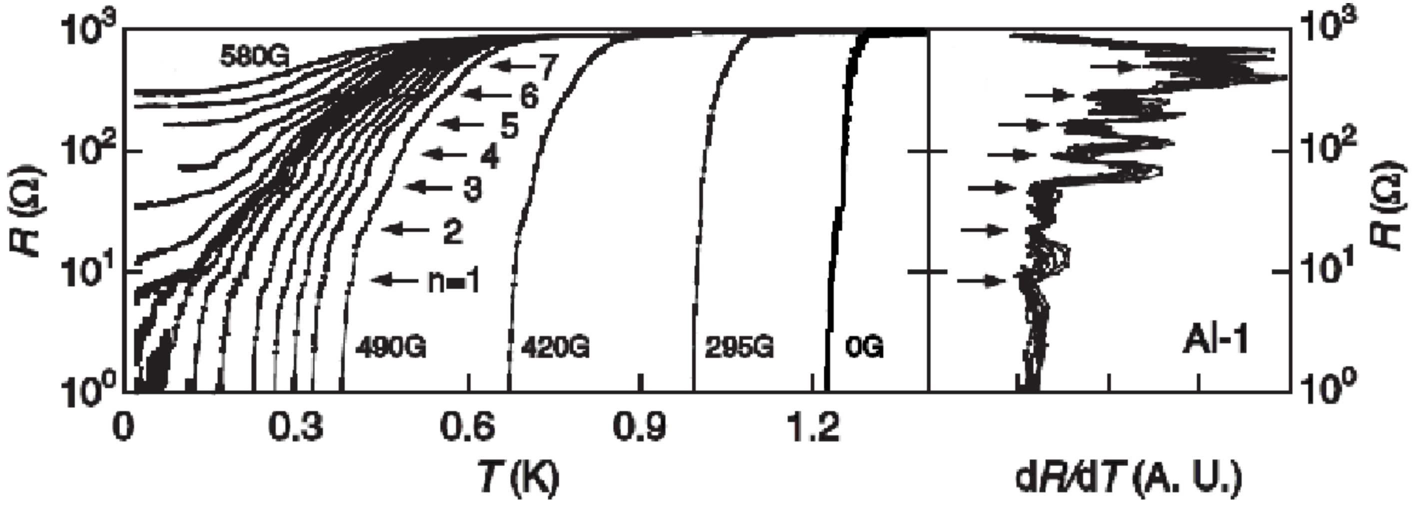


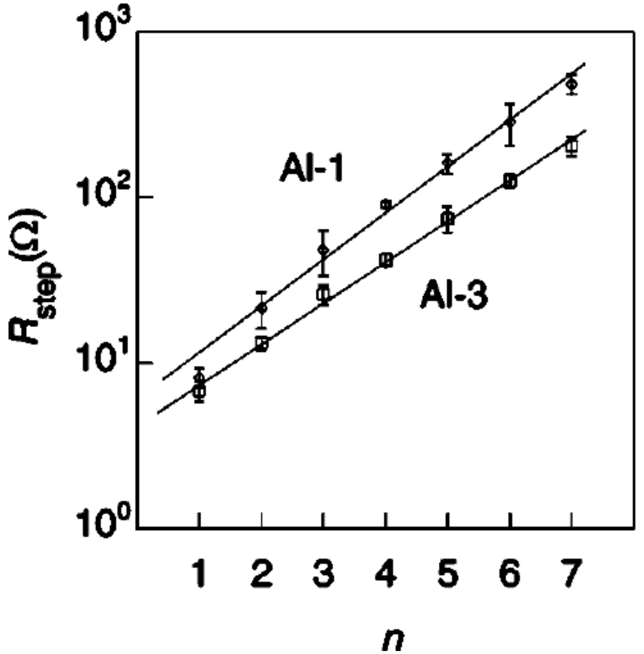


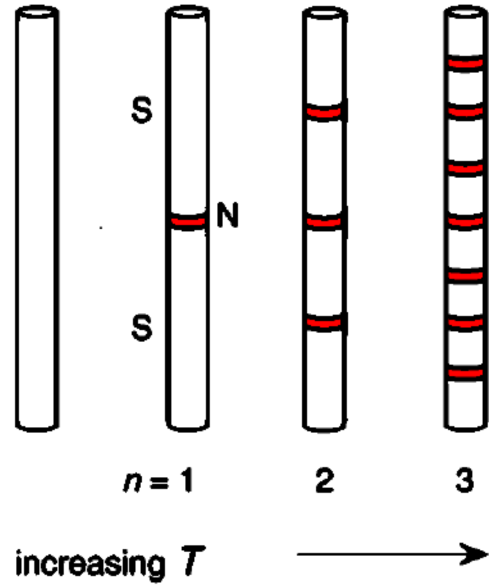
Little-Parks in a small diameter cylinder



Quantum phase transition hypothesis

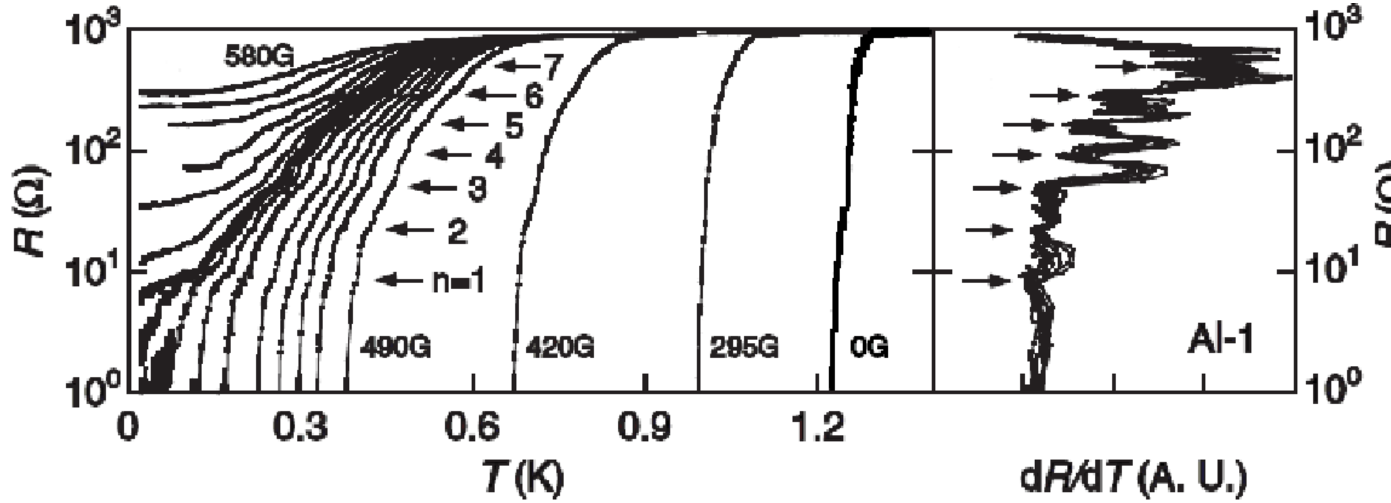


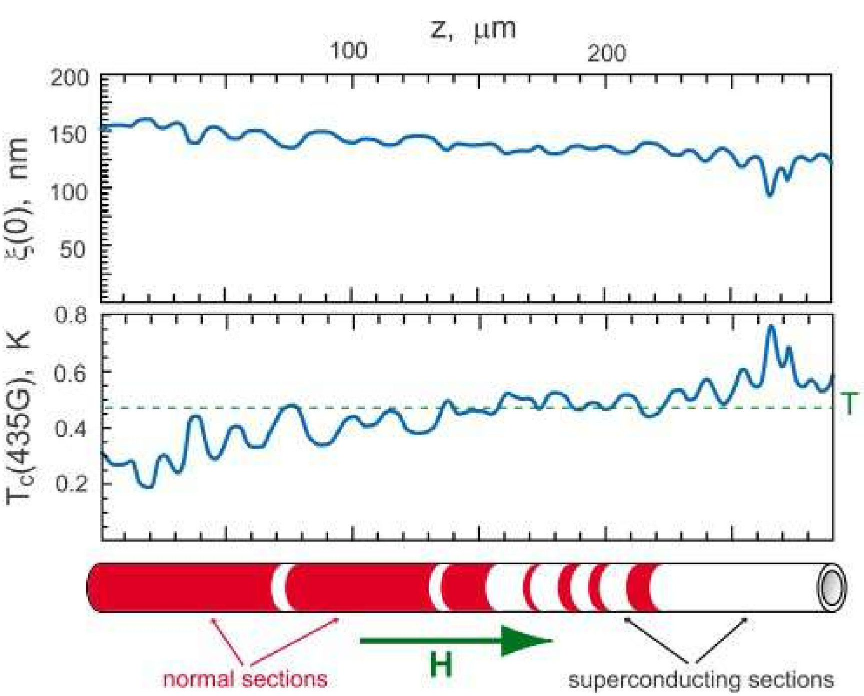


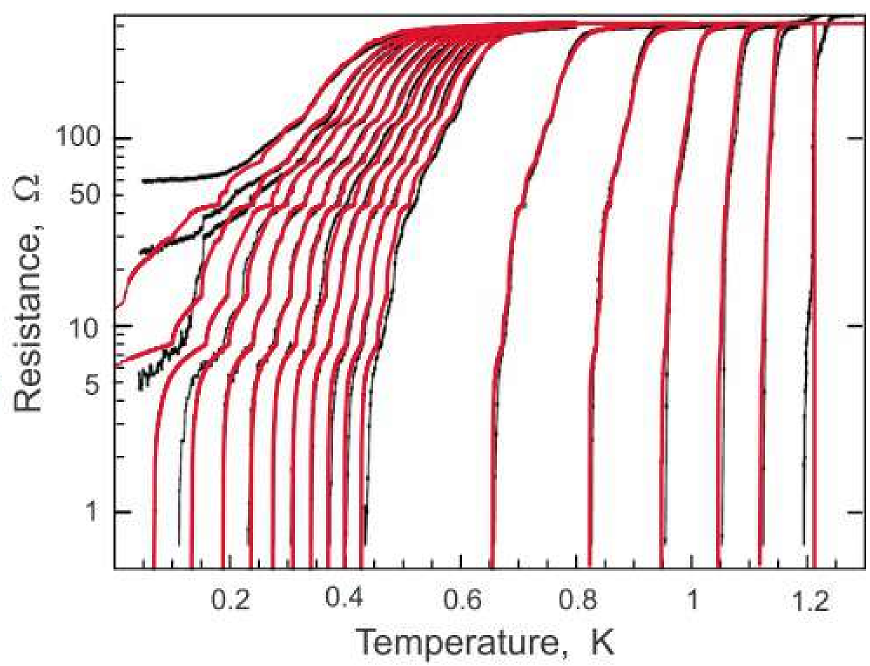


Wang et al. PRL (2005)

