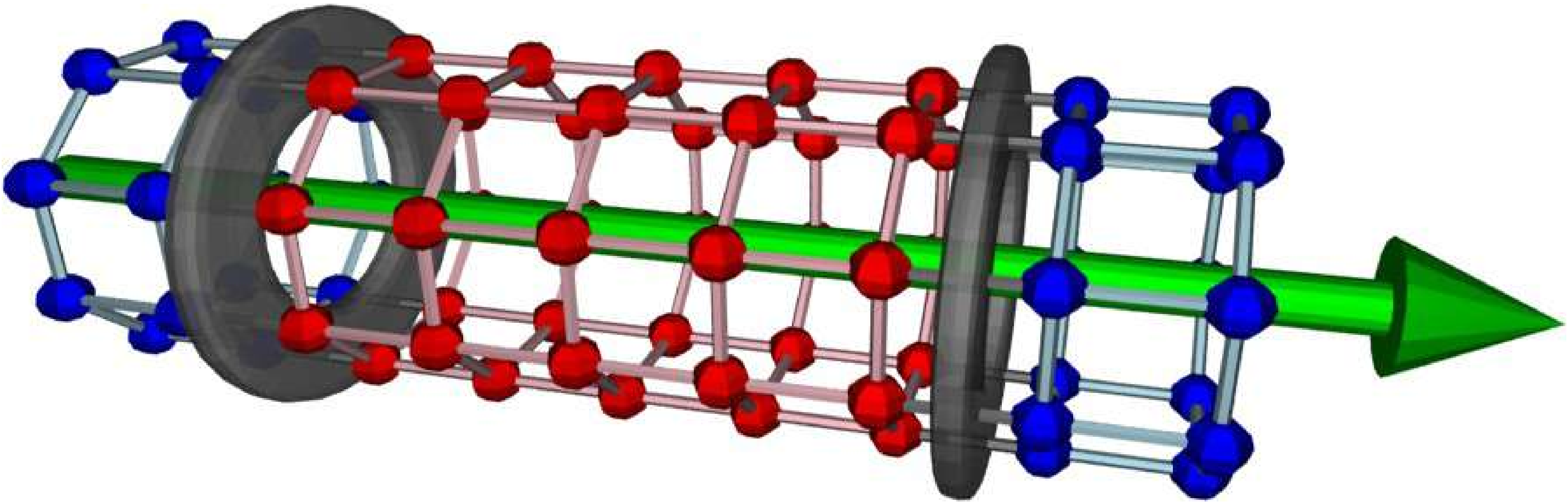
An *ab initio* study of the Little-Parks effect in ultrathin cylinders

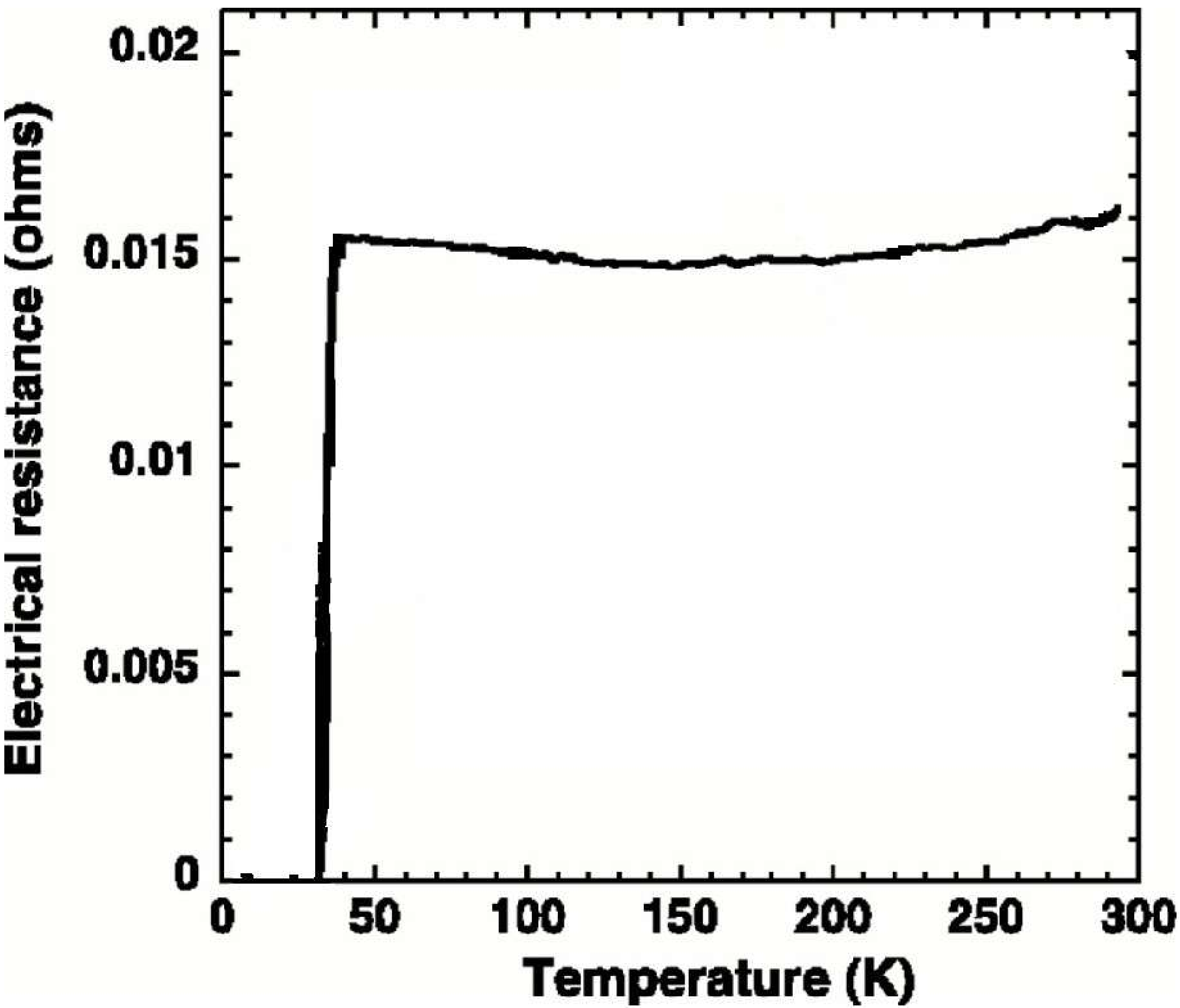


Gareth Conduit, Yigal Meir

Ben Gurion University & Weizmann Institute of Science

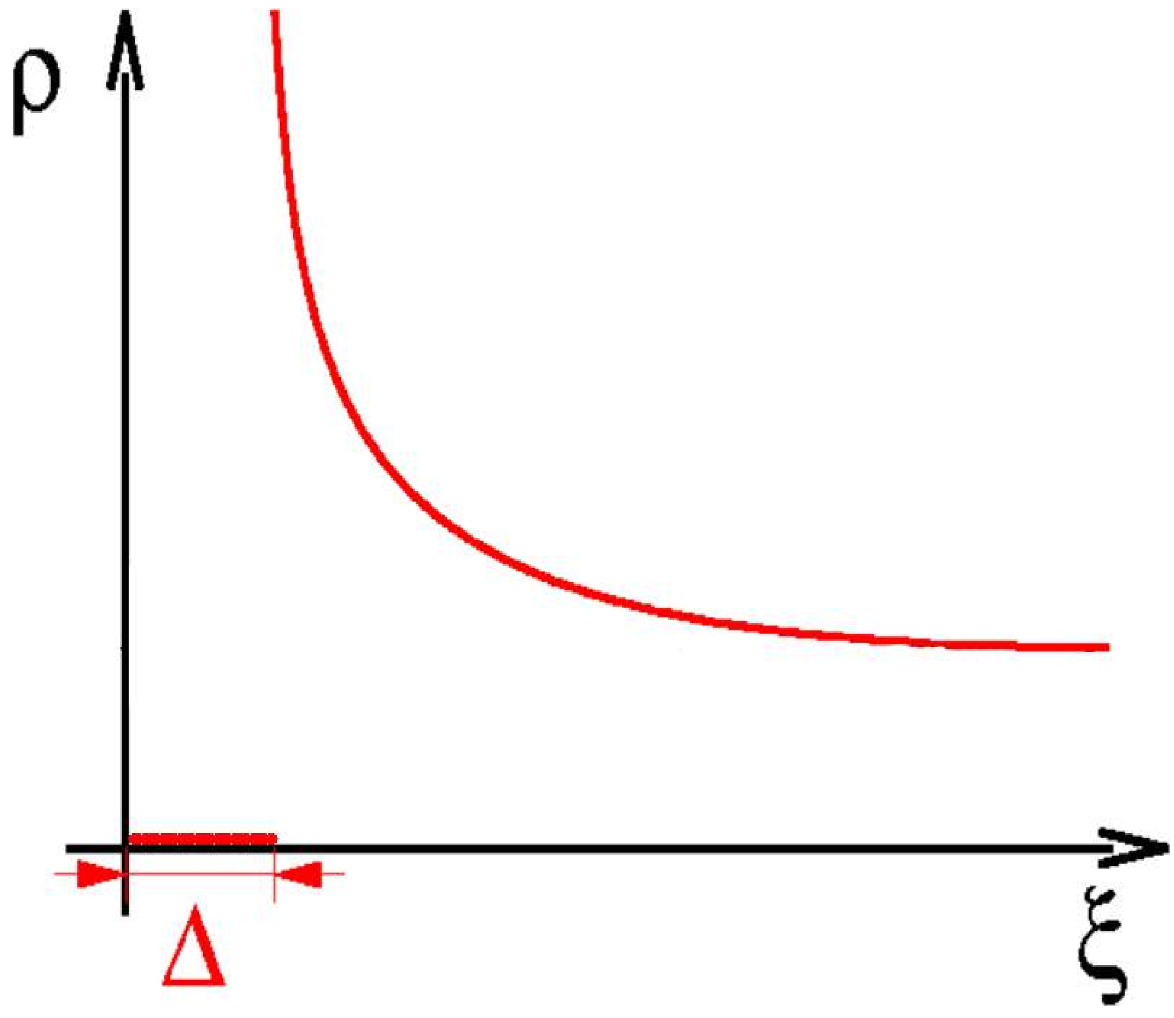
arXiv:1102.1604

BCS superconductivity in MgB_2

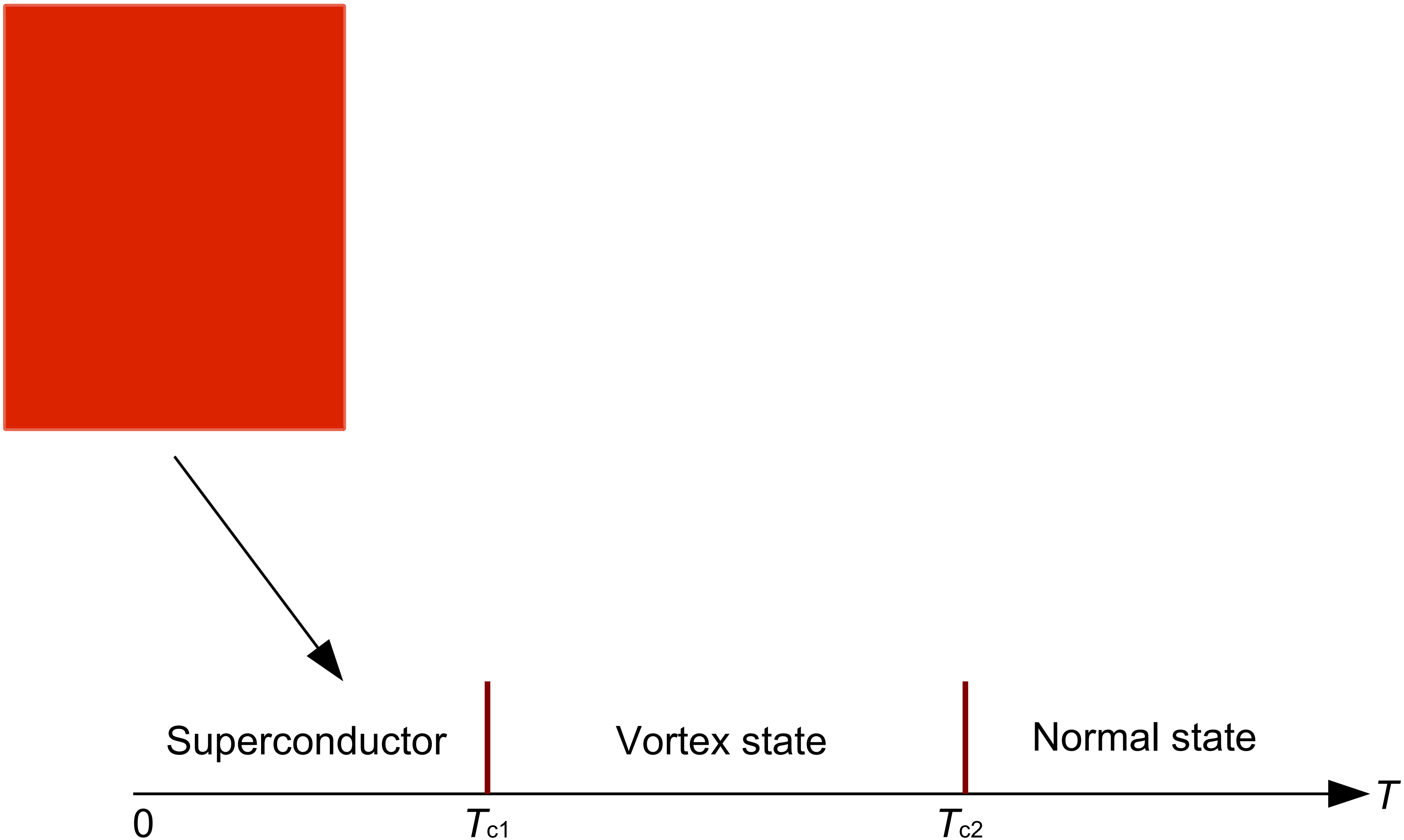


Monteverde et al., Science **292**, 75 (2001)

BCS superconductivity



Kosterlitz Thouless transition



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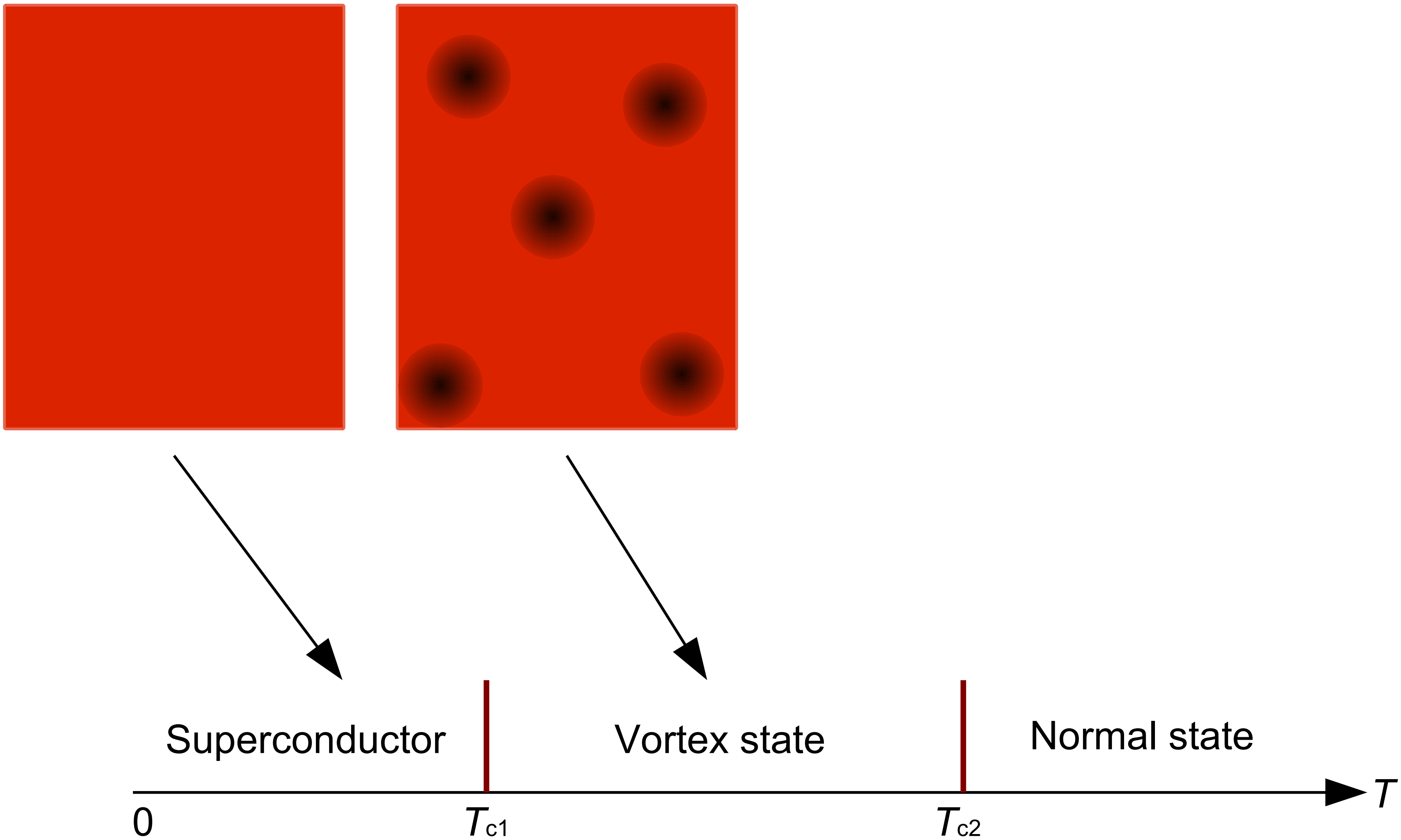