Mean-field BCS transition hypothesis



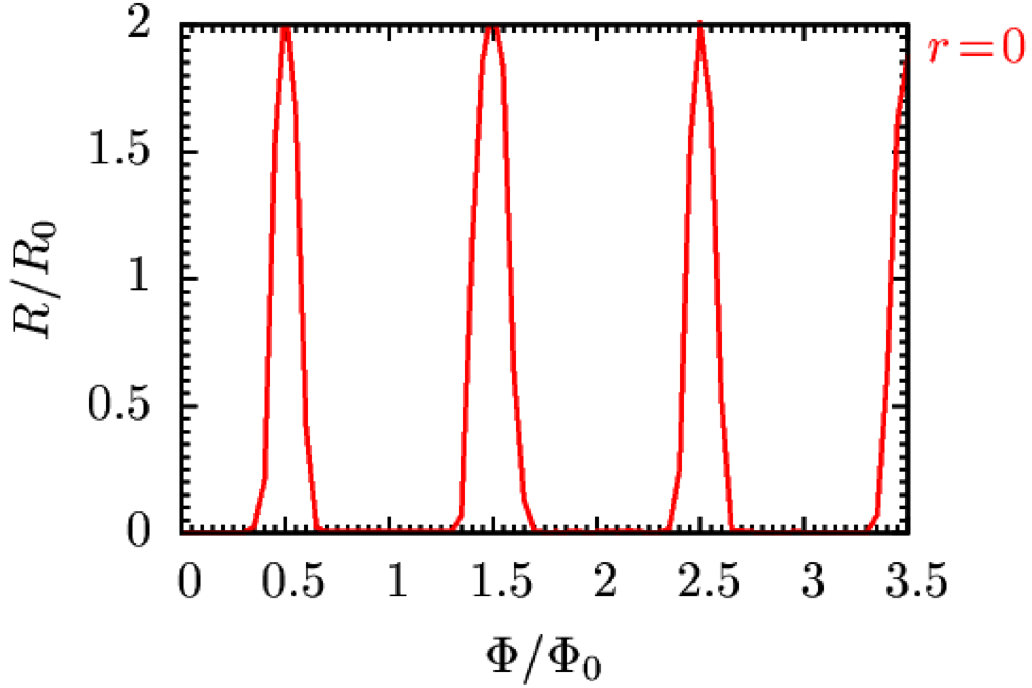


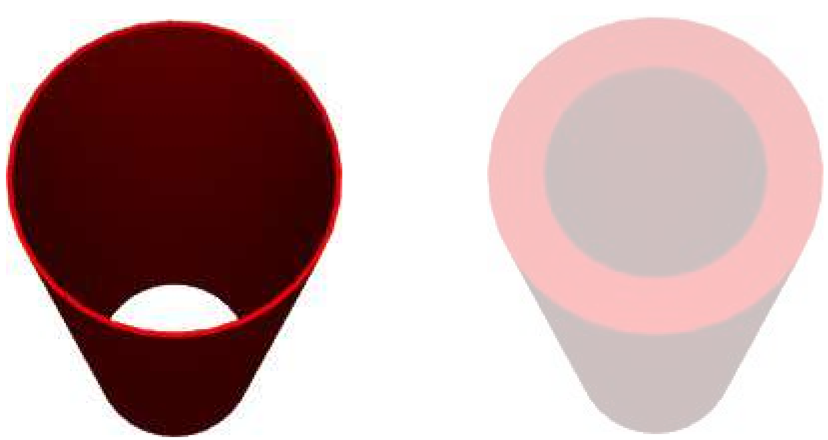


Dao & Chibotaru, PRB (2009)

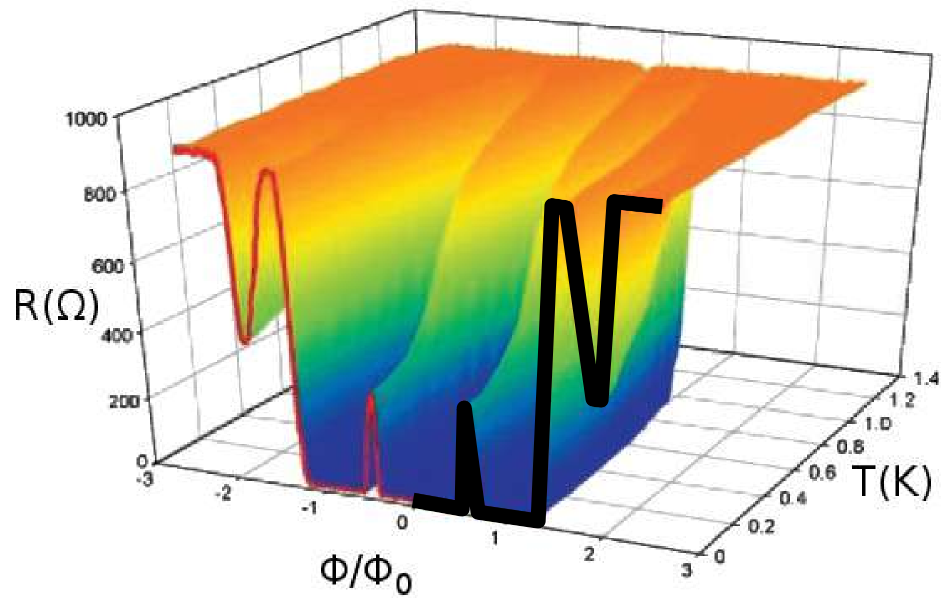
Little-Parks in a small diameter cylinder

Theory:





Experiment:



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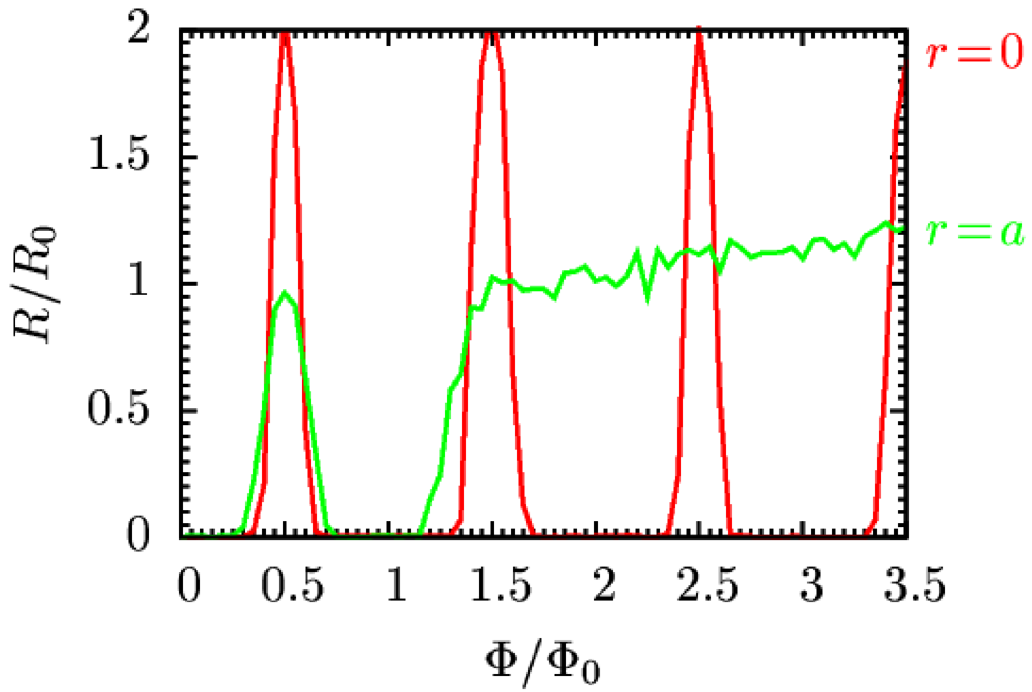

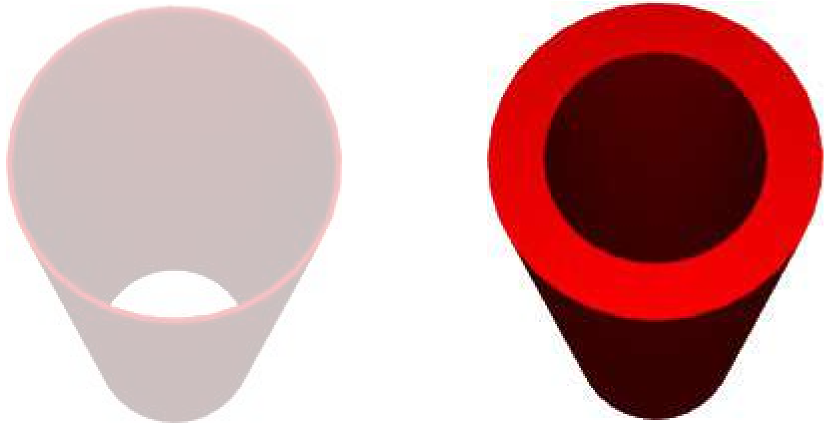

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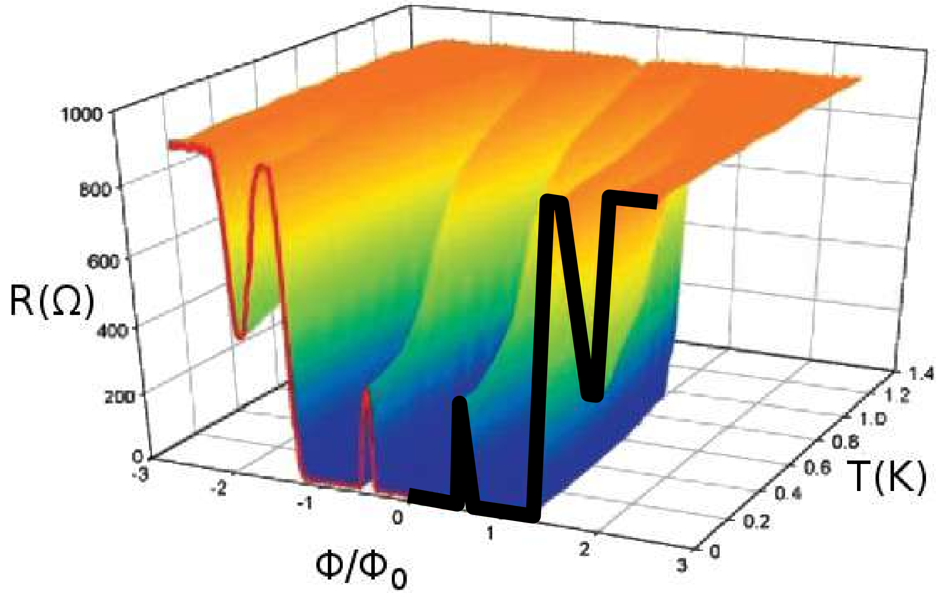
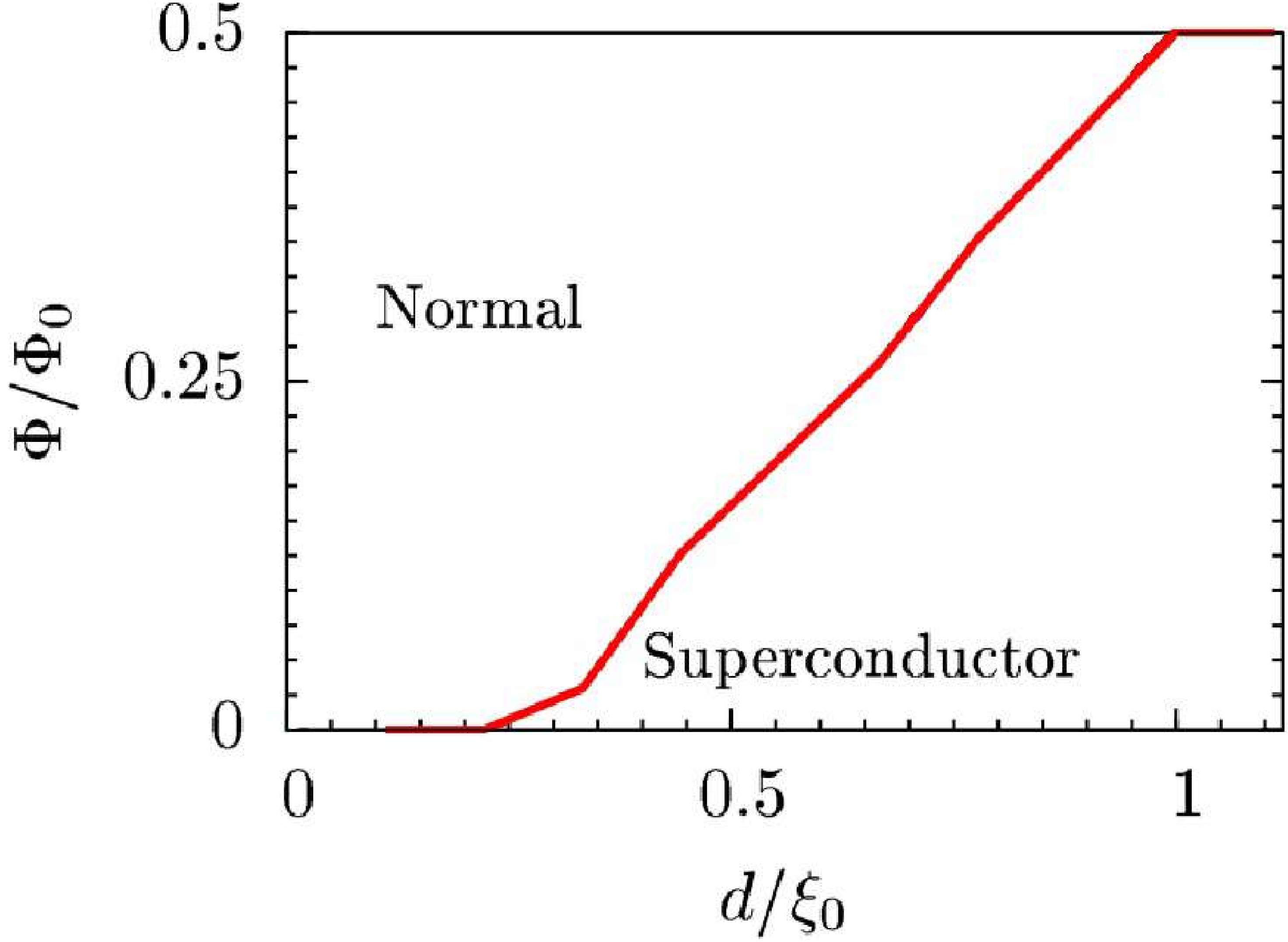


Variation with diameter



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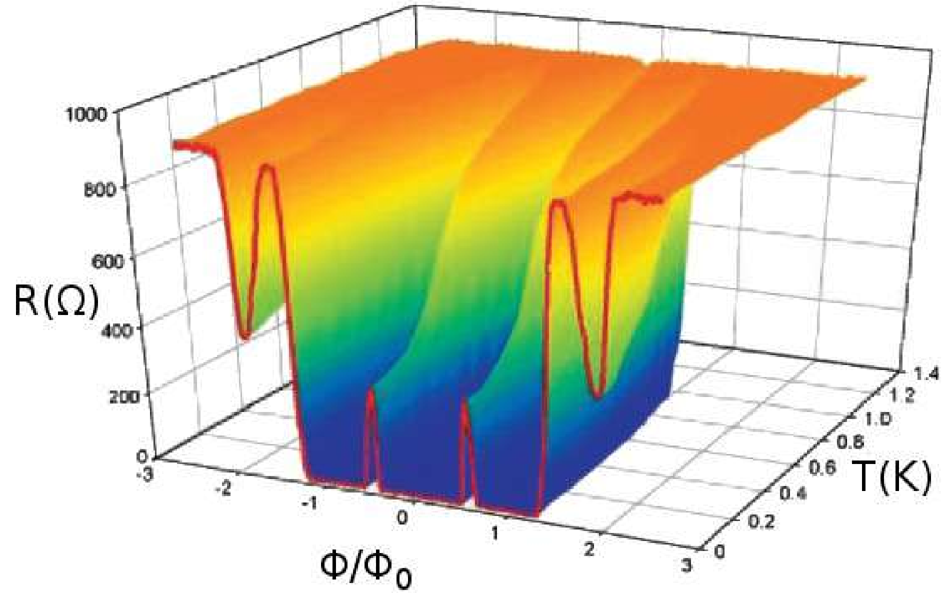

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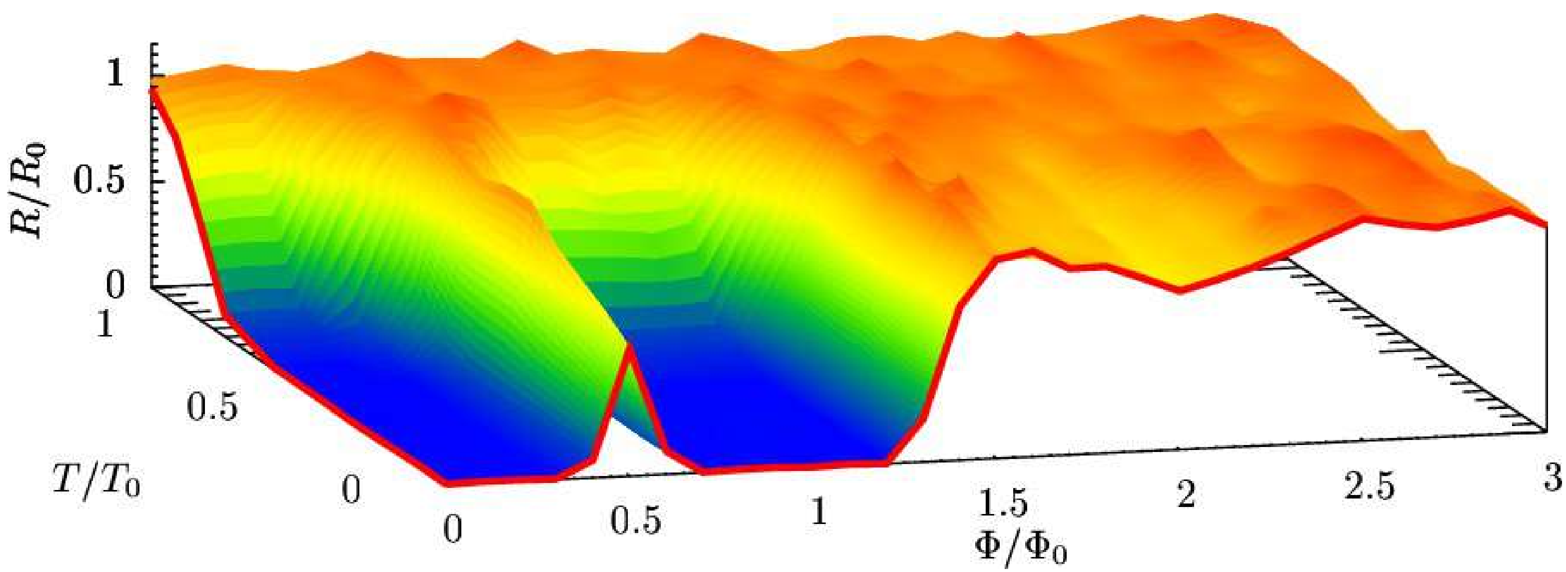

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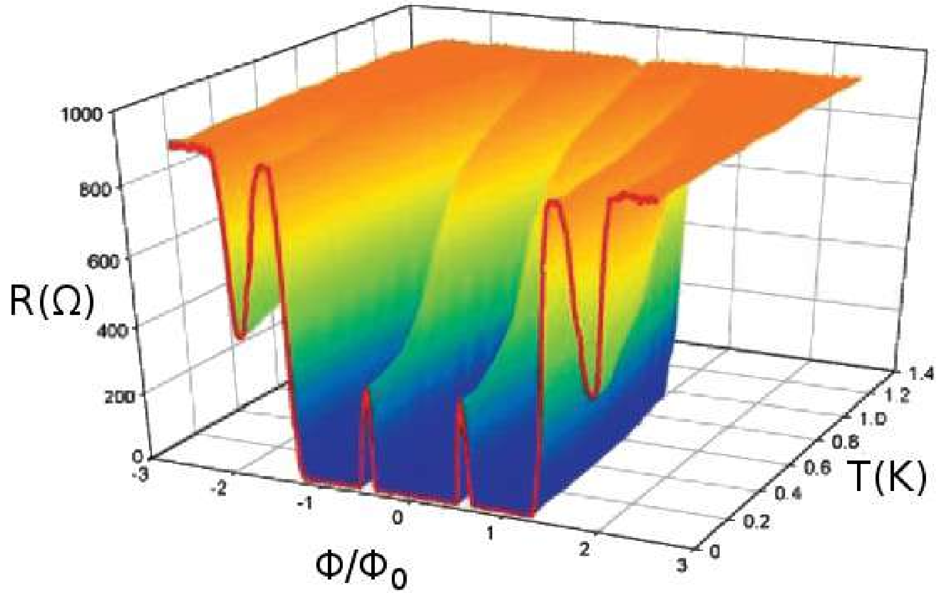