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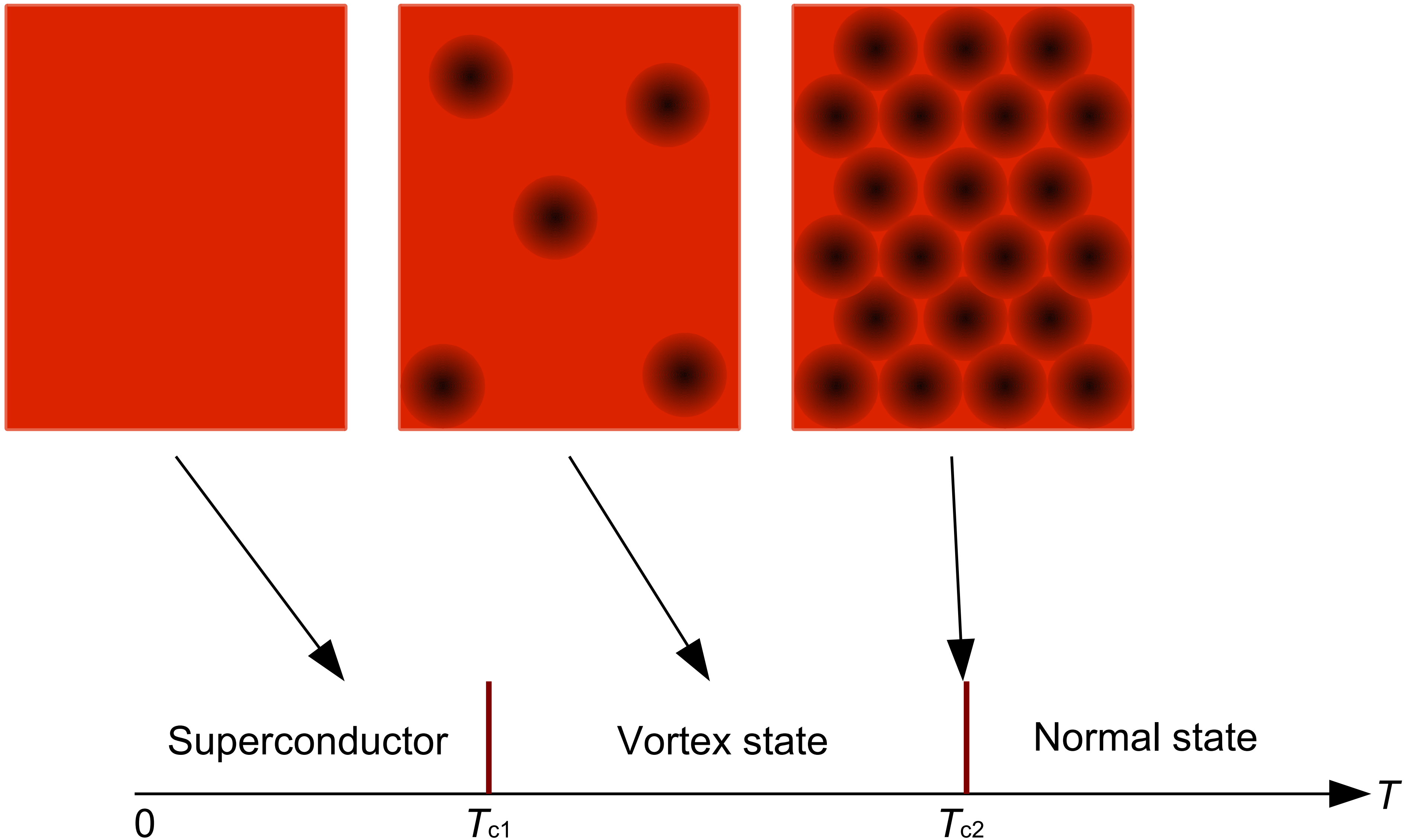
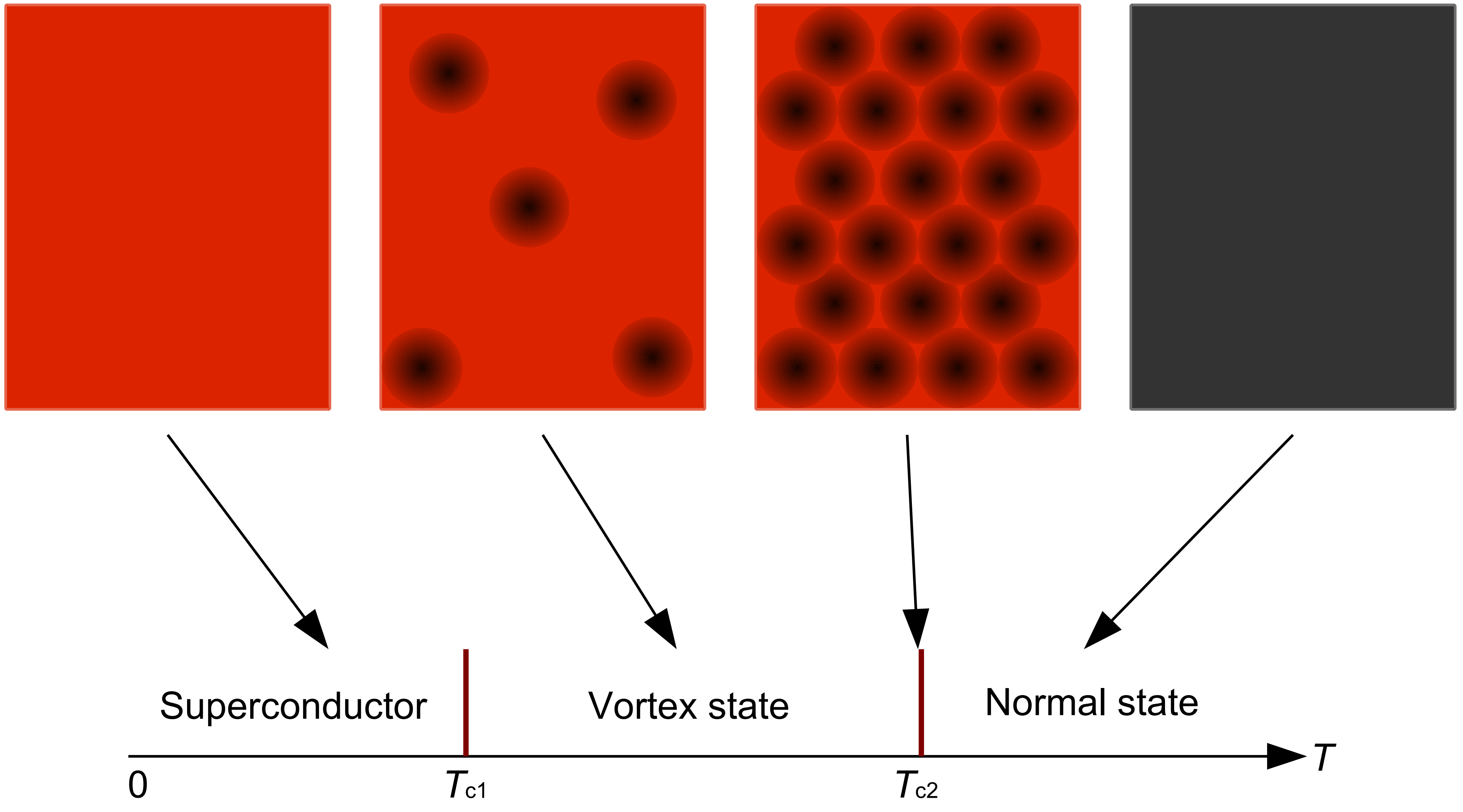
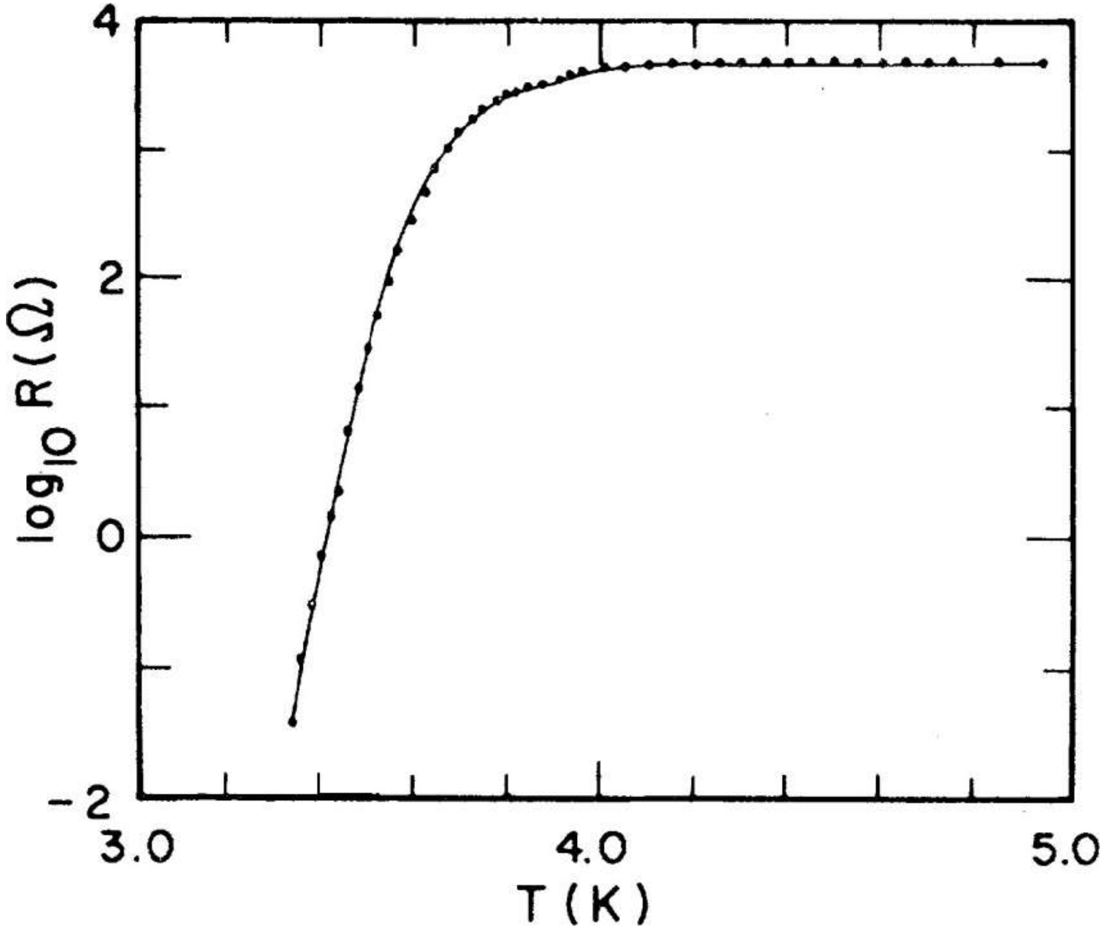