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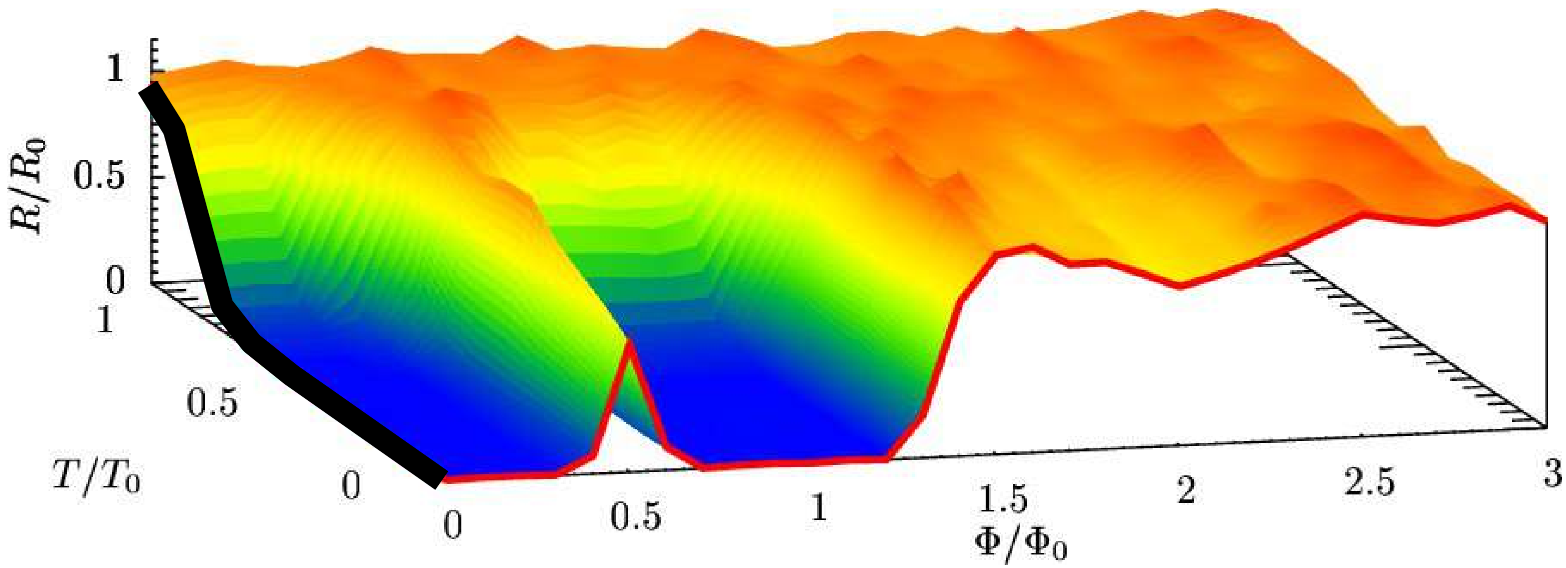
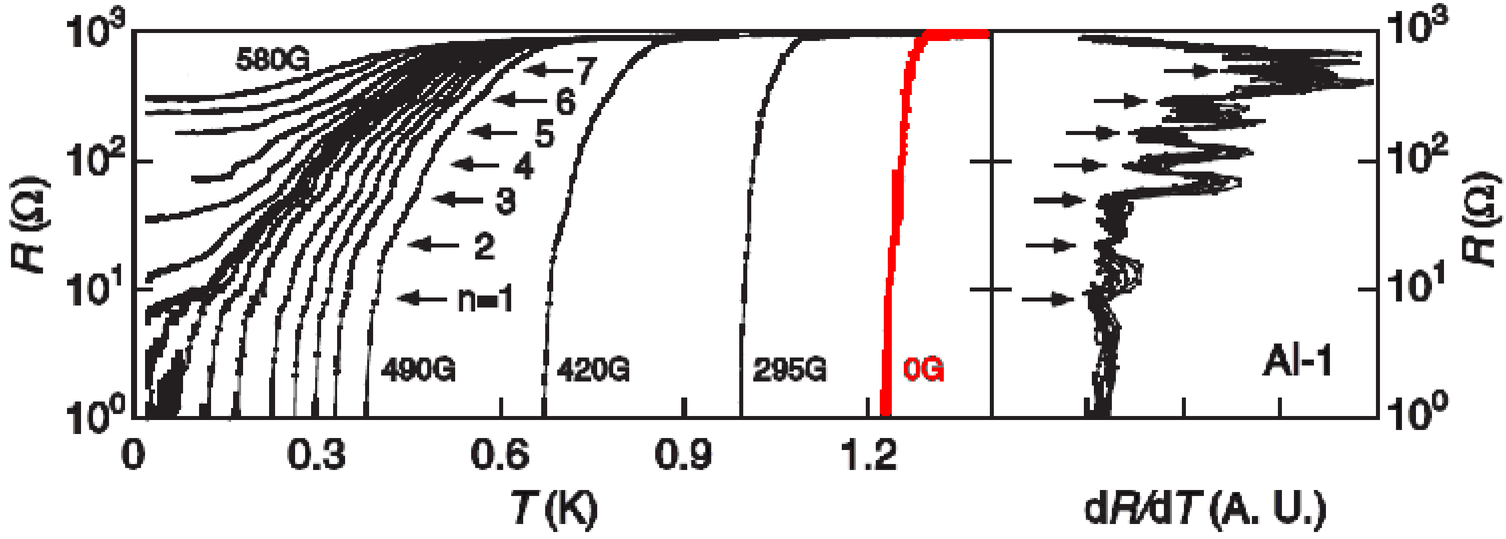
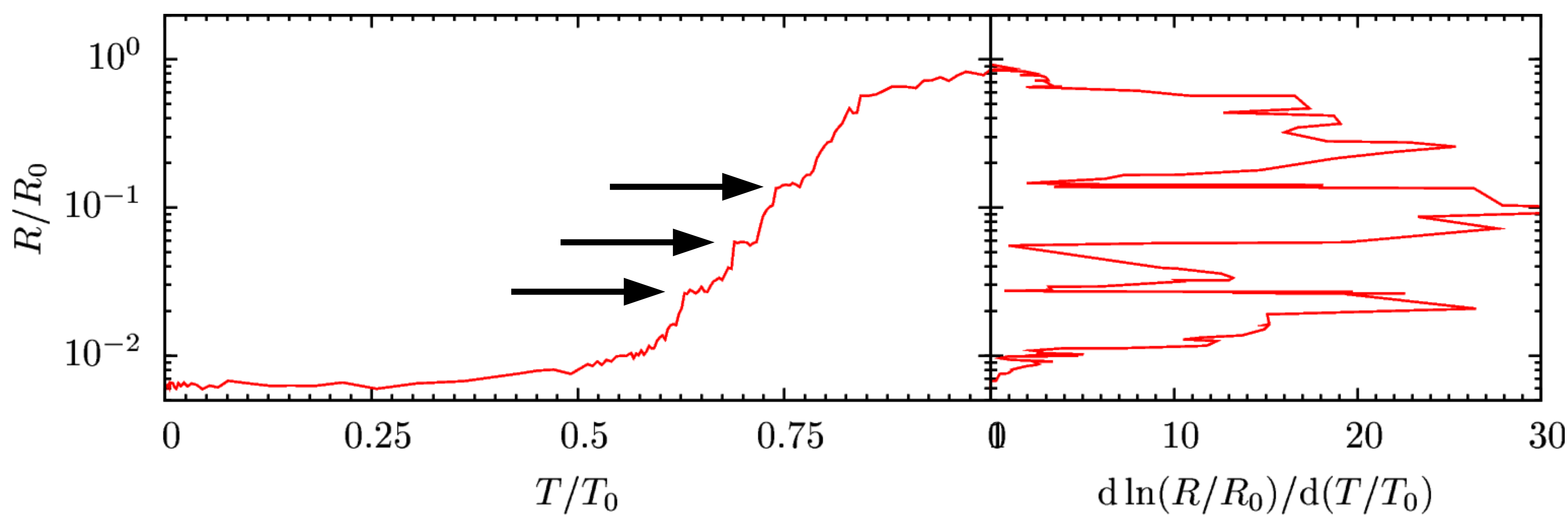


Evidence of phase reconstruction

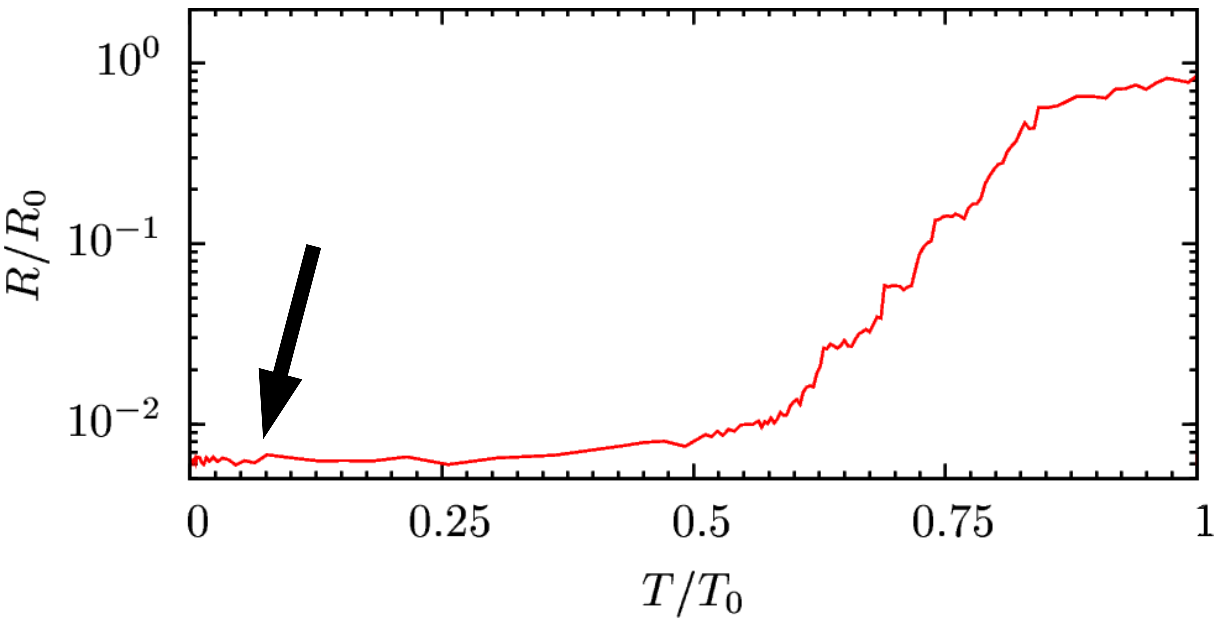
- Experiment:

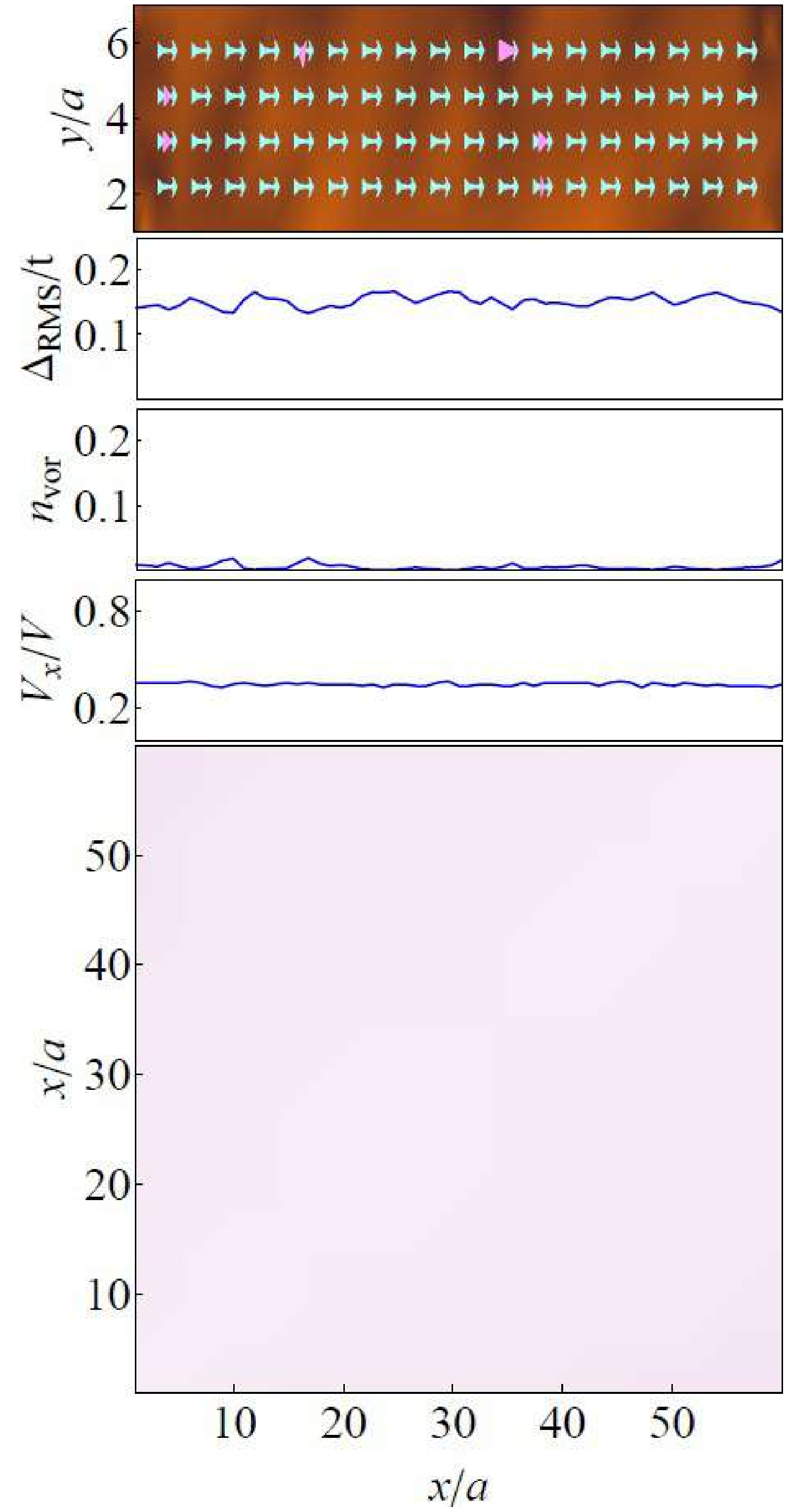


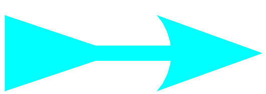
- Theory:

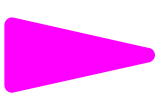


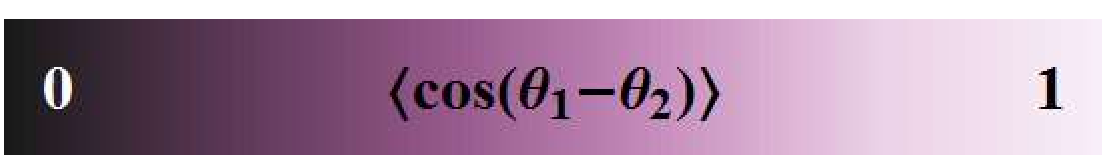
Completely superconducting



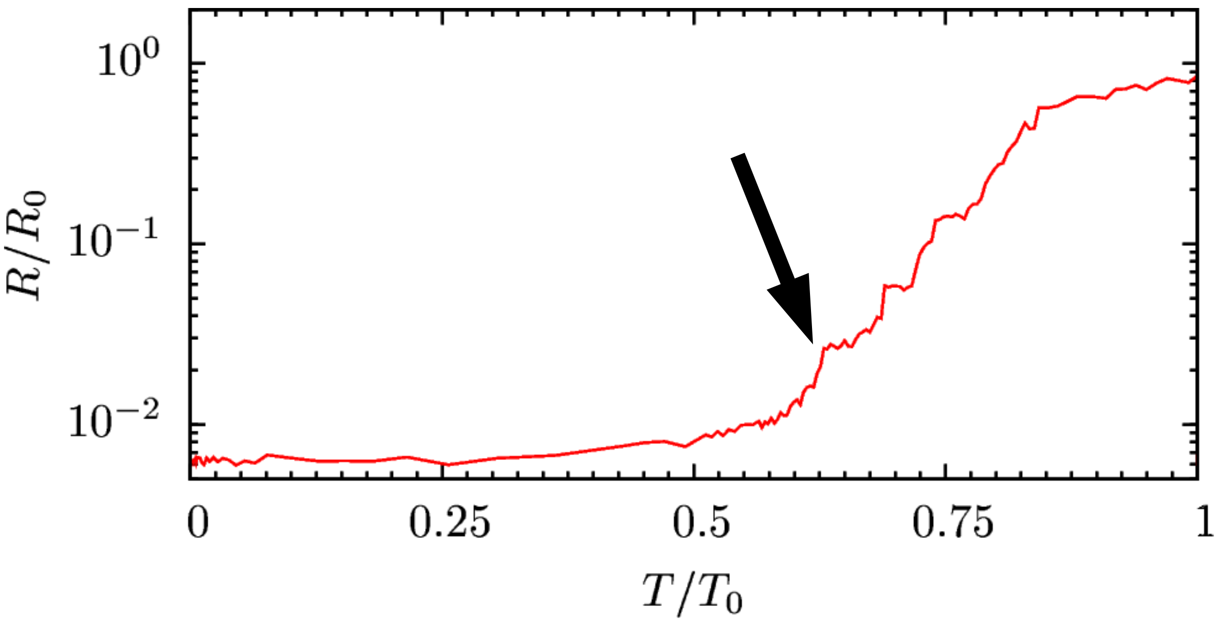


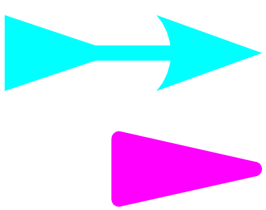

Superconducting current


Normal current



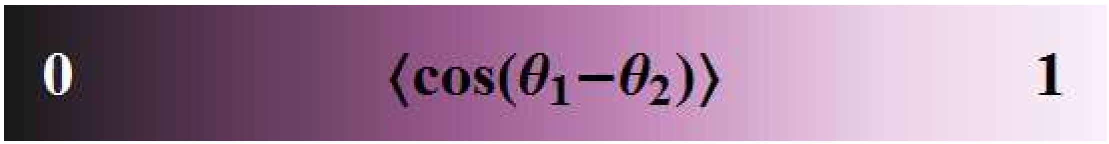
Two superconducting regions

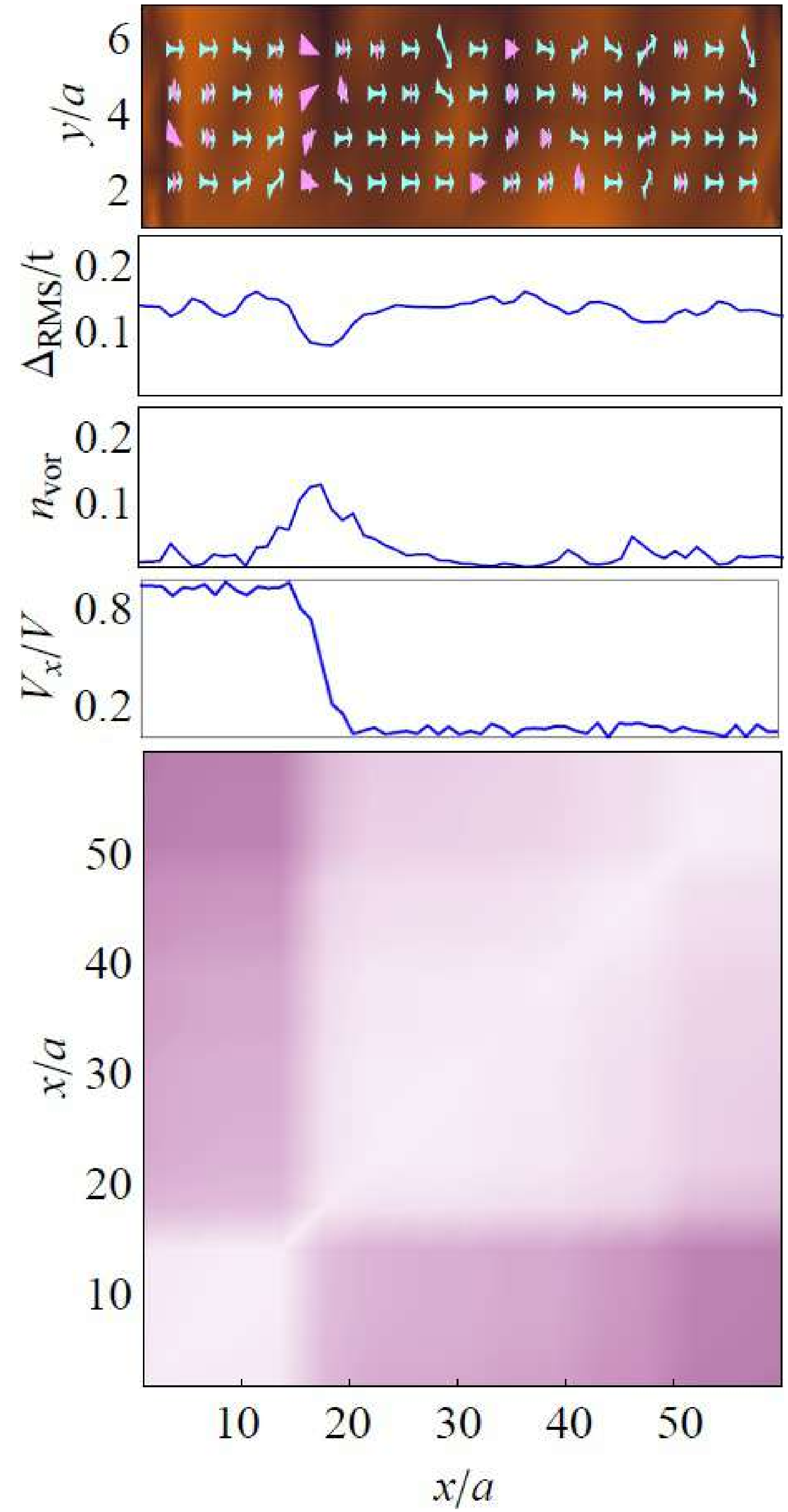




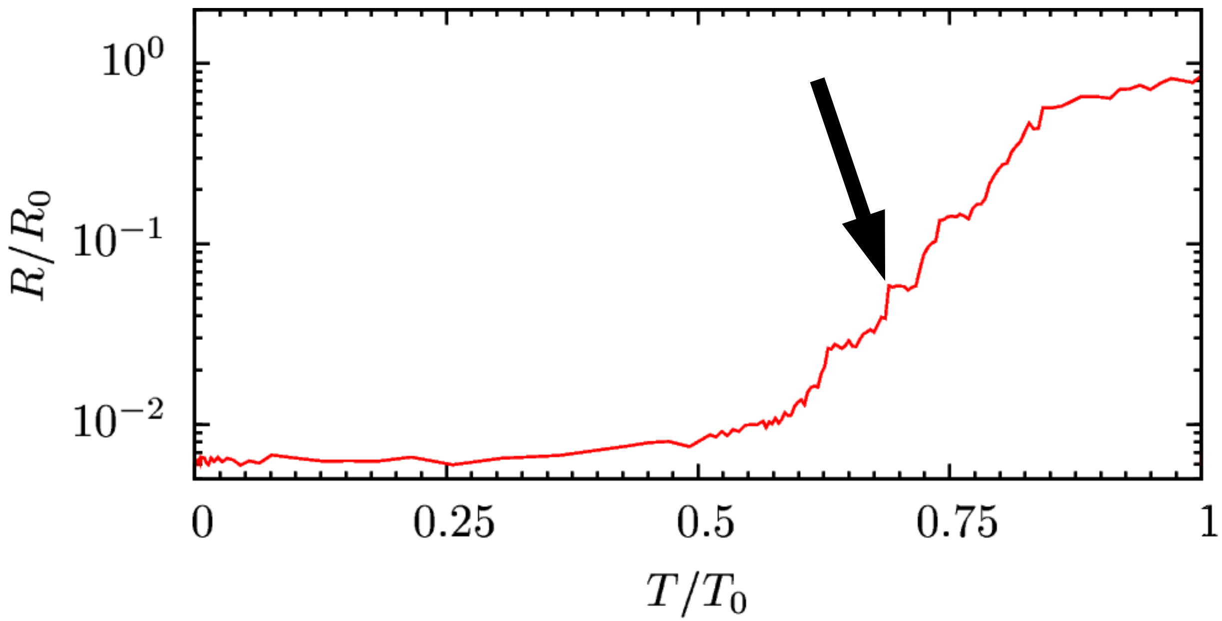
Superconducting current

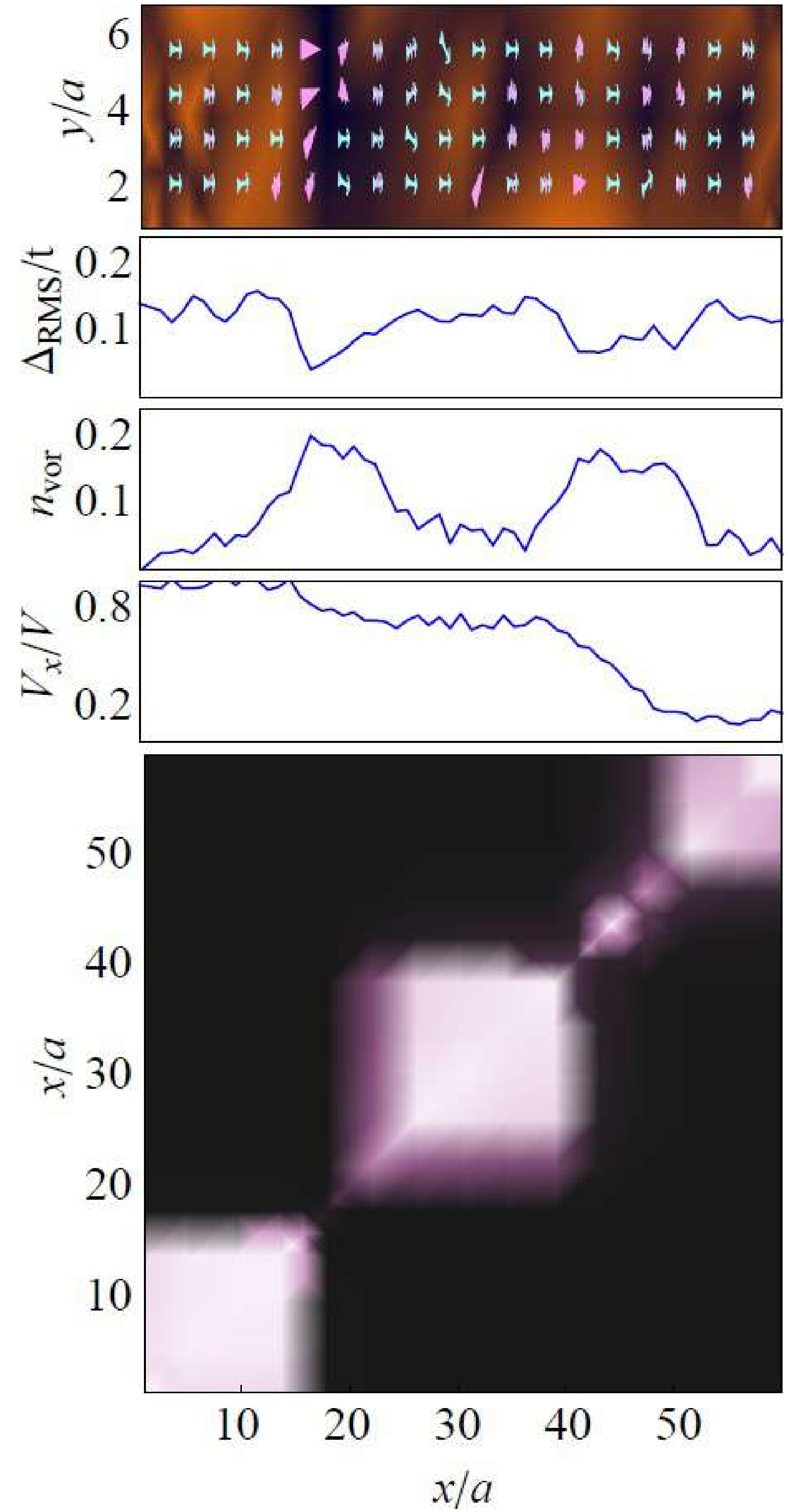