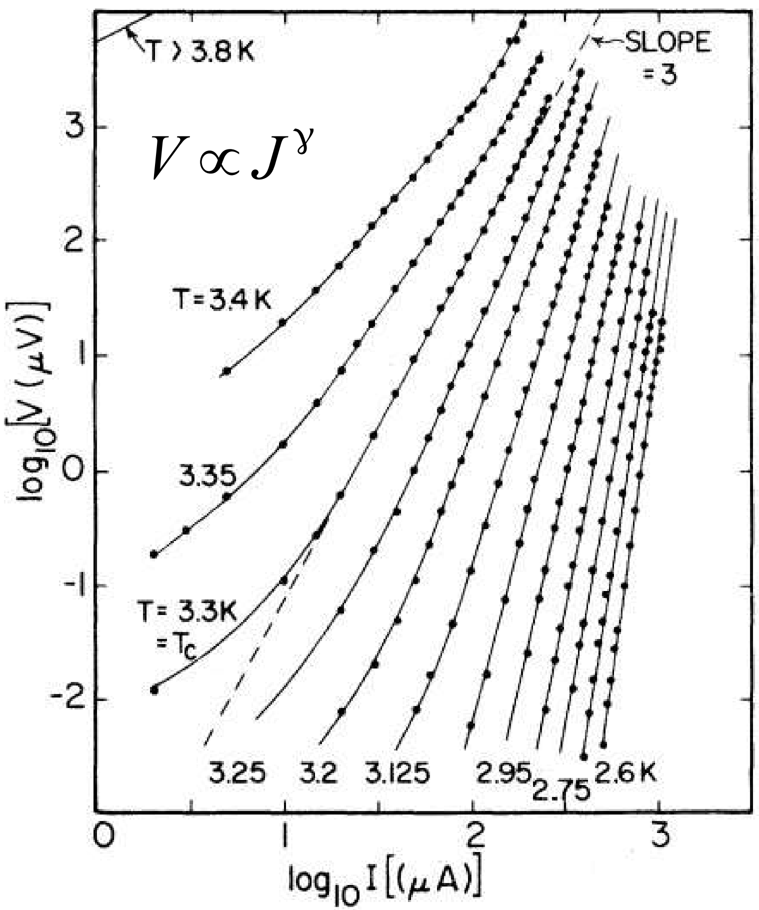
Kosterlitz Thouless transition

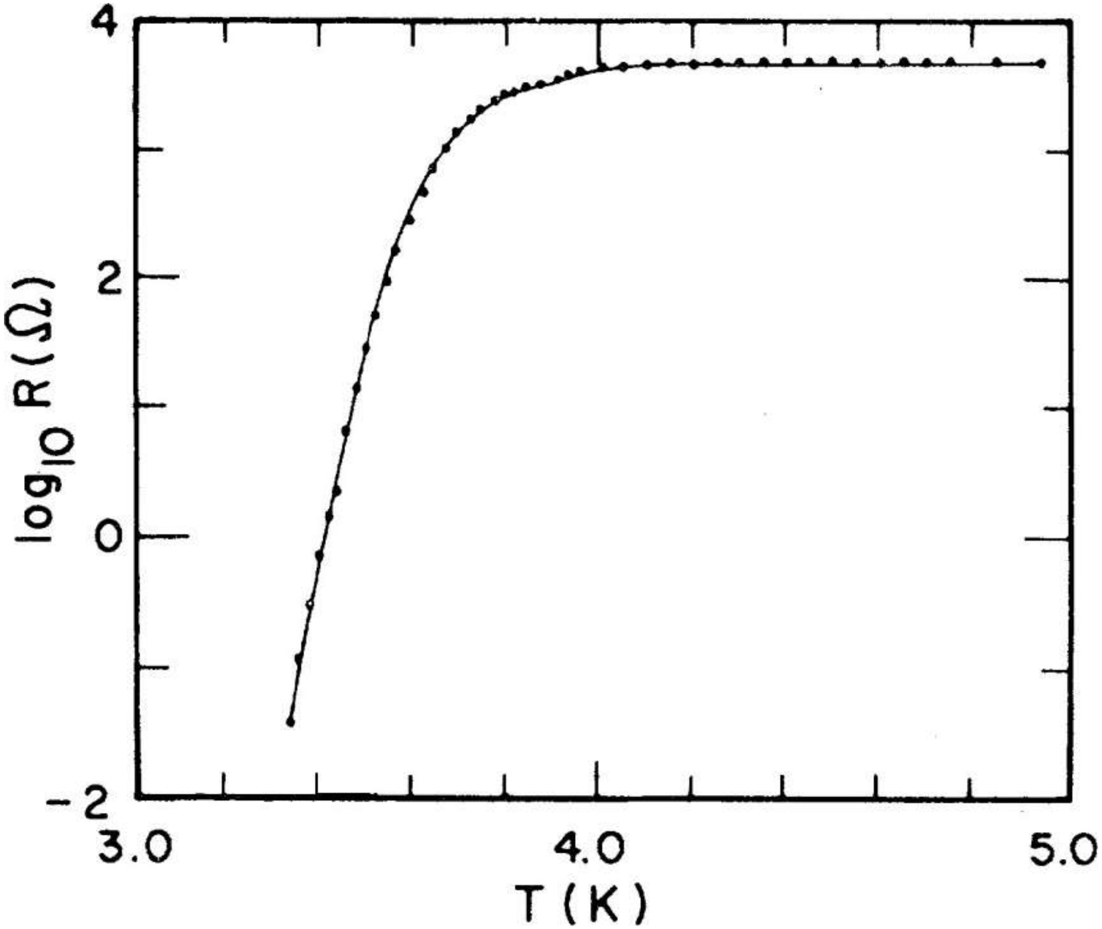


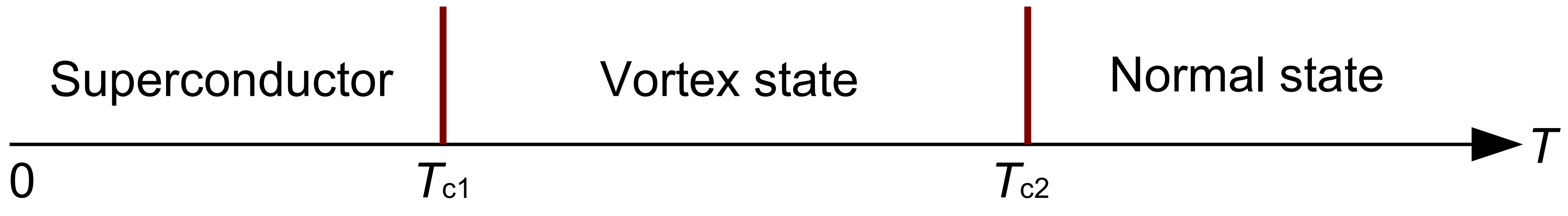
KT transition conductivity



KT transition conductivity

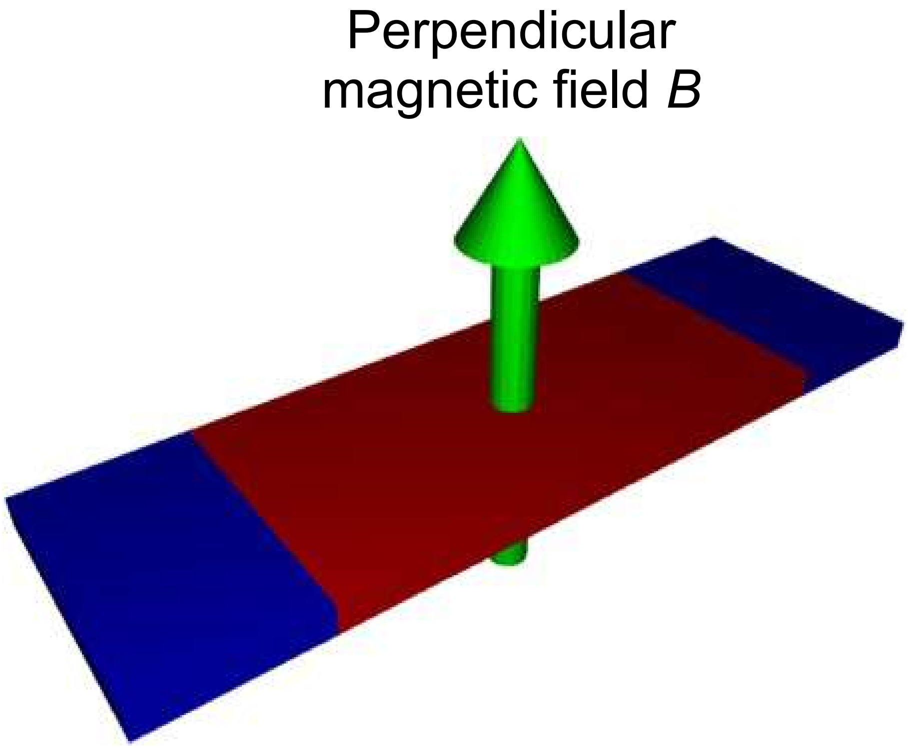


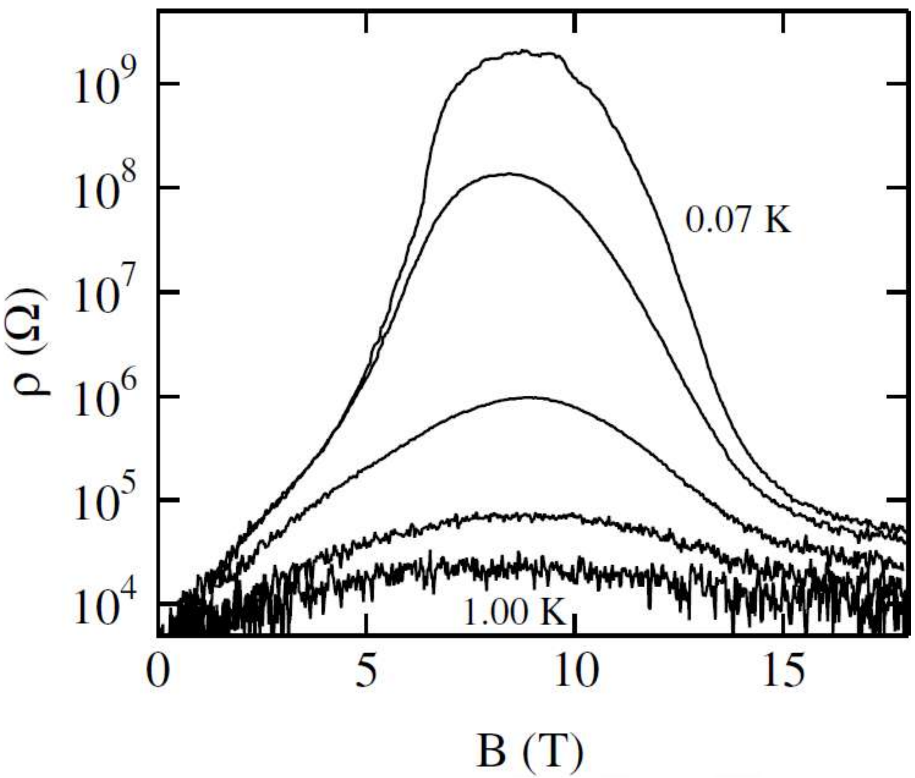




Transition in highly disordered systems

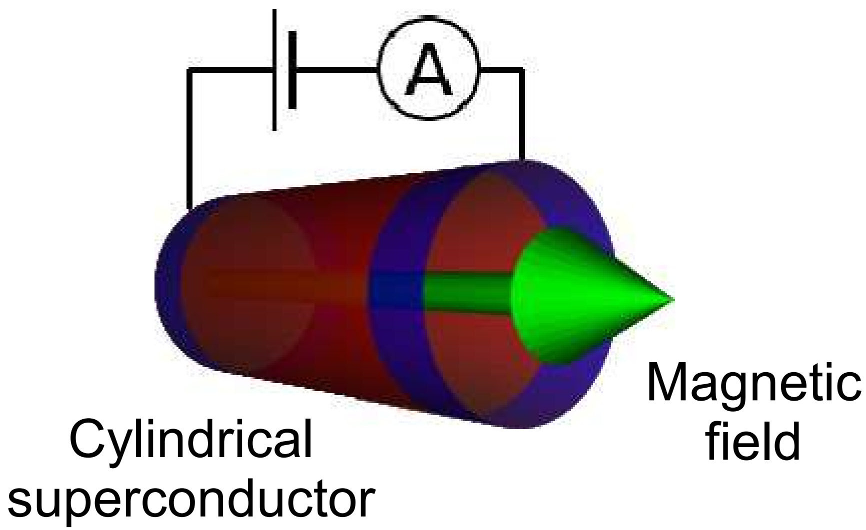
- Magnetoresistance peak [Sambandamurthy 04]

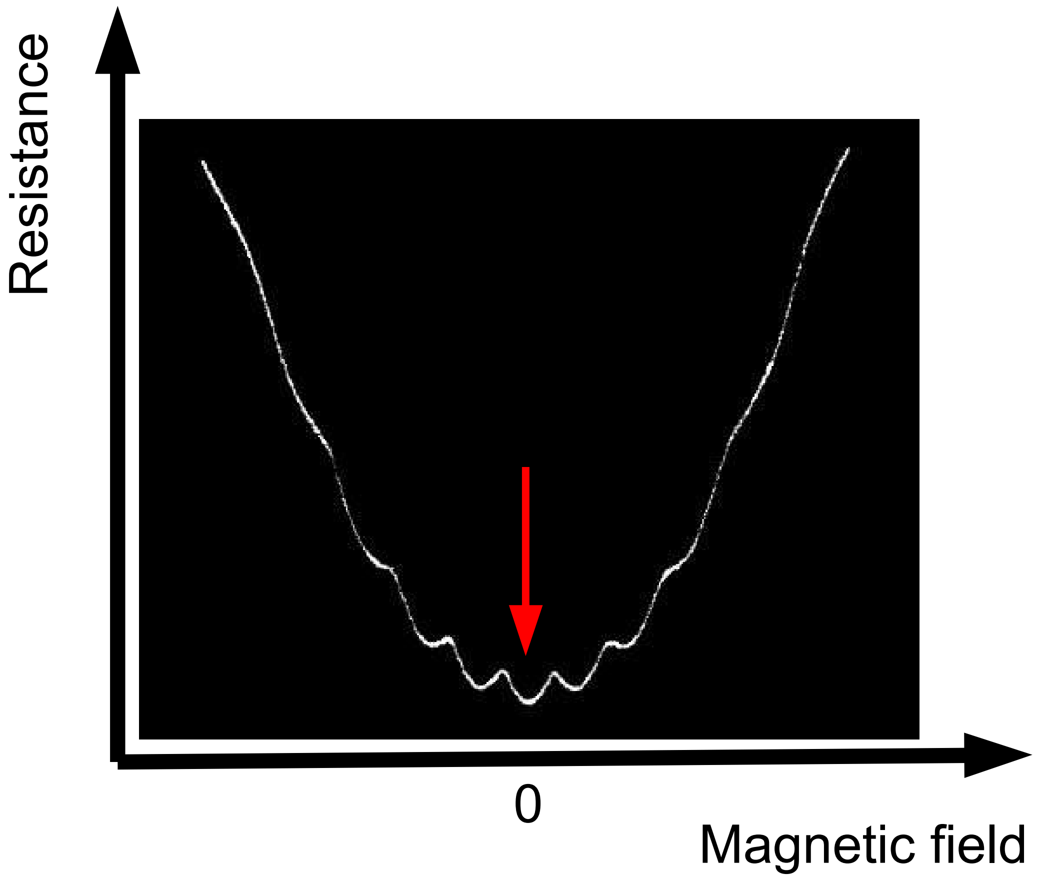




Little-Parks in a large diameter cylinder

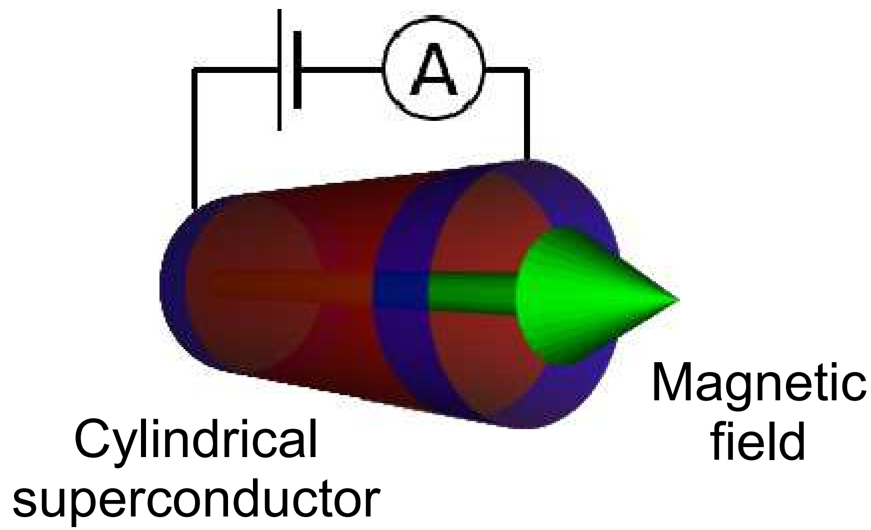
- Cylindrical superconductor held at transition temperature and zero threading flux [Little & Parks, PRL 1962]

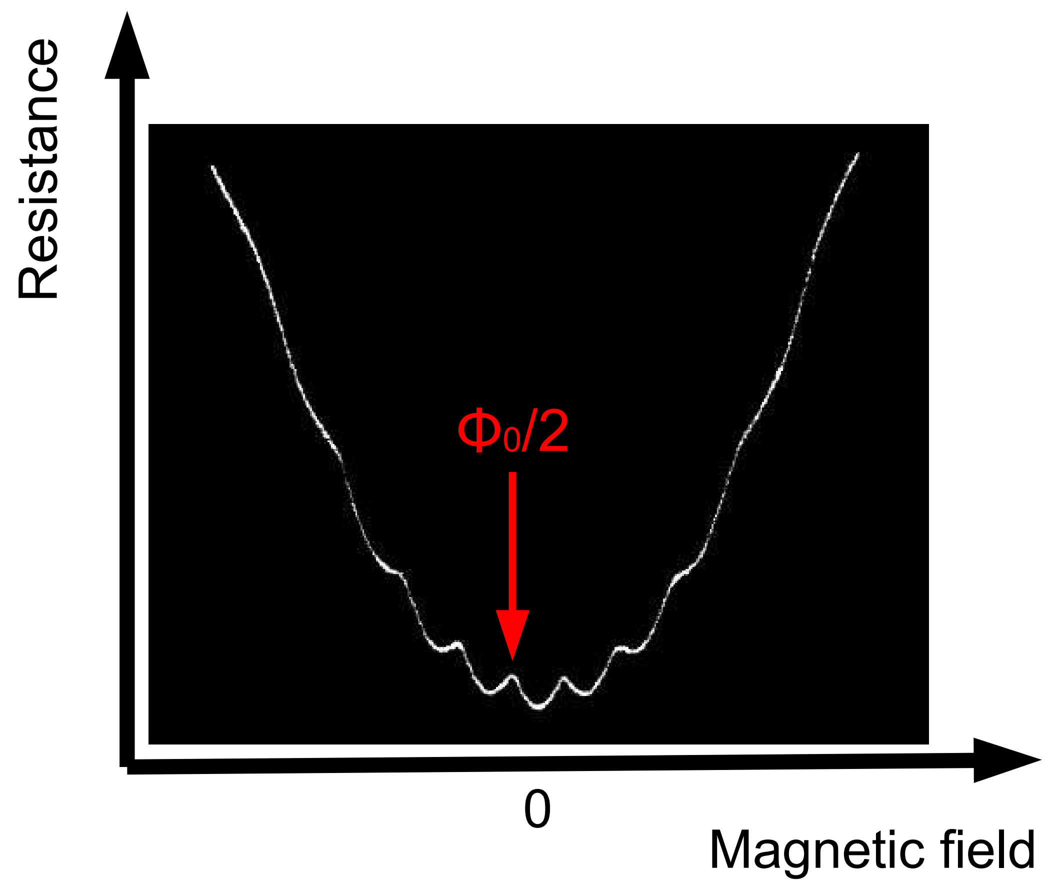




Little-Parks in a large diameter cylinder

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





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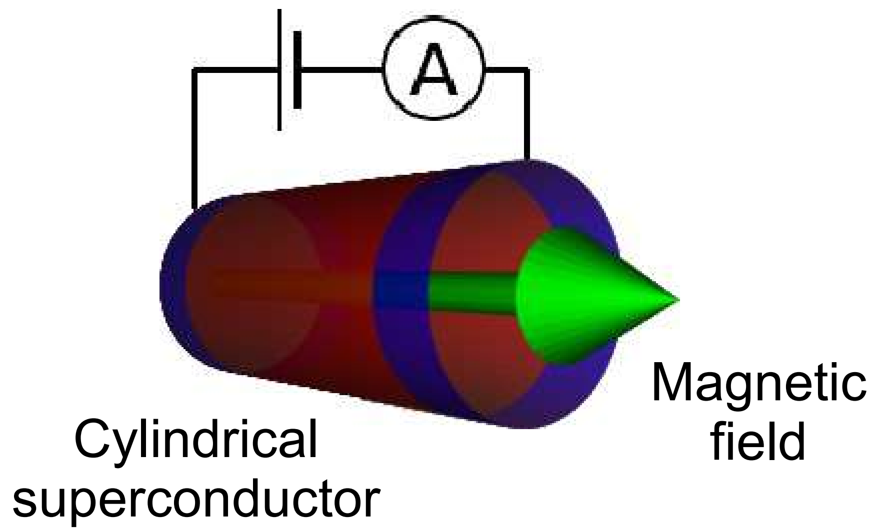
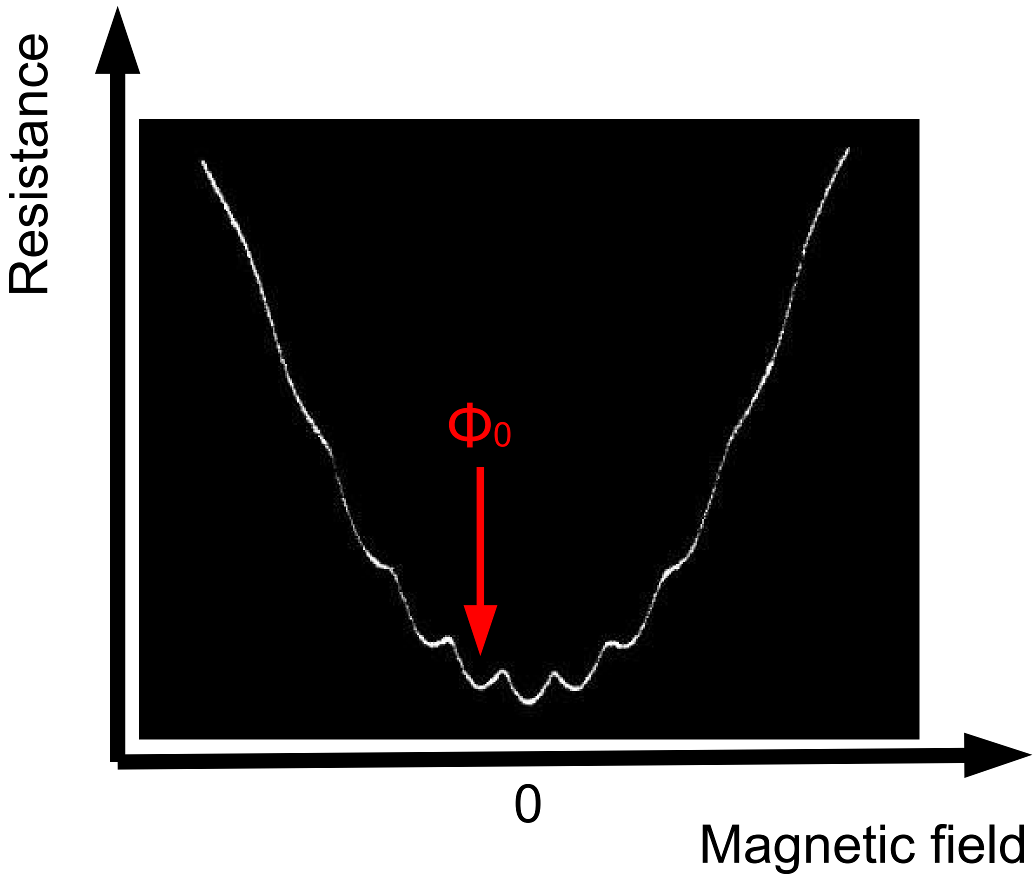
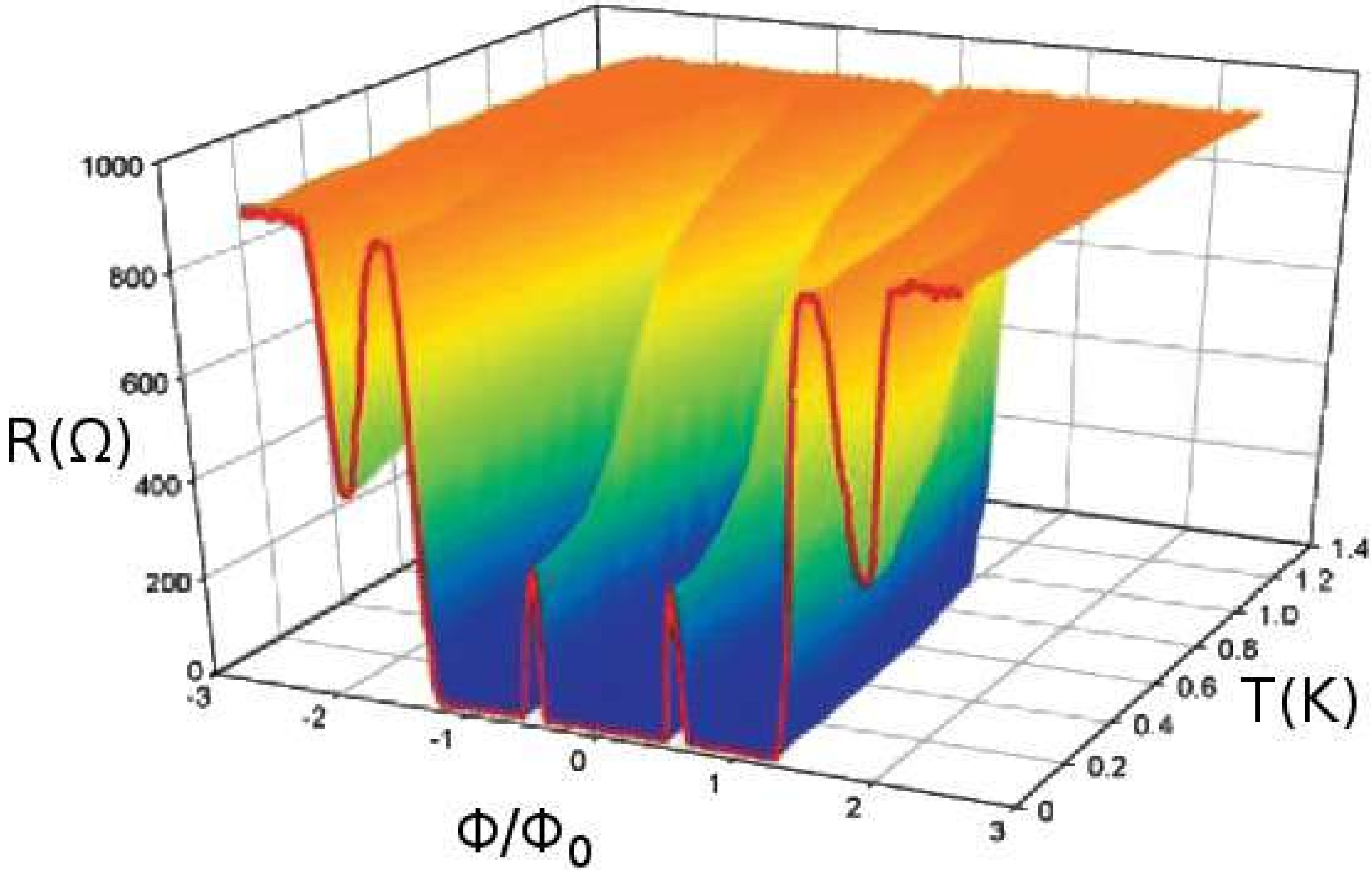




Little-Parks in a small diameter cylinder

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



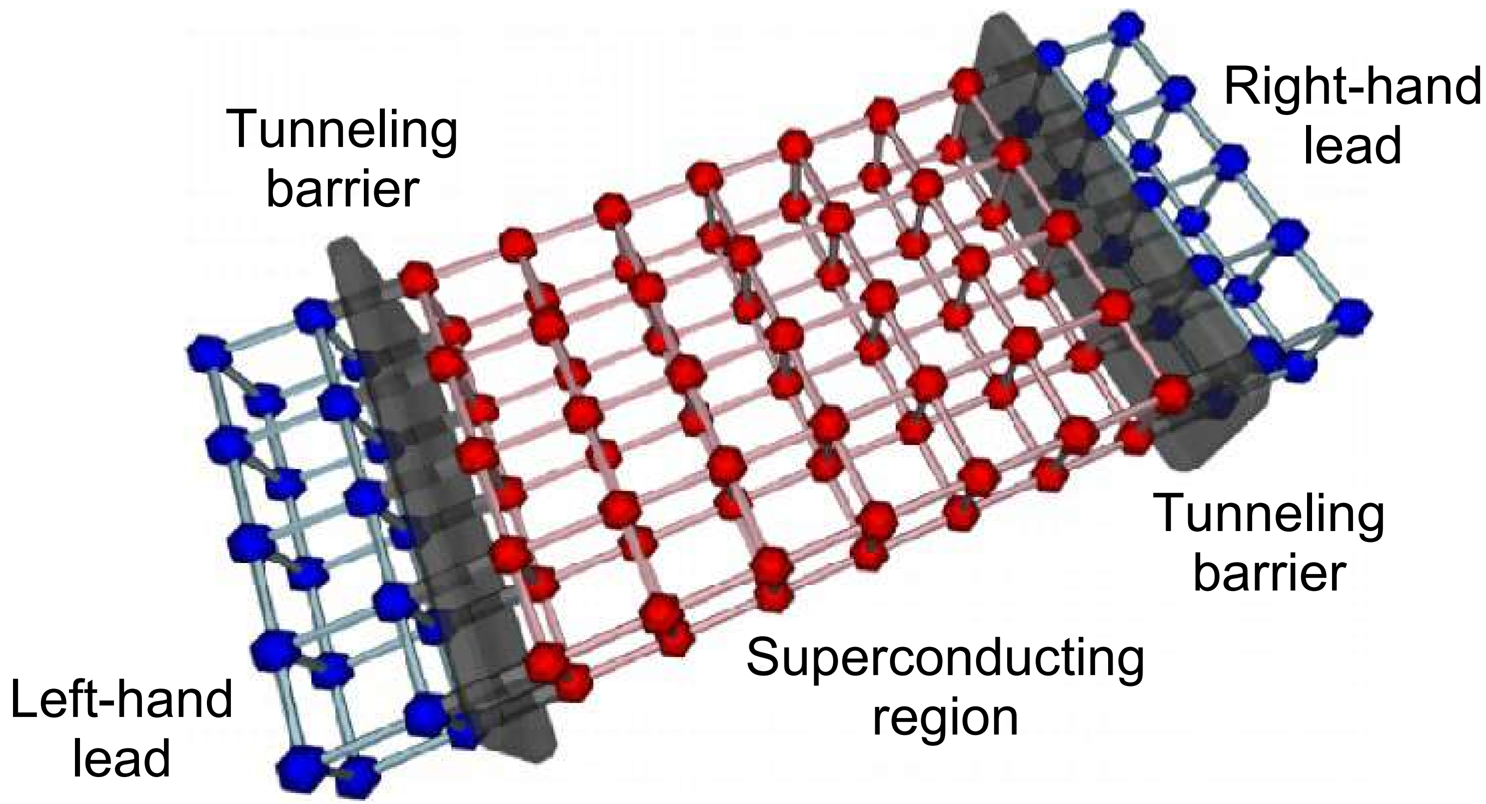
Strategy to study superconductors

- 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

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

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

- 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

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

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

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

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

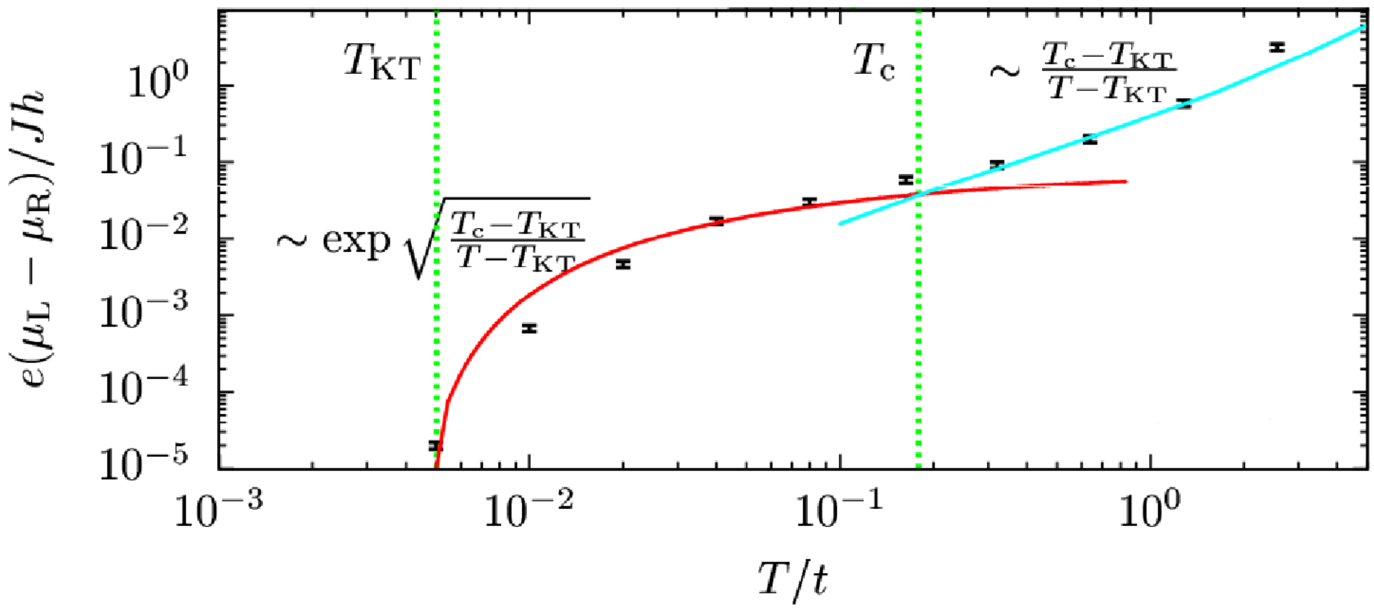
- Propose new configuration of Δ and ρ, accept with probability

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

- 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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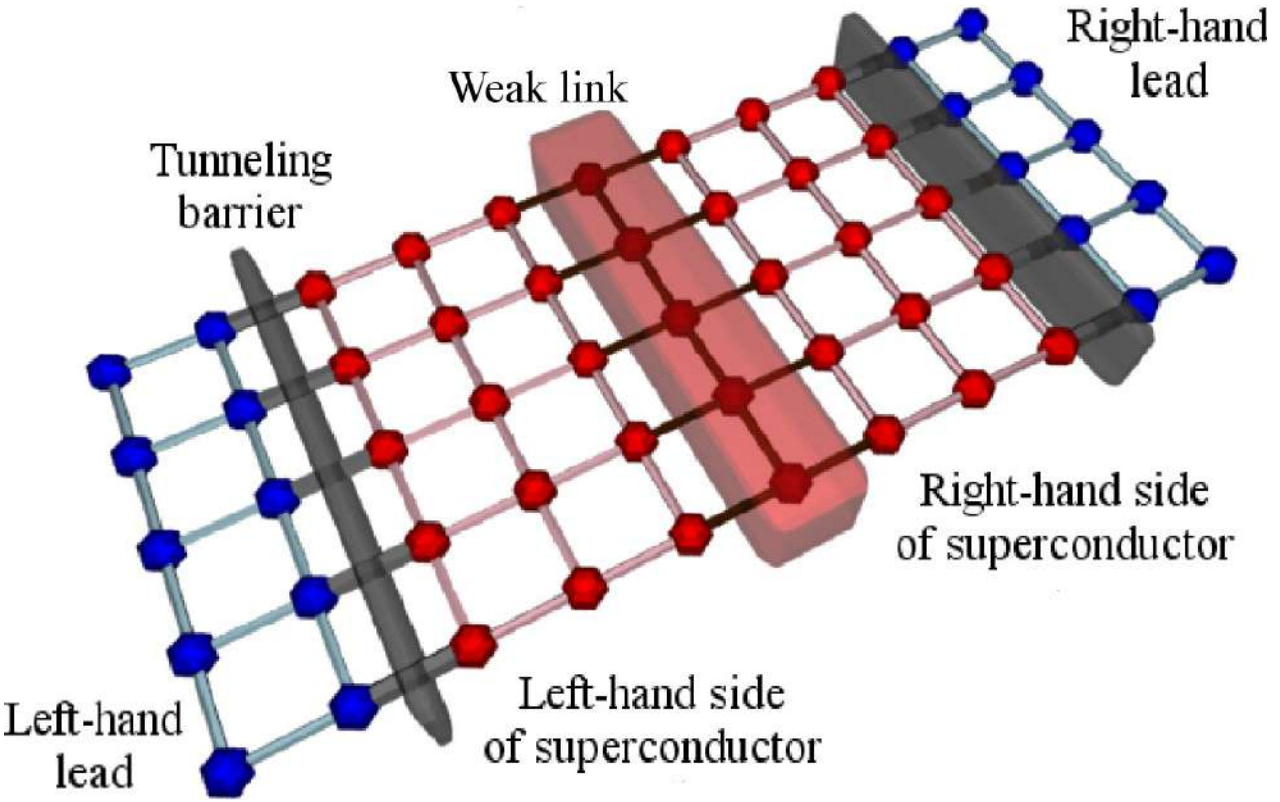

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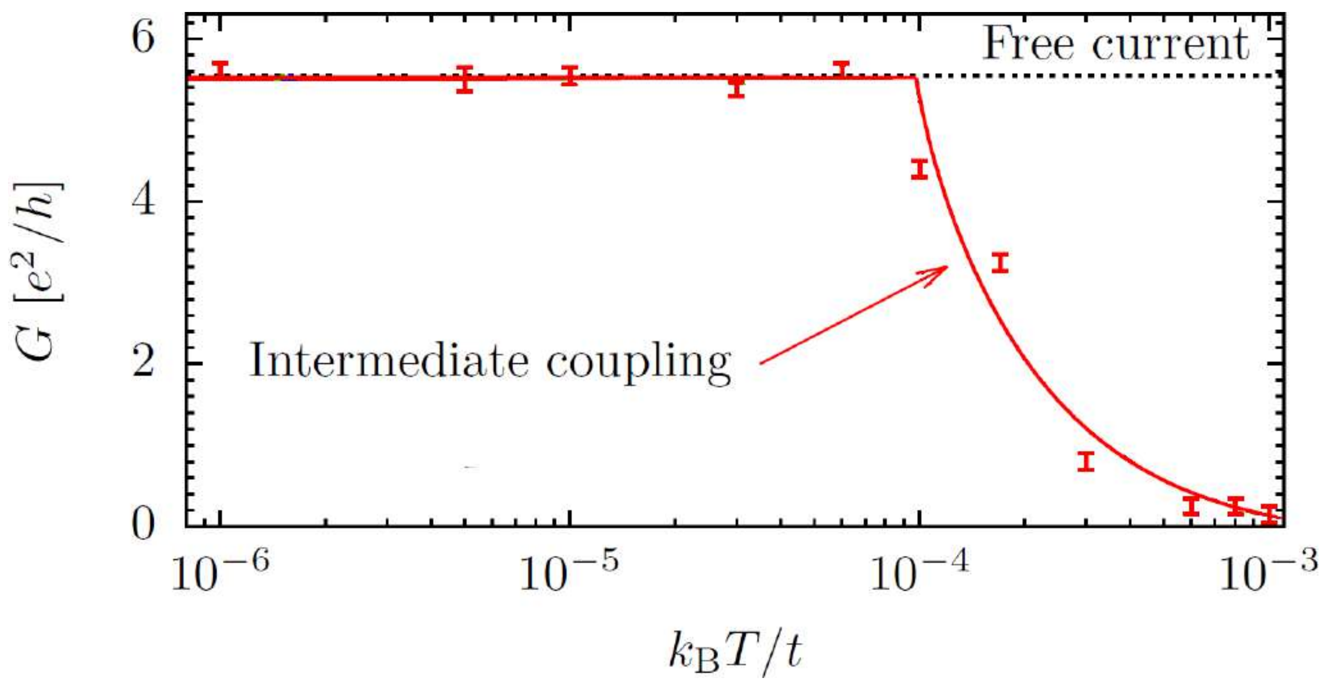

Ambegaokar & Baratoff, PRL **10**, 486 (1963)

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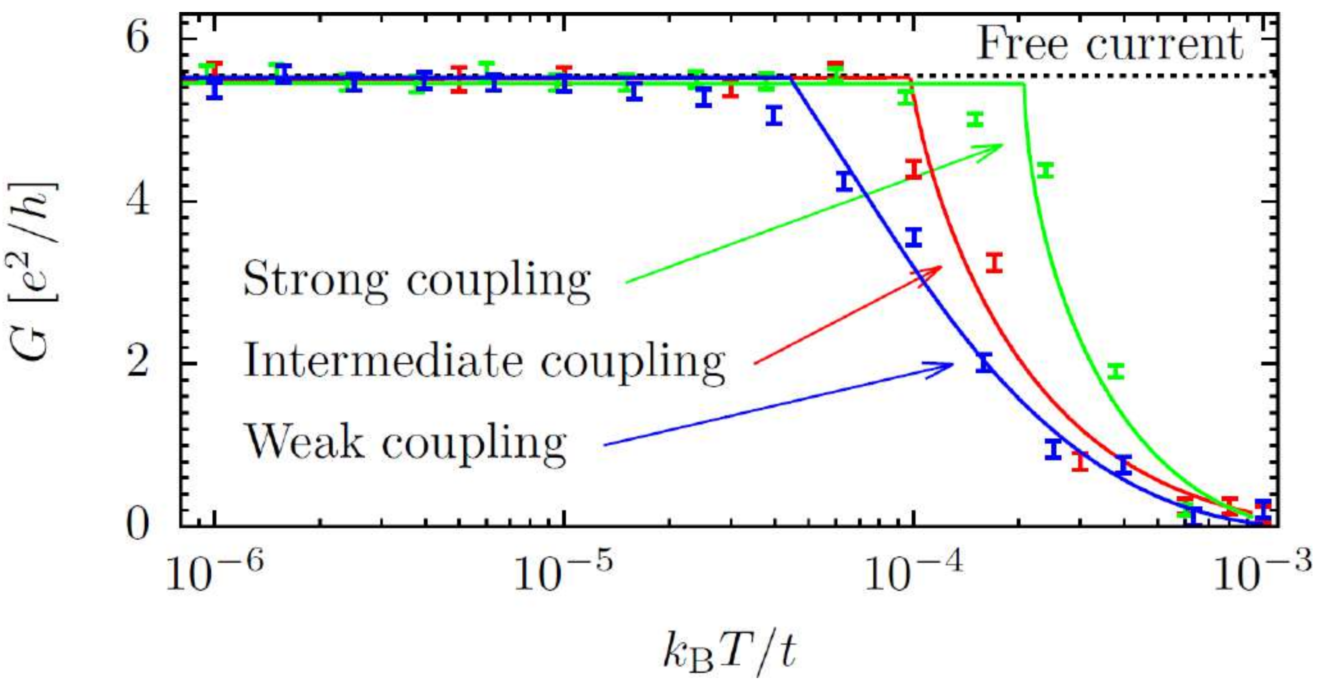

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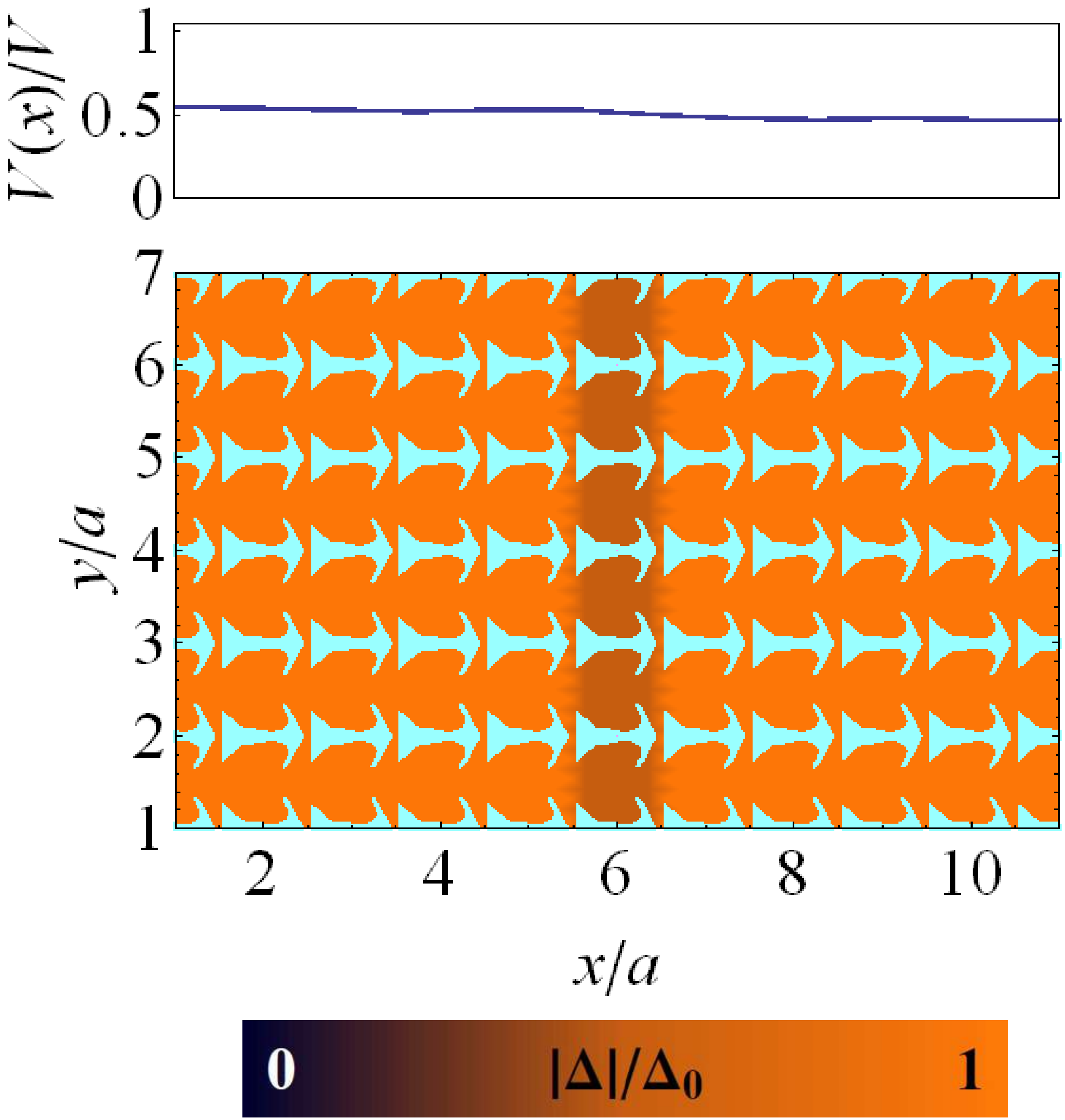