Normal current

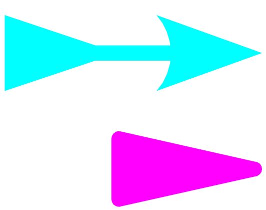




Three superconducting regions

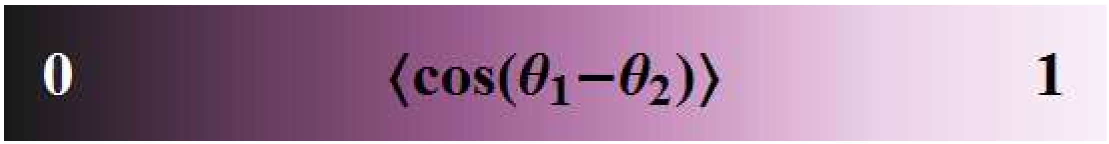




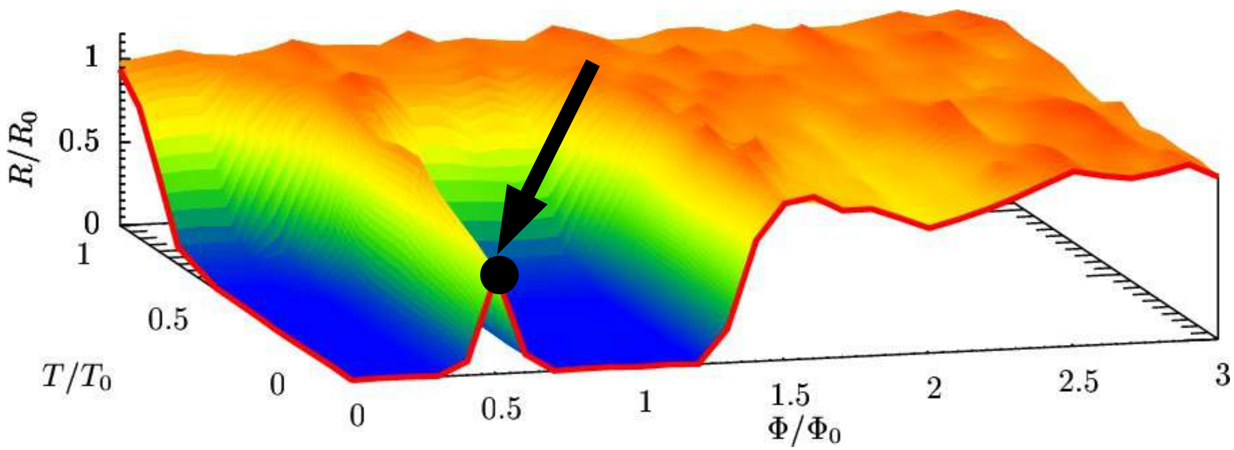


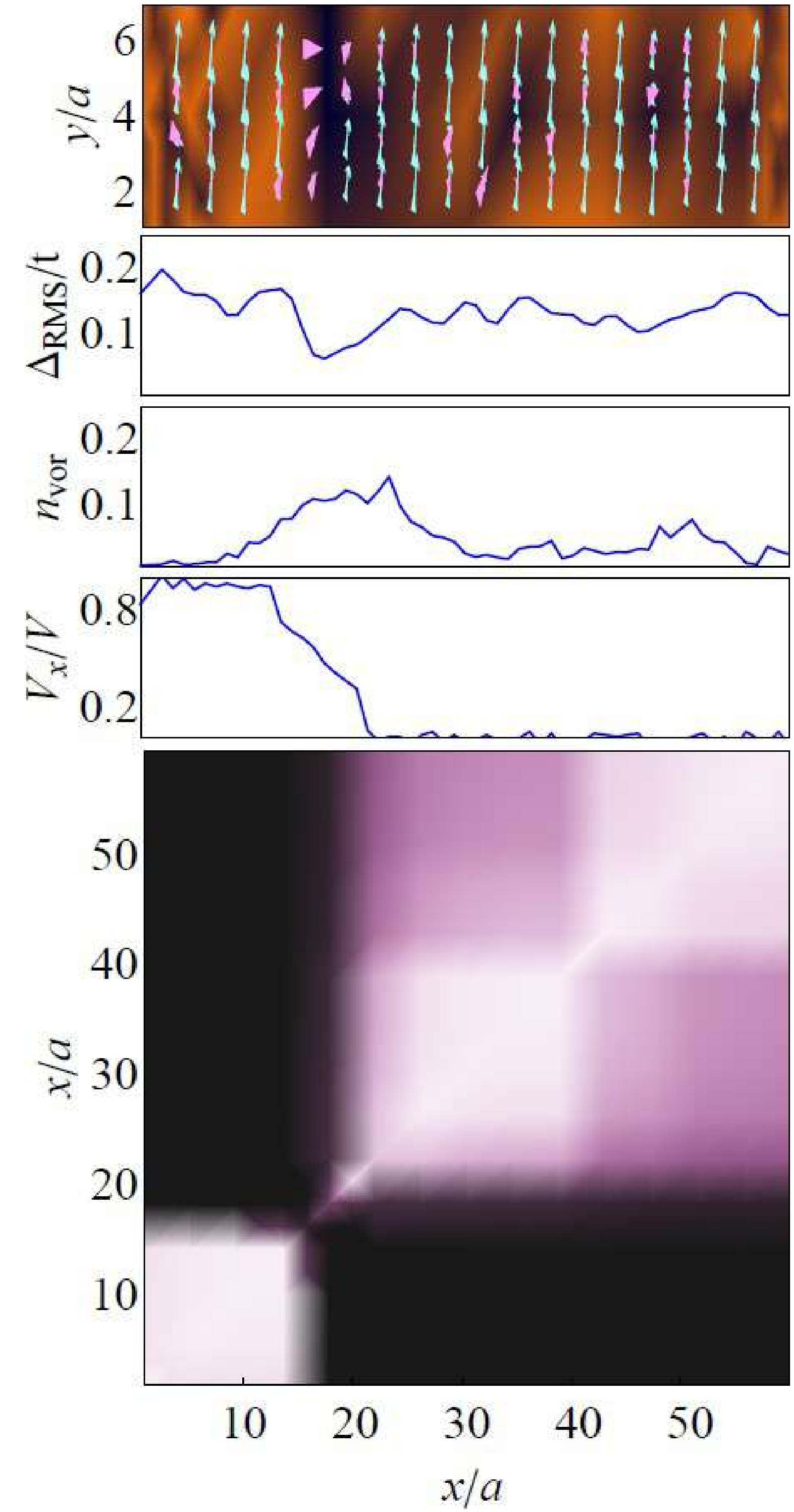
Superconducting current

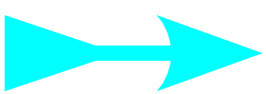
Normal current



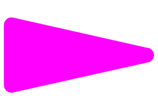
Half flux quantum normal state



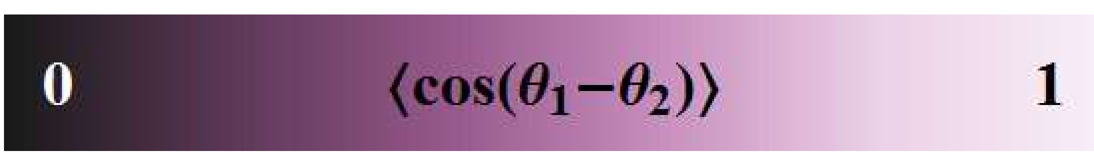




Superconducting current

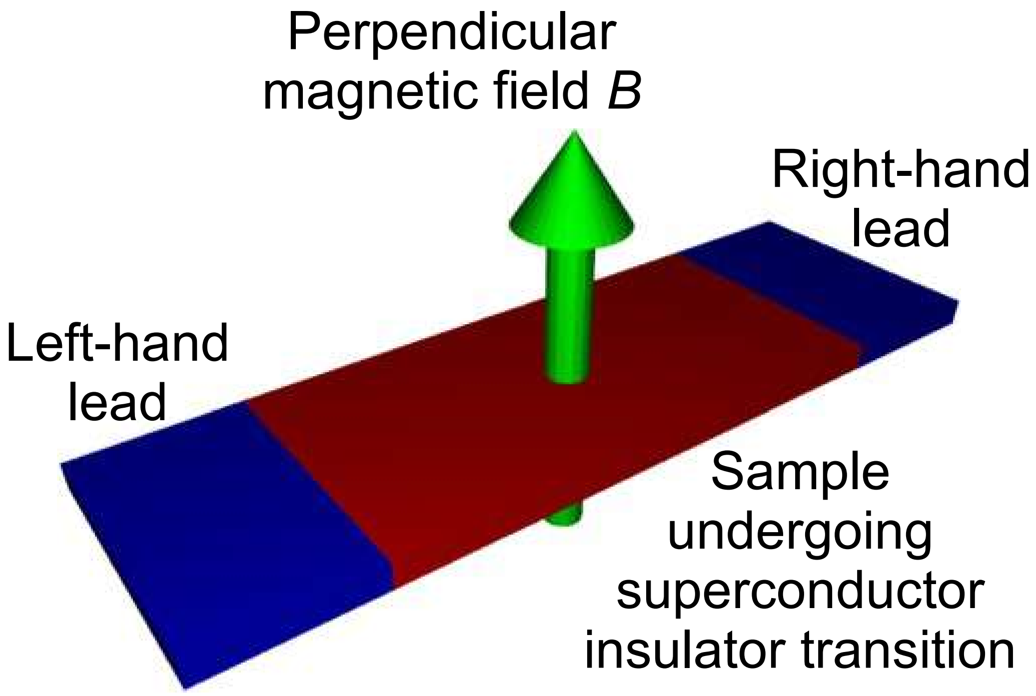


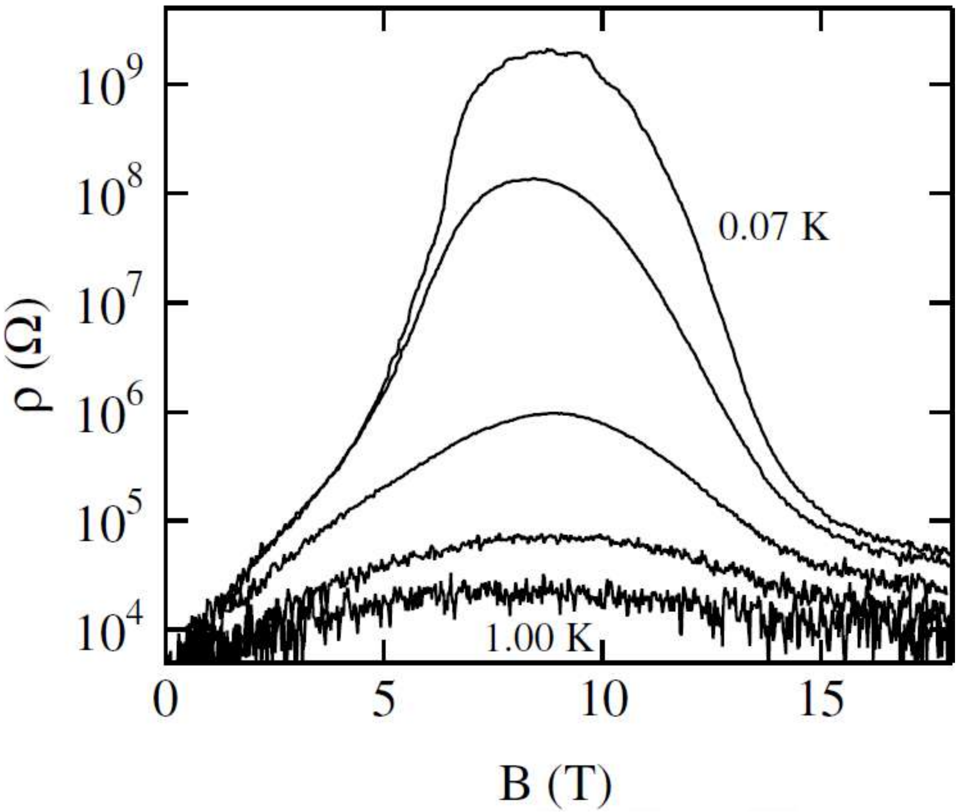
Normal current



Magnetoresistance peak

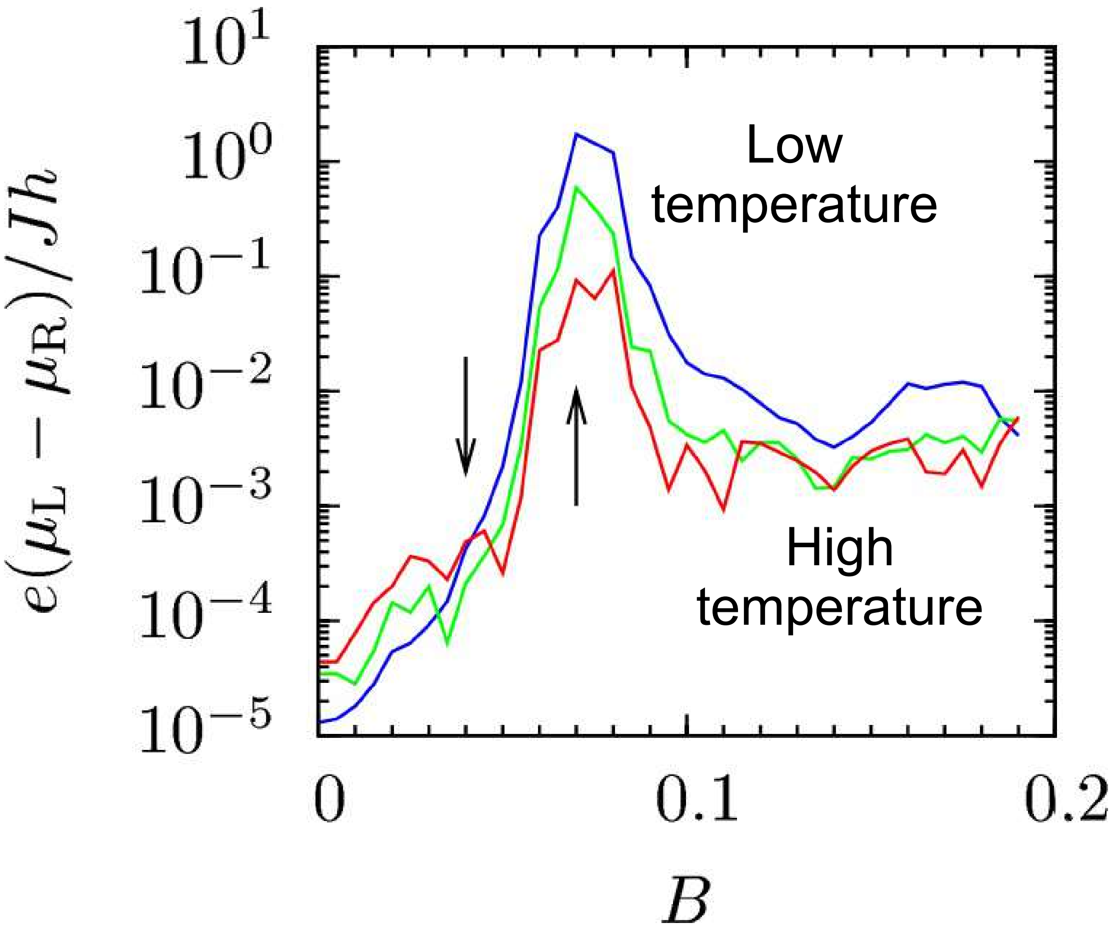
- Study superconductor-insulator transition in dirty sample with perpendicular magnetic field

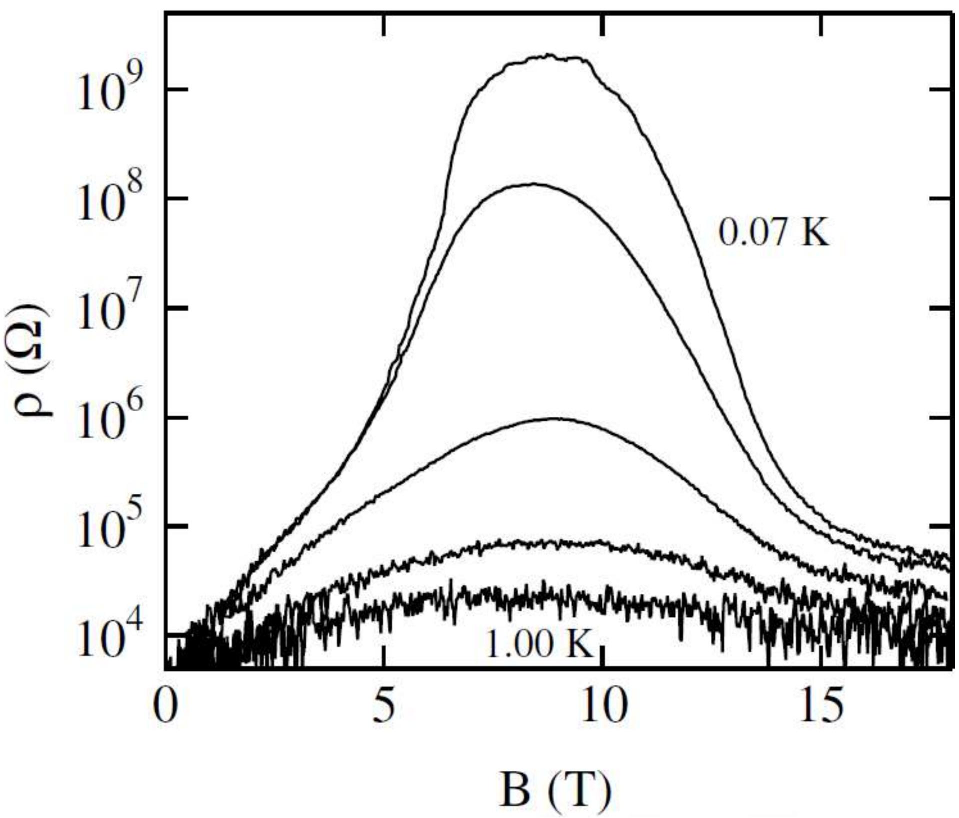




Magnetoresistance peak

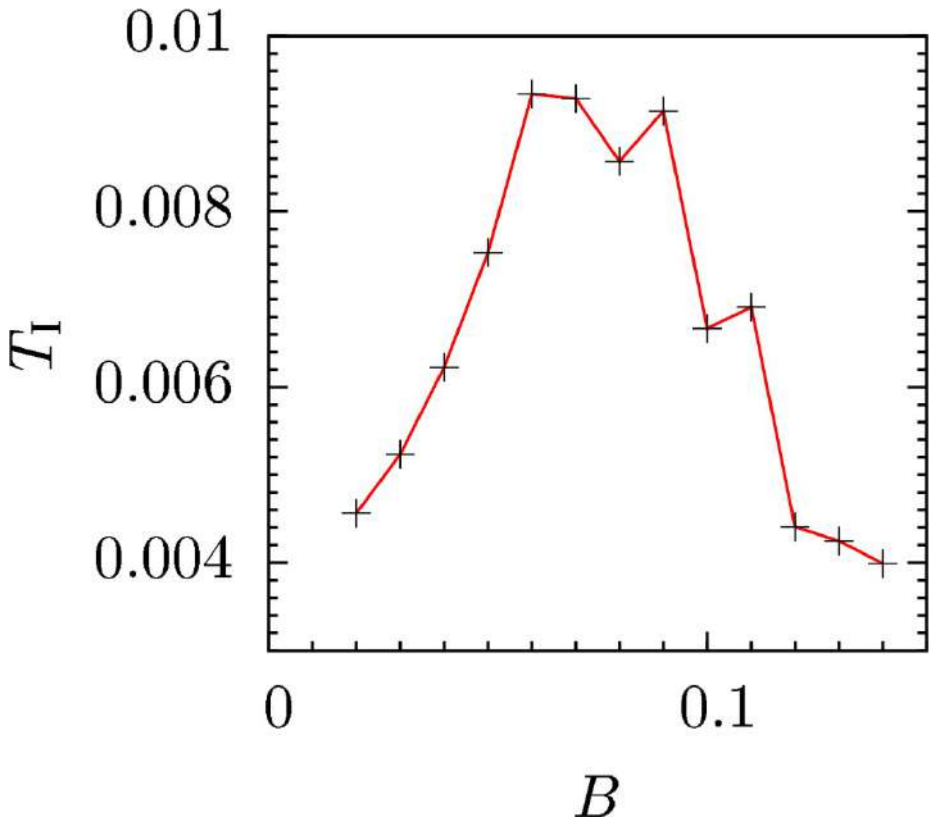
- Study superconductor-insulator transition in dirty sample with perpendicular magnetic field