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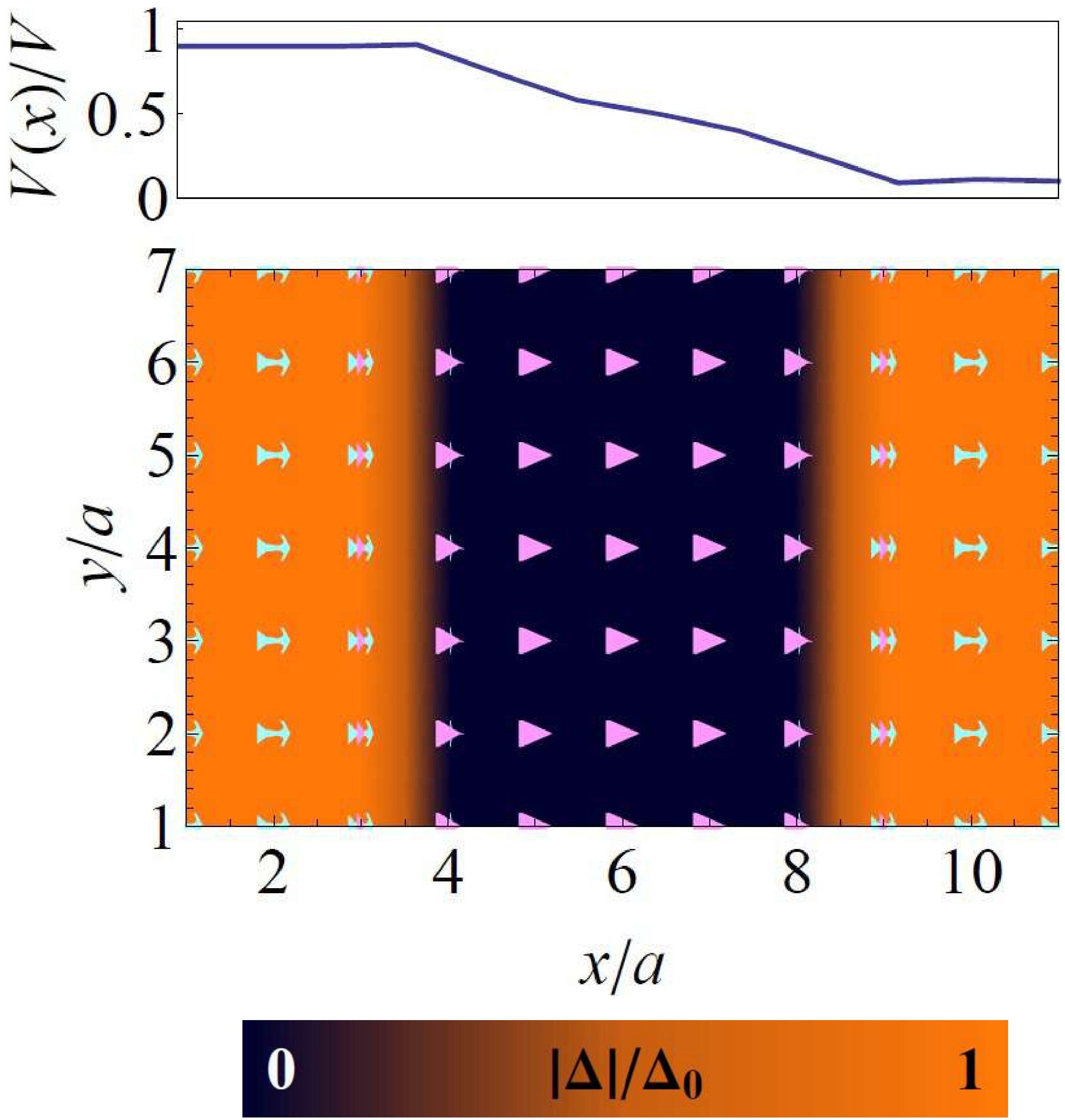

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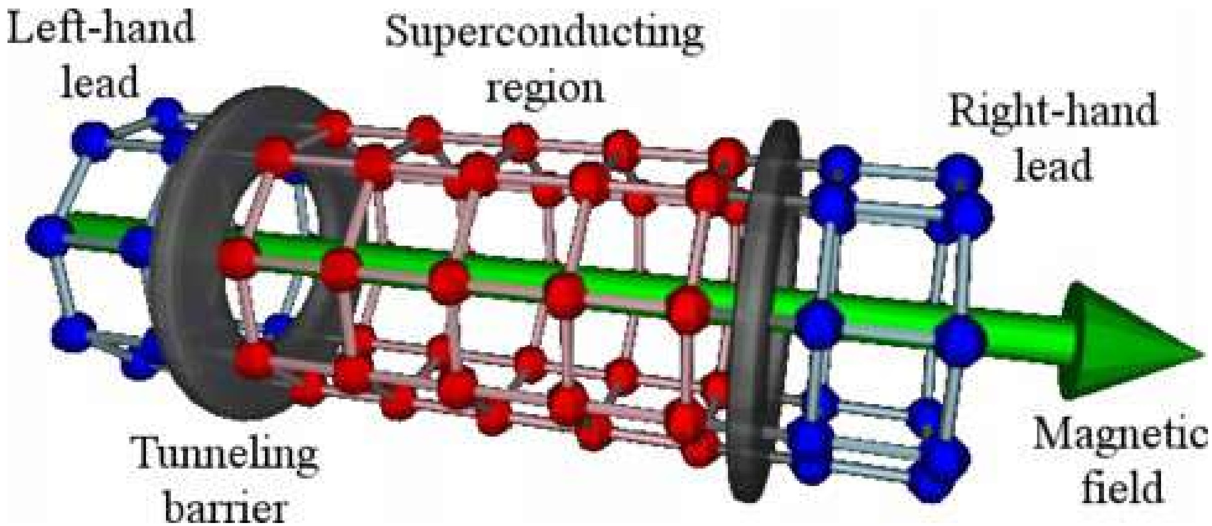
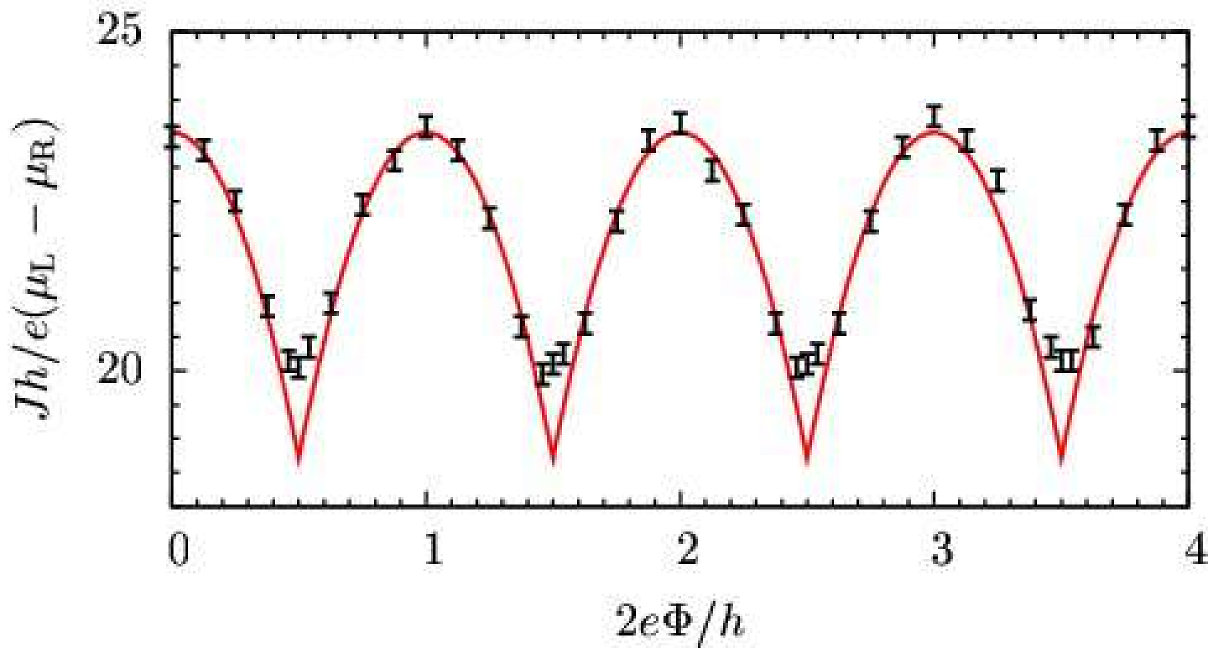
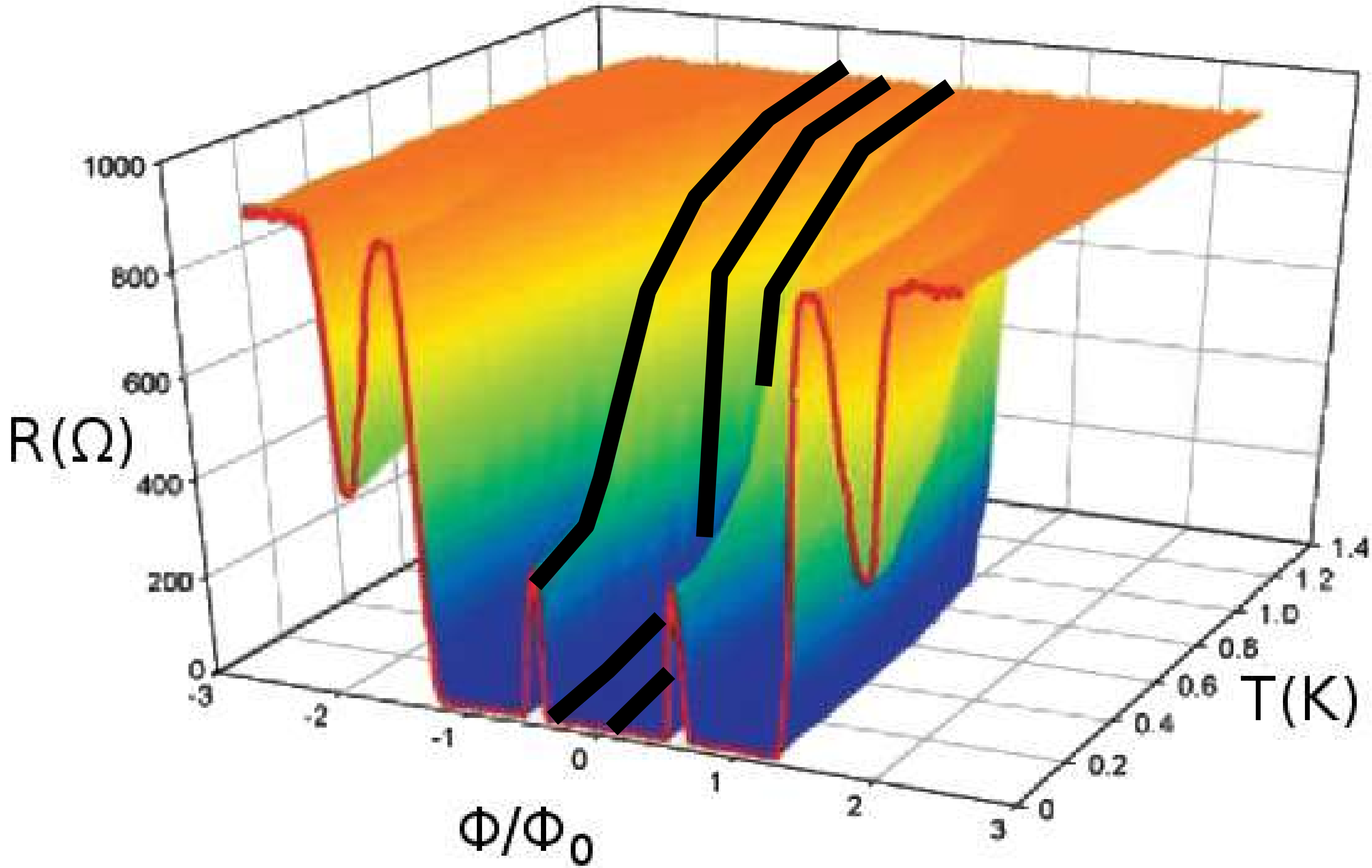
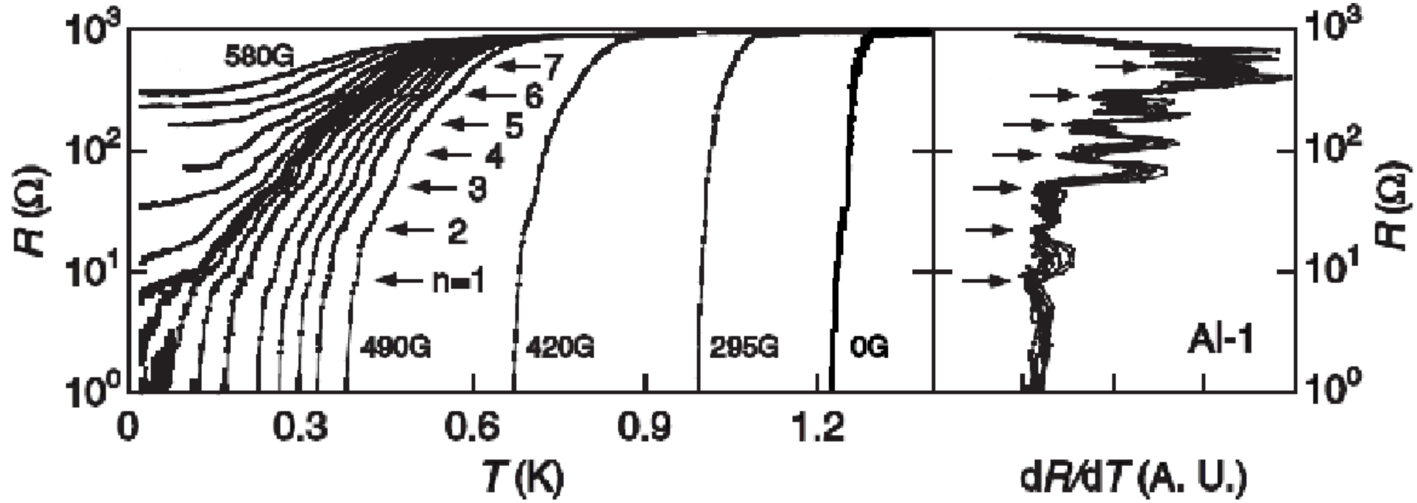


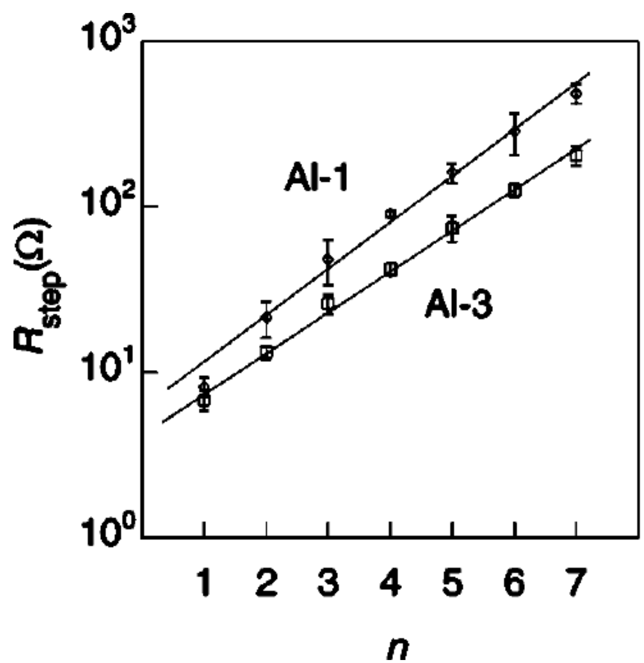


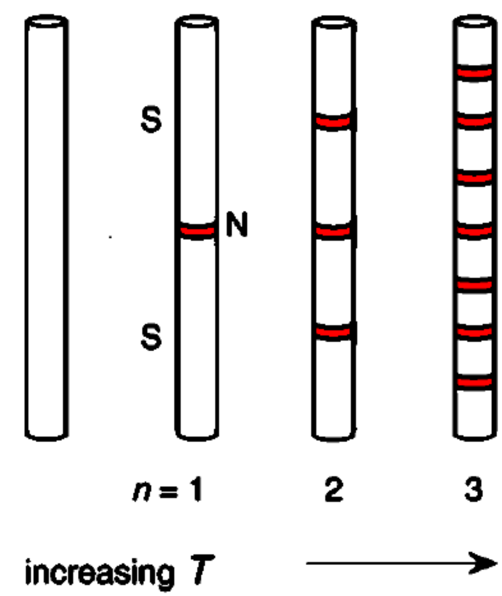
Little-Parks in a small diameter cylinder



Quantum phase transition hypothesis

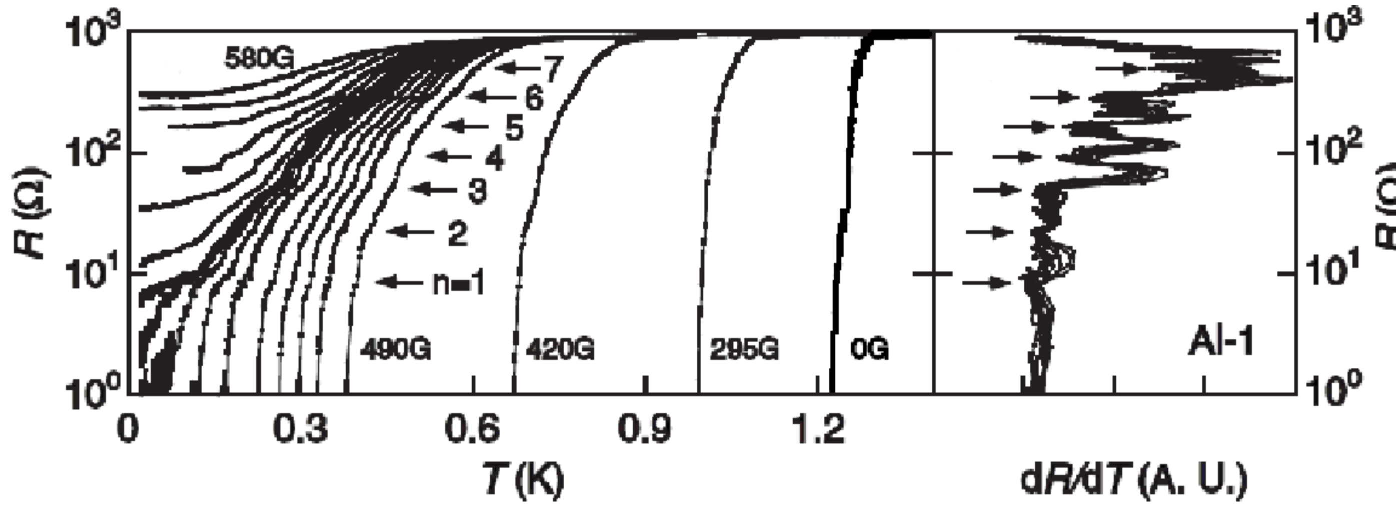


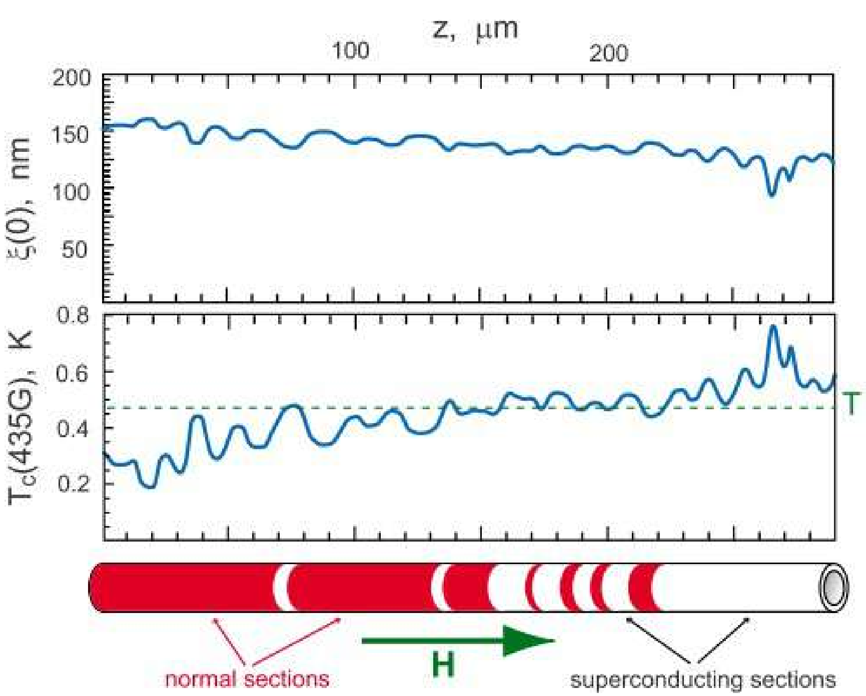


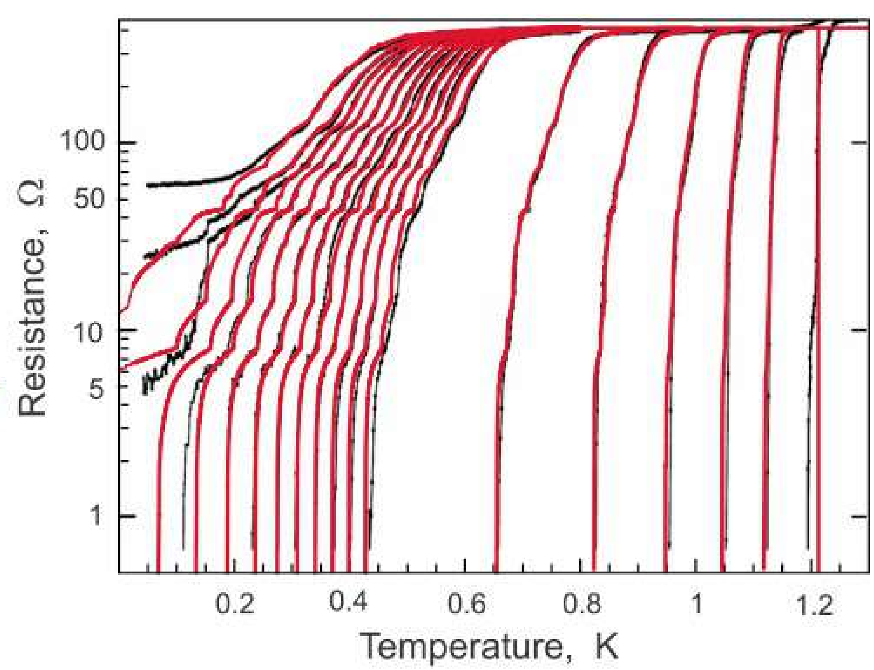


Wang et al. PRL (2005)

Mean-field BCS transition hypothesis



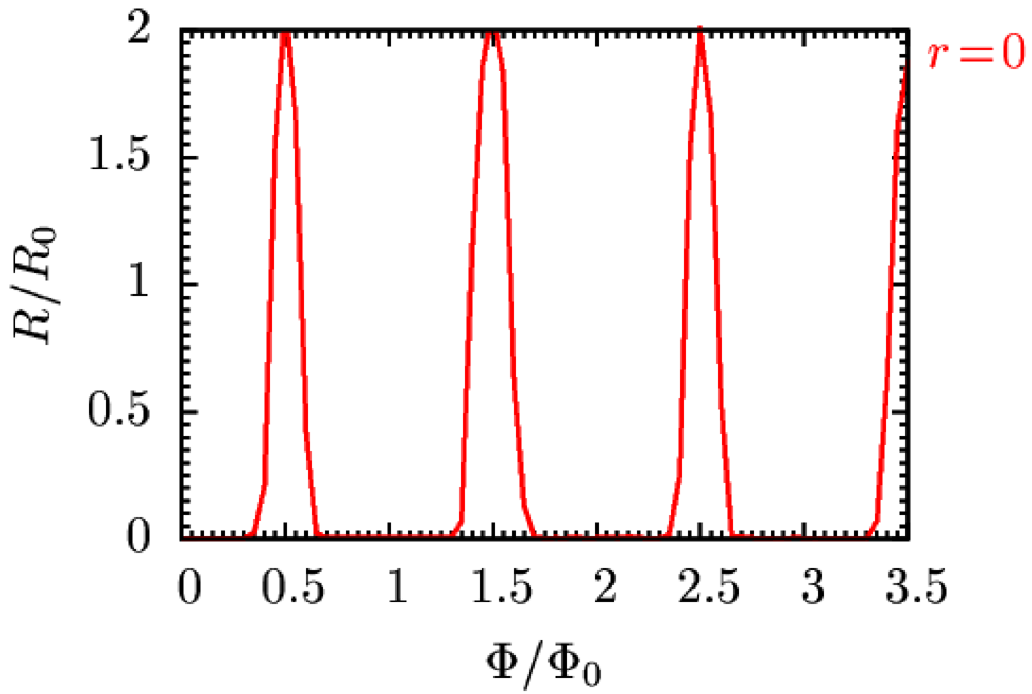




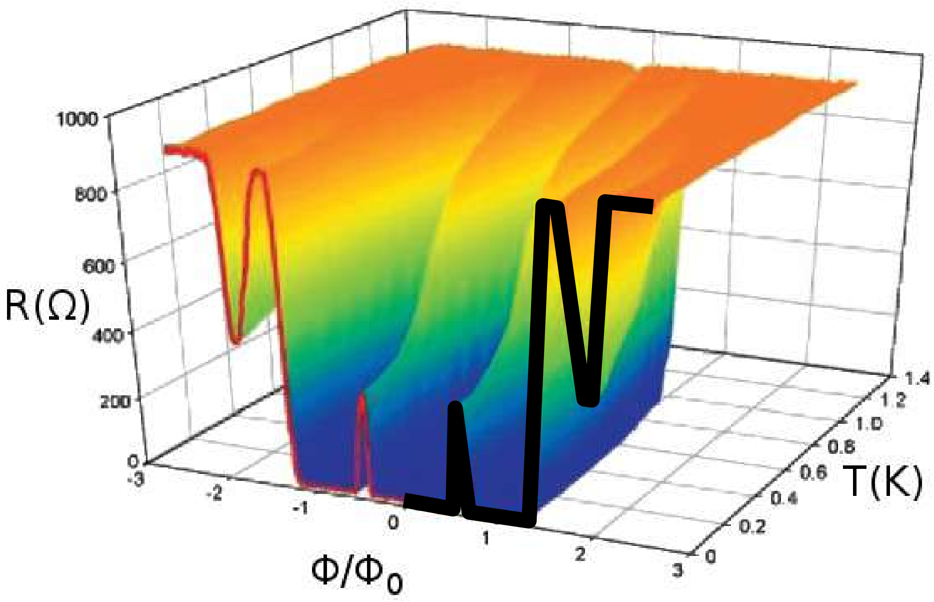
Dao & Chibotaru, PRB (2009)

Little-Parks in a small diameter cylinder

Theory:



Experiment:



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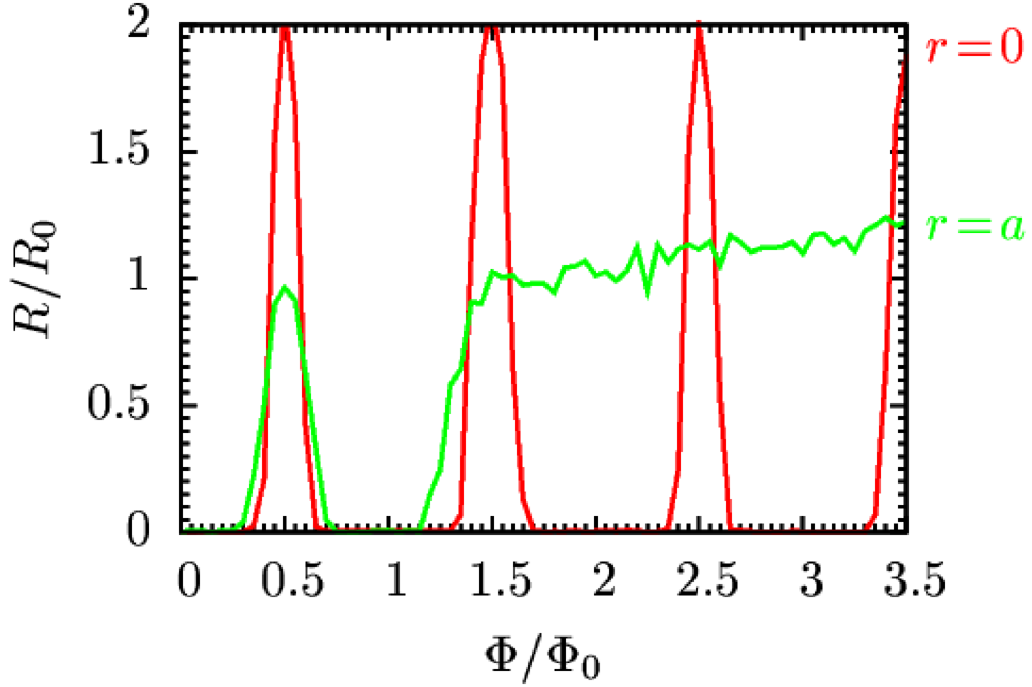

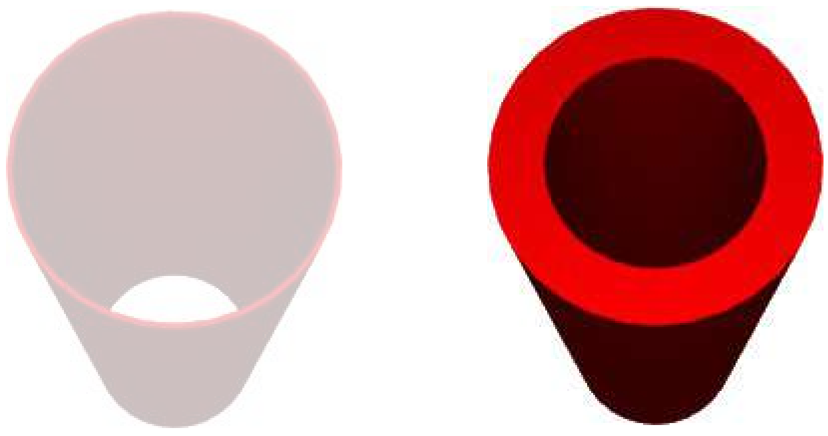

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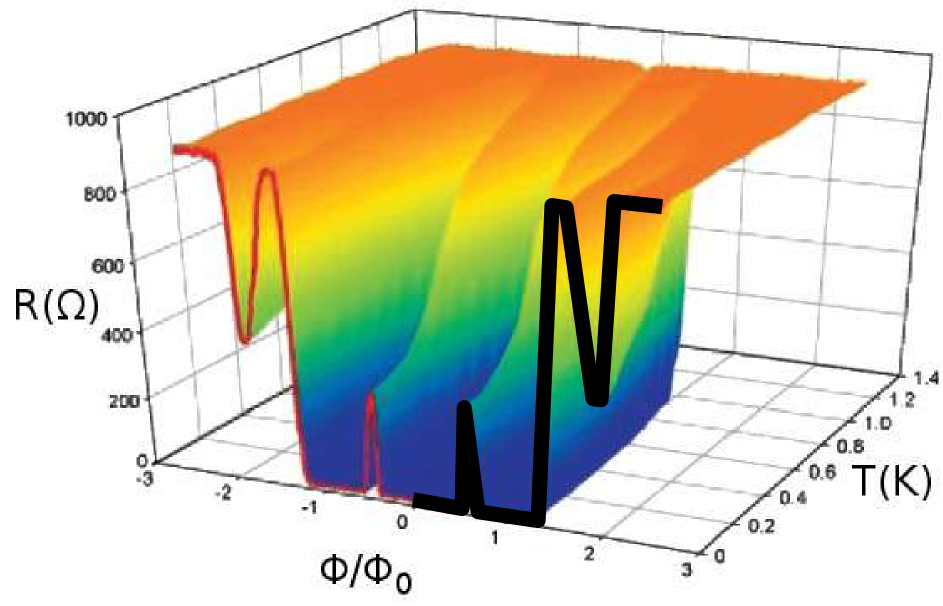
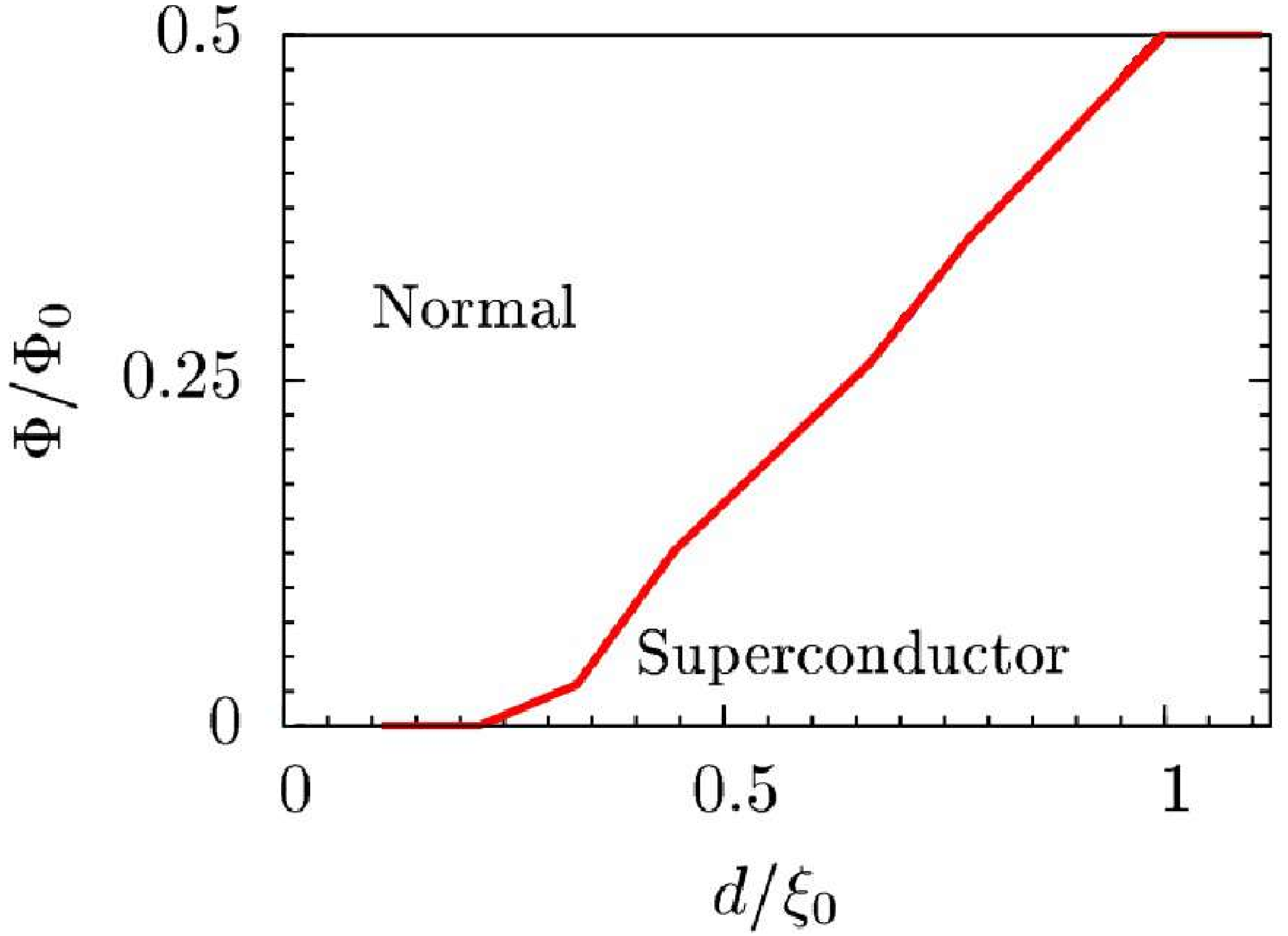


Variation with diameter



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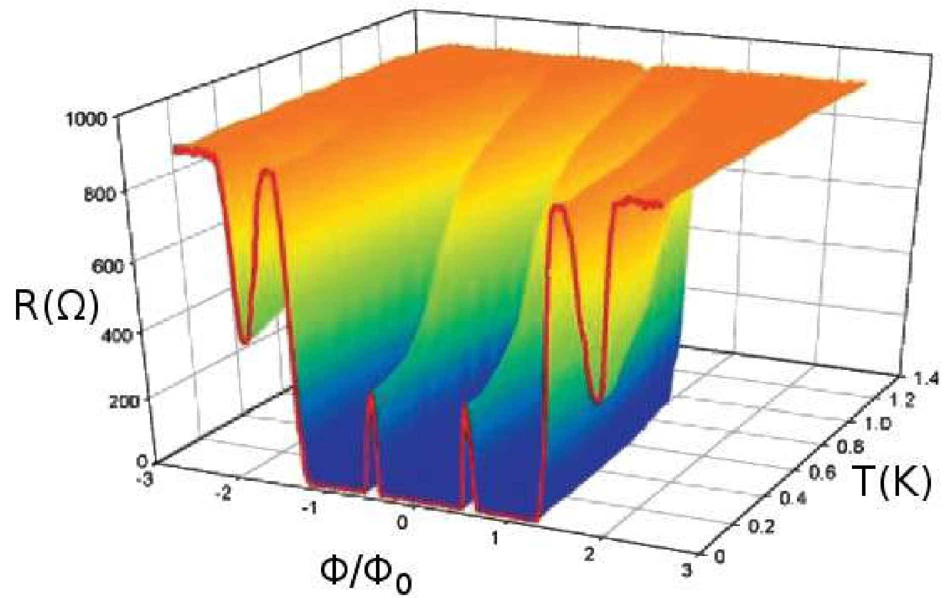

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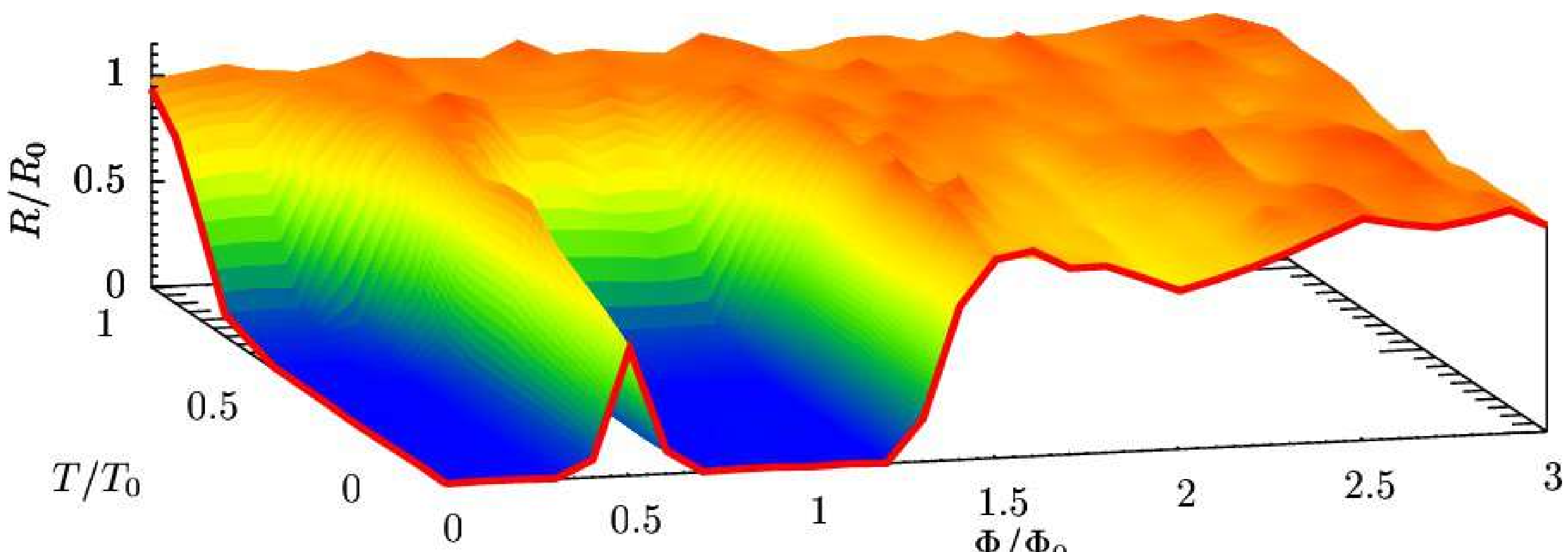

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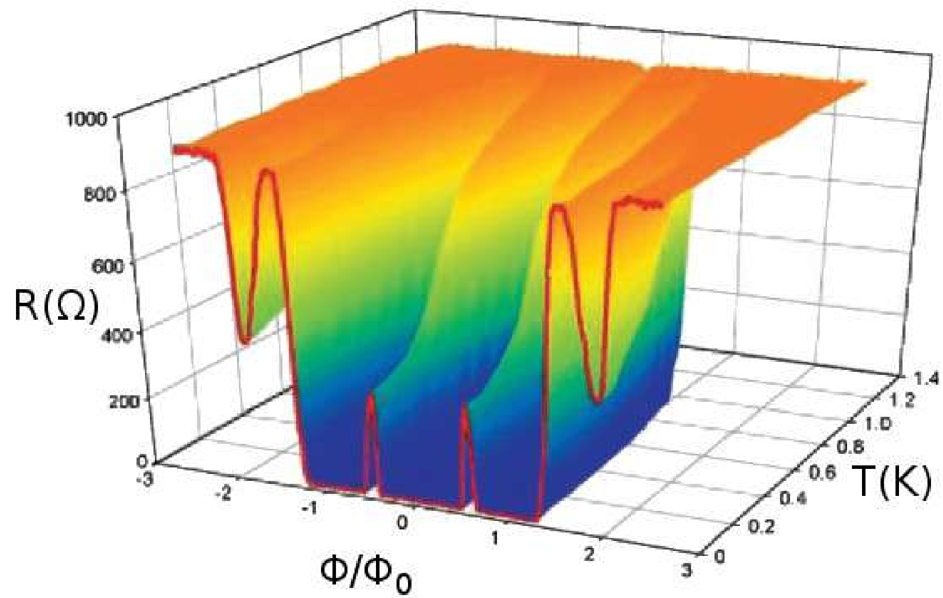

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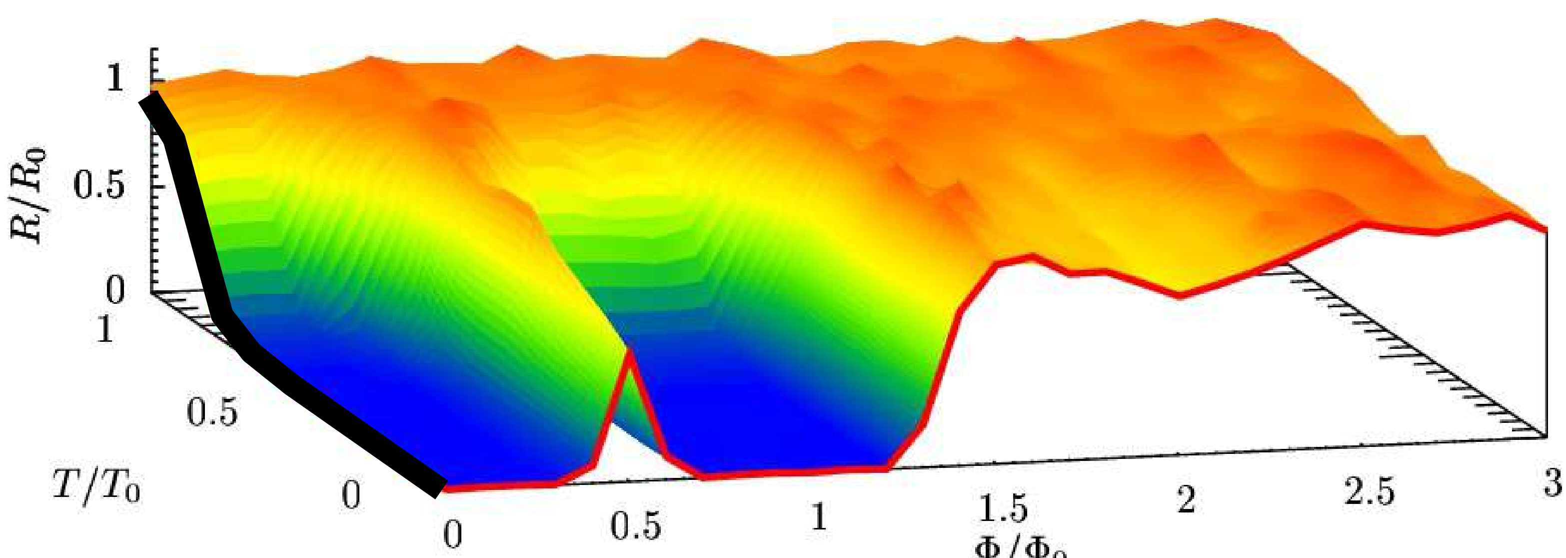
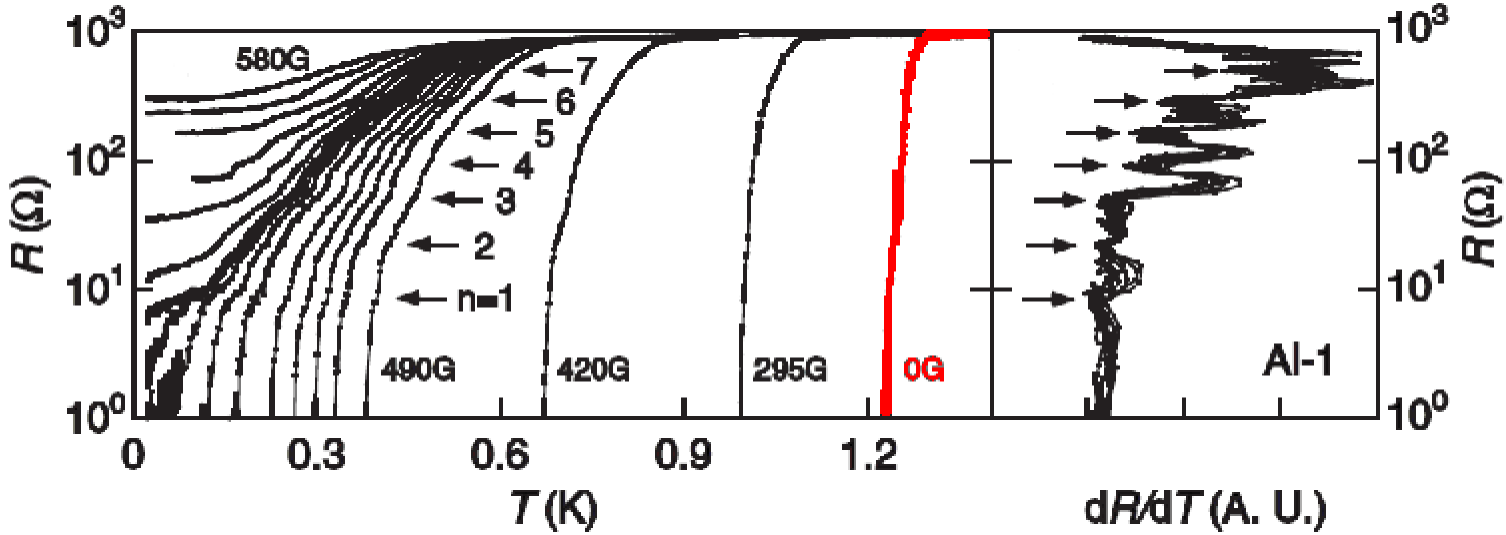
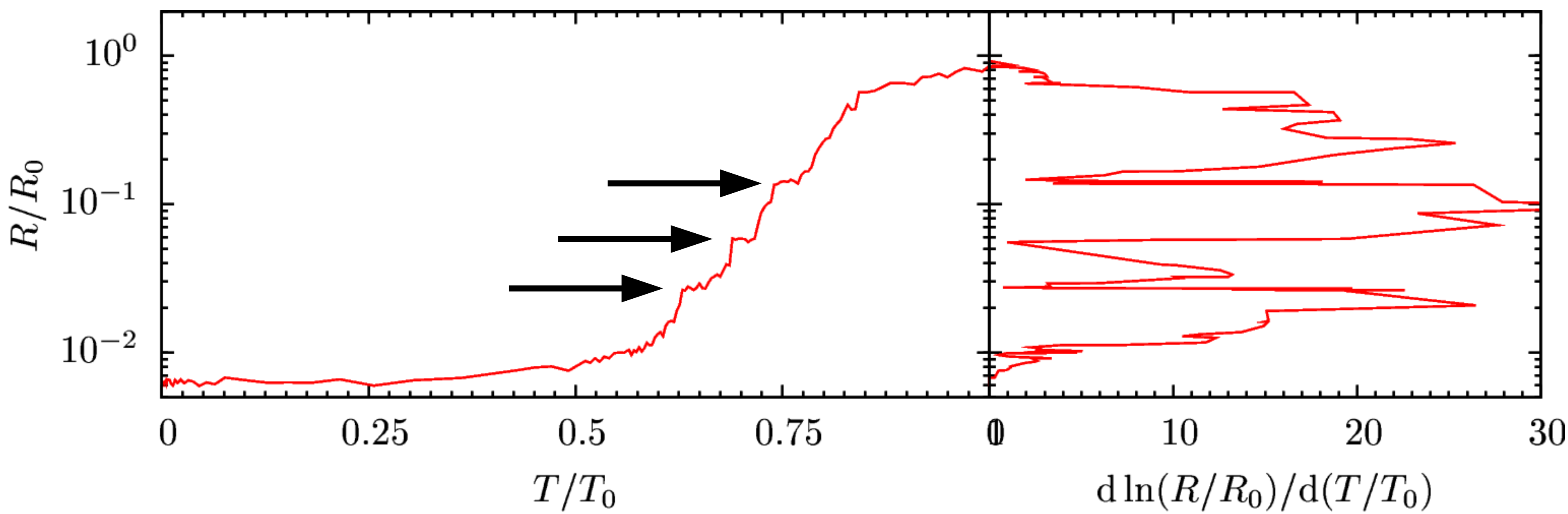


Evidence of phase reconstruction

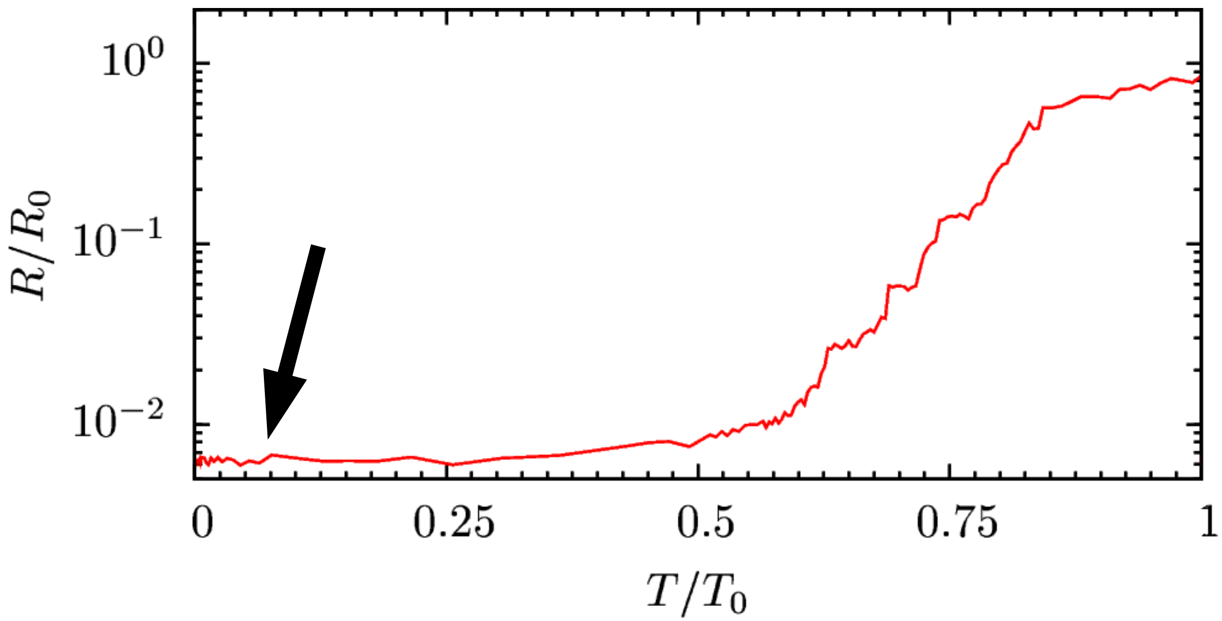
- Experiment:

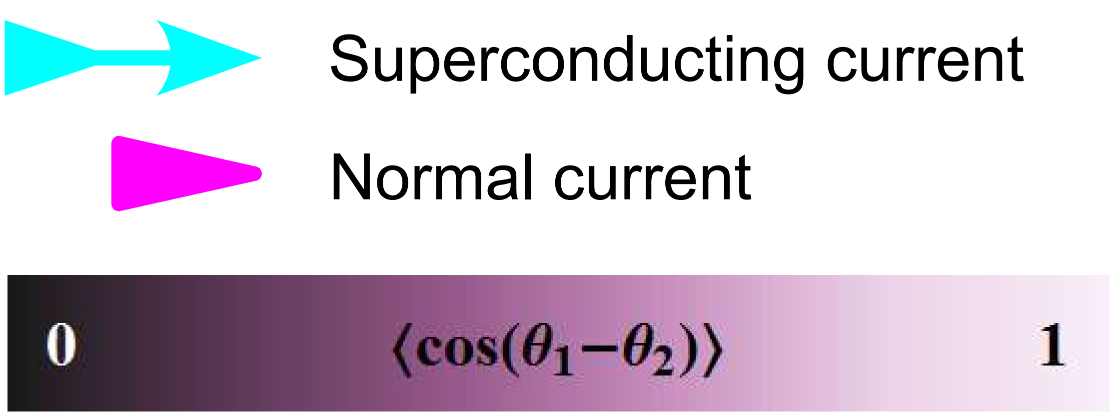


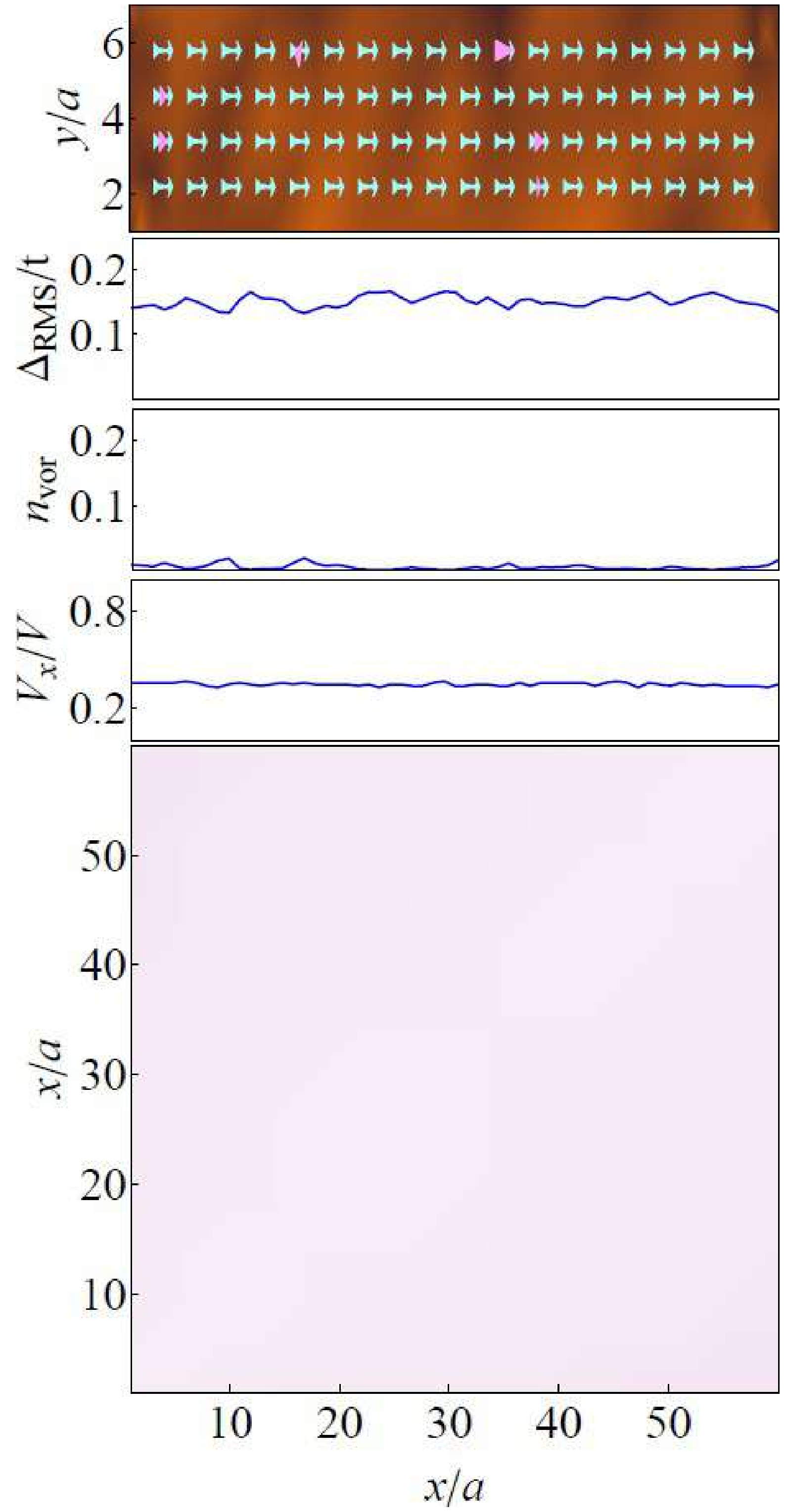
- Theory:



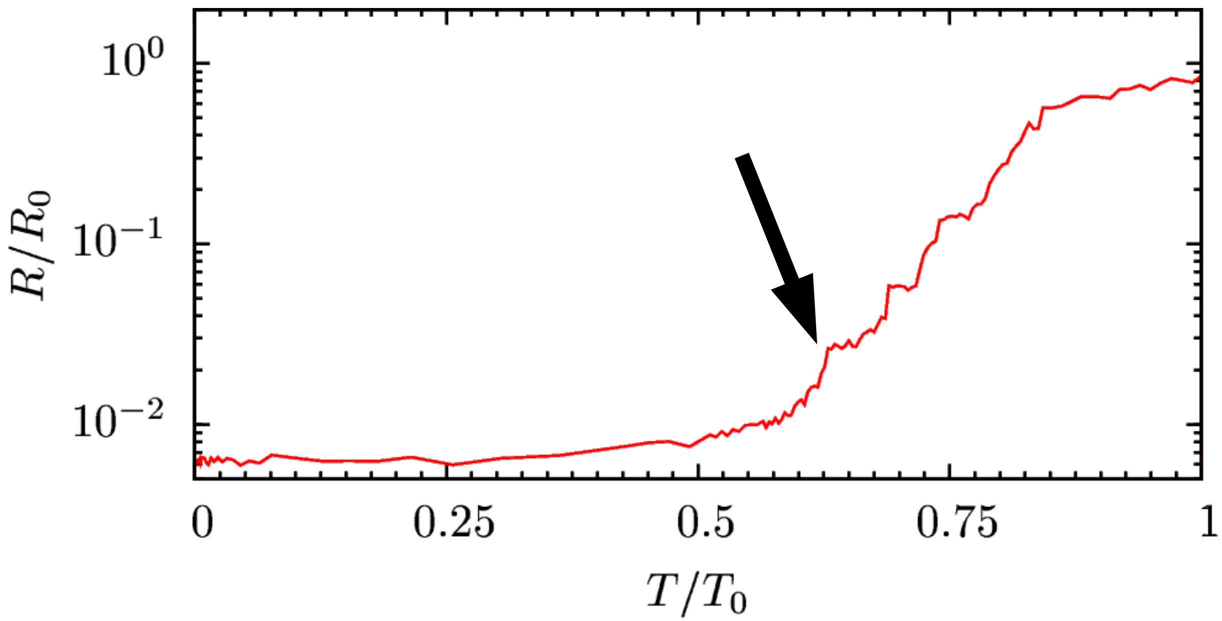
Completely superconducting

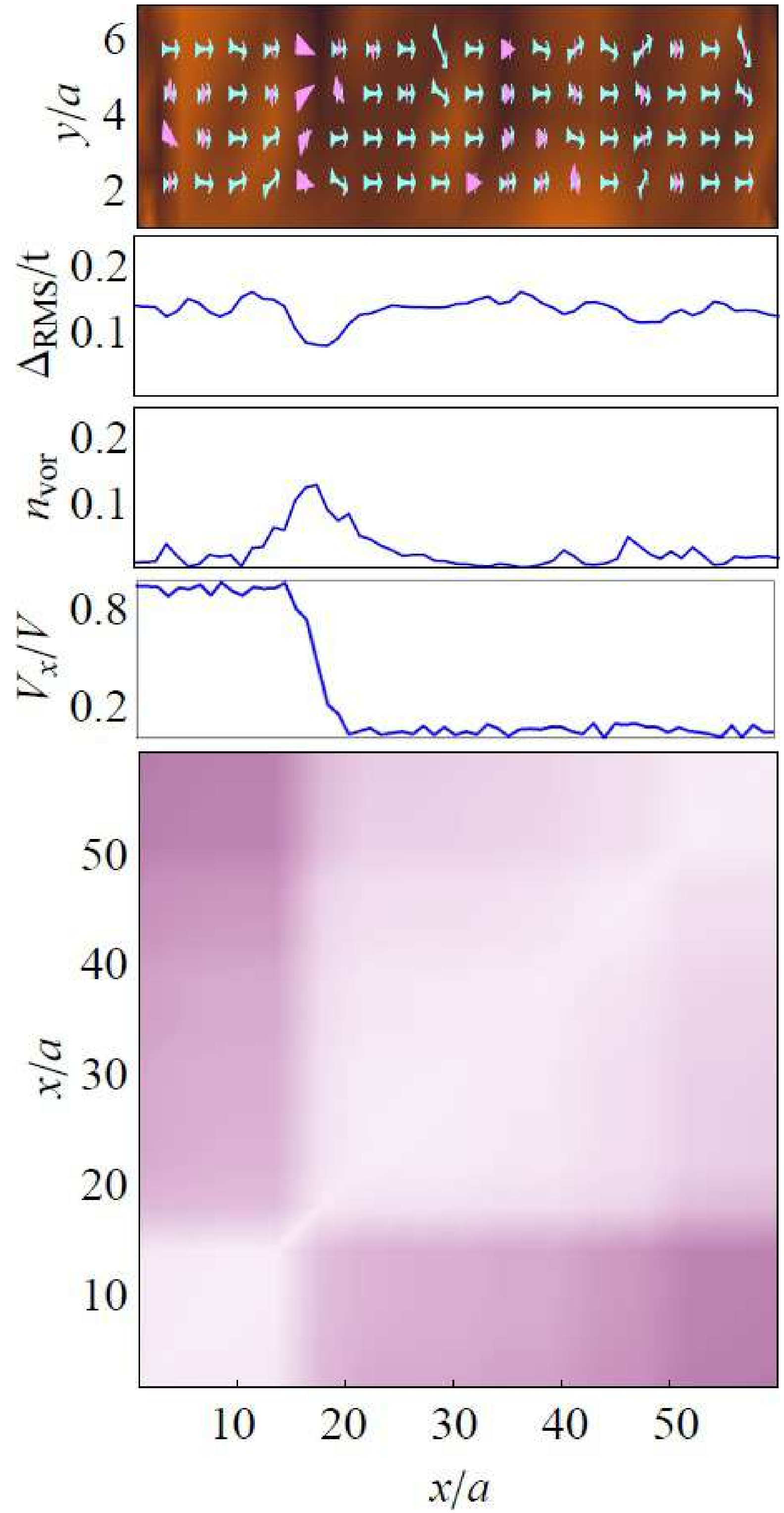






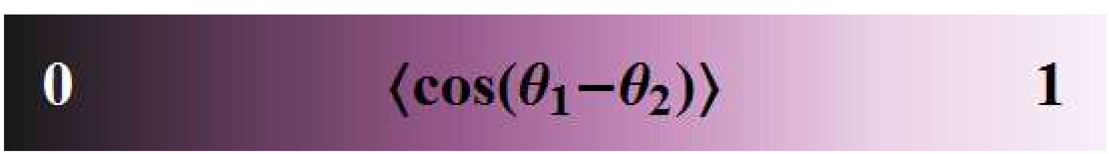
Two superconducting regions





Superconducting current

Normal current



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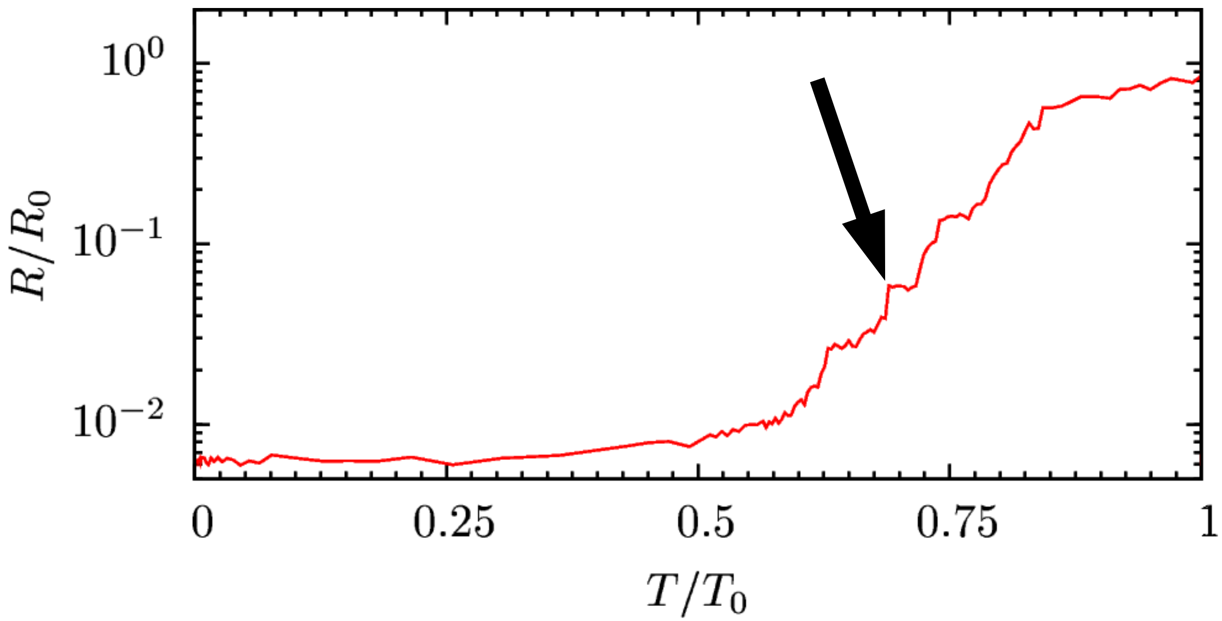

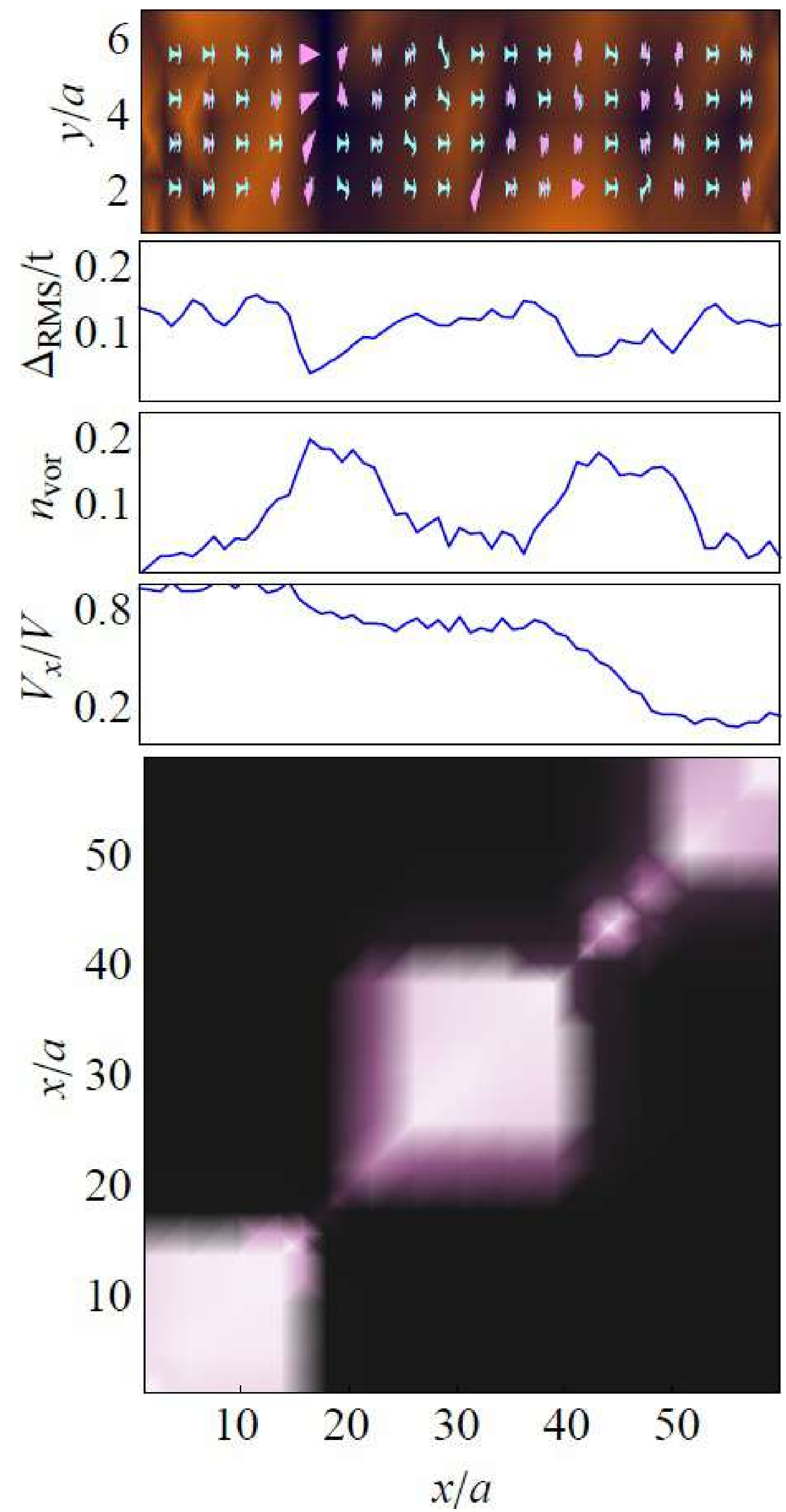

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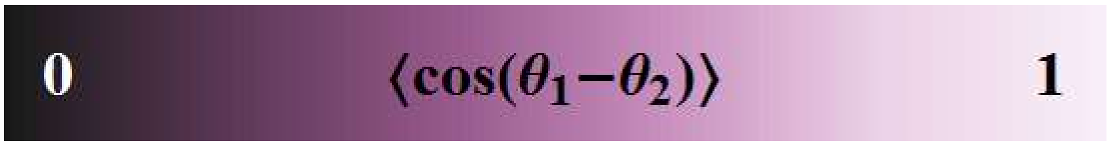
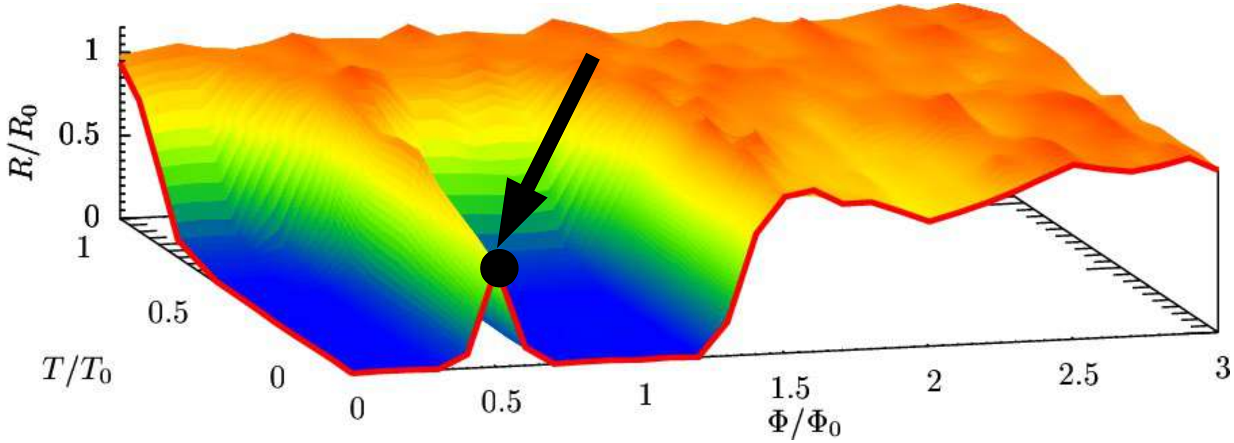