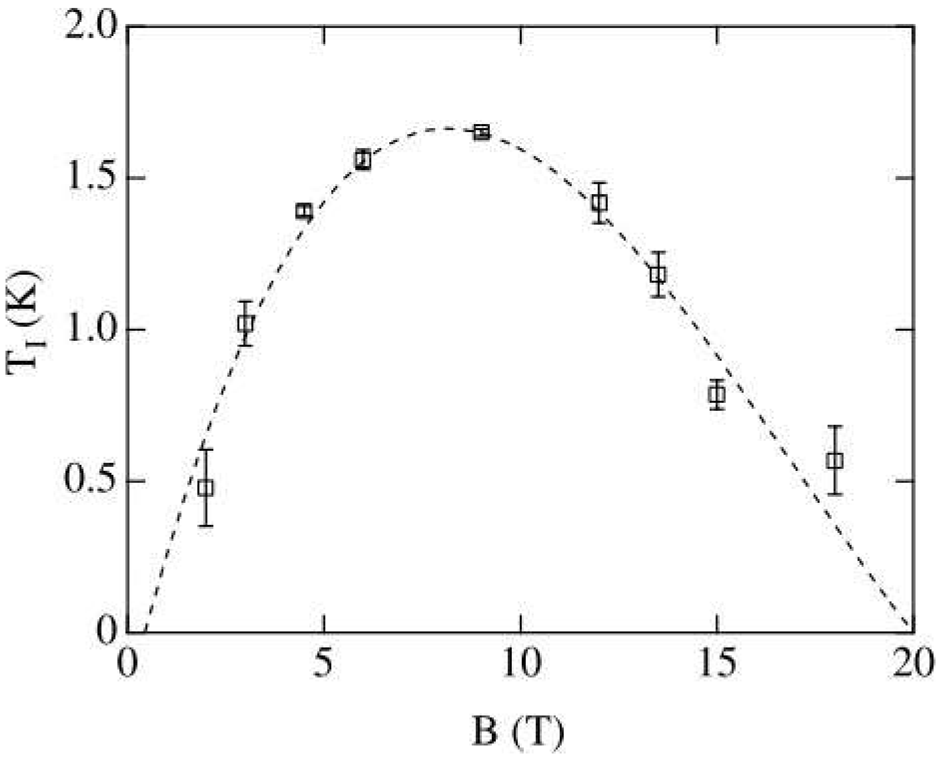




Clues: activated transport

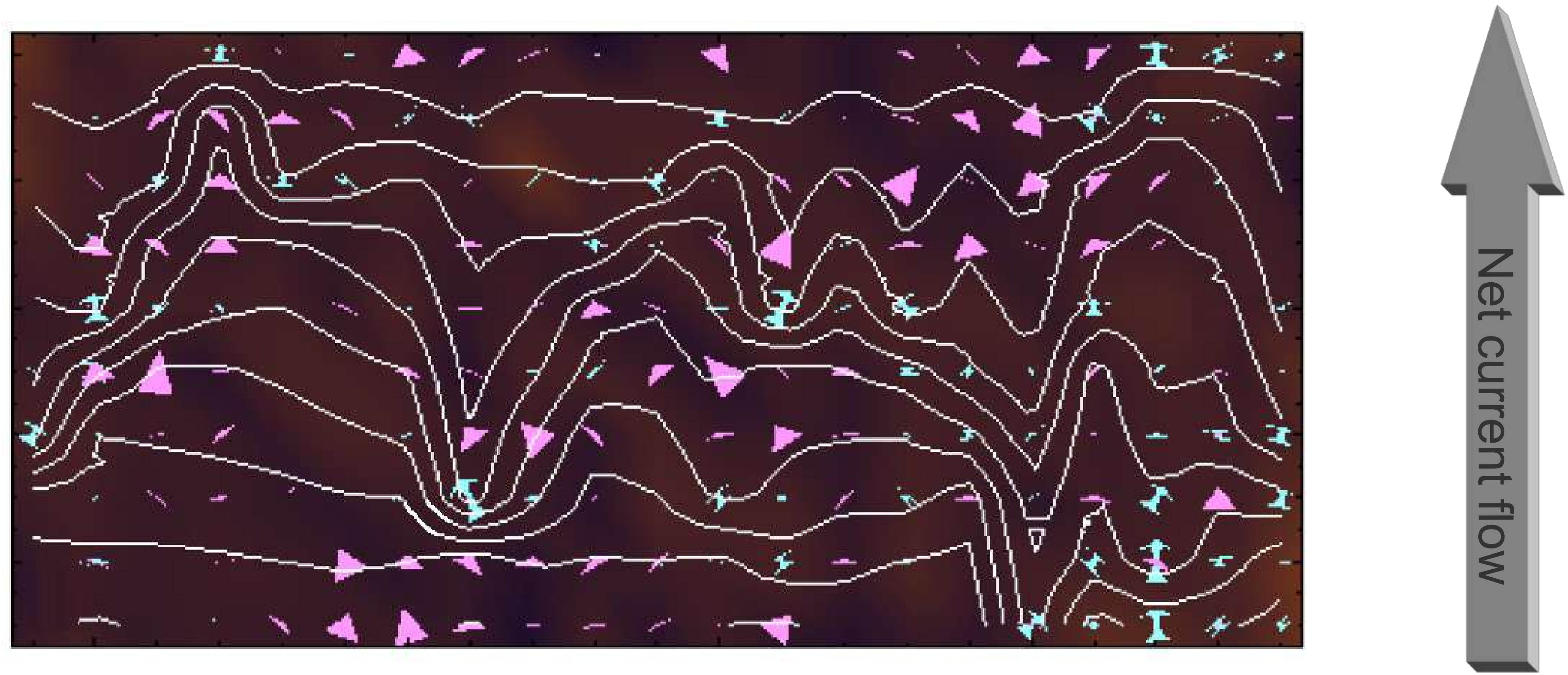
- Activated transport $\rho = \rho_0 e^{T_\mathrm{I}/T}$



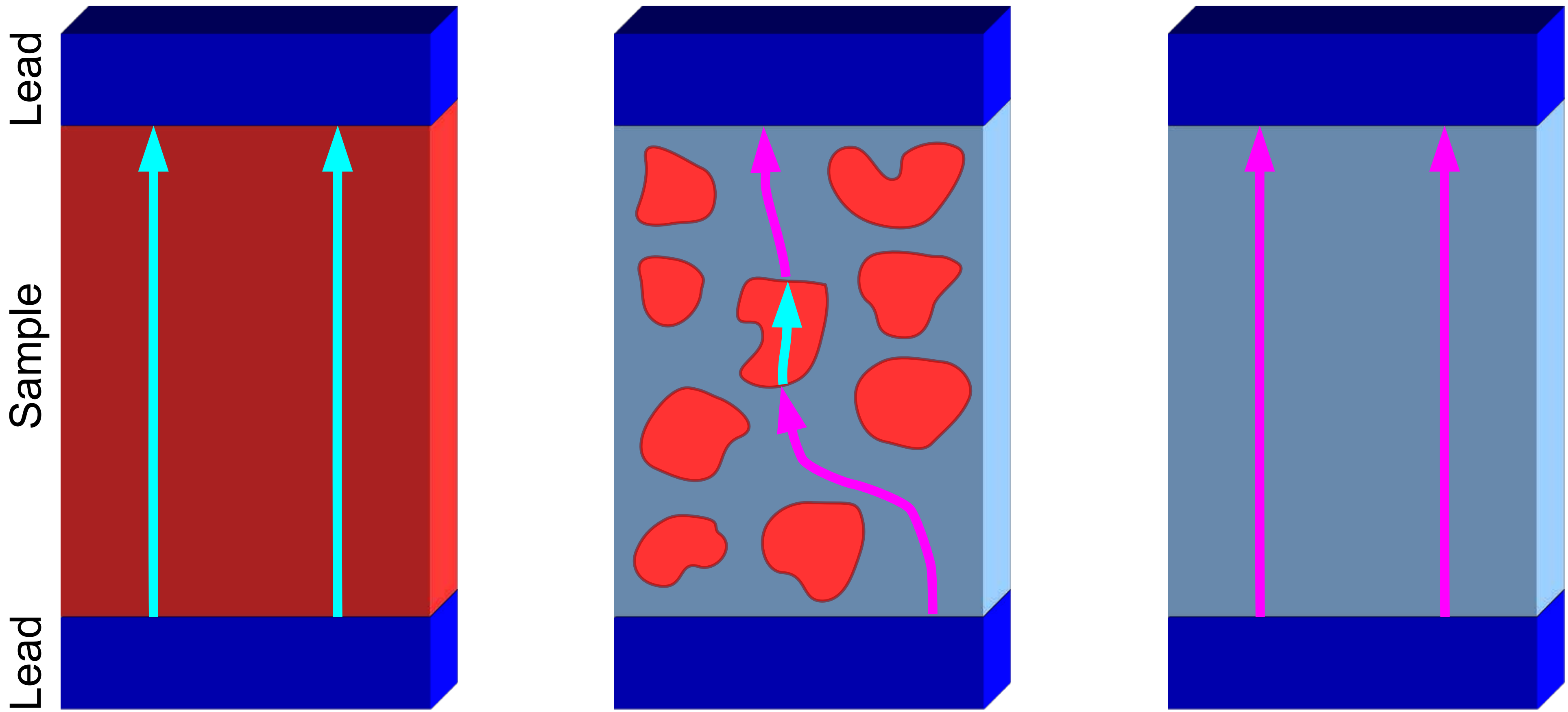


Clues: current maps

- Weak links across superconducting puddles



Working hypothesis



Sample entirely superconducting

Superconducting puddles have a charging energy and a tunneling barrier

Sample entirely normal

Summary & future prospects

- Developed new formalism that includes thermal phase fluctuations to calculate and probe transport in superconductors
- New numerical techniques permit access to large systems
- Tested formalism against a series of well established results
- Shown that superconductor-insulator transition in small diameter cylinders is driven by phase fluctuations
- Shown that magnetoresistance peak could be driven by condensation of superconducting puddles
- Flexibility allows us to study wide range of unexplained effects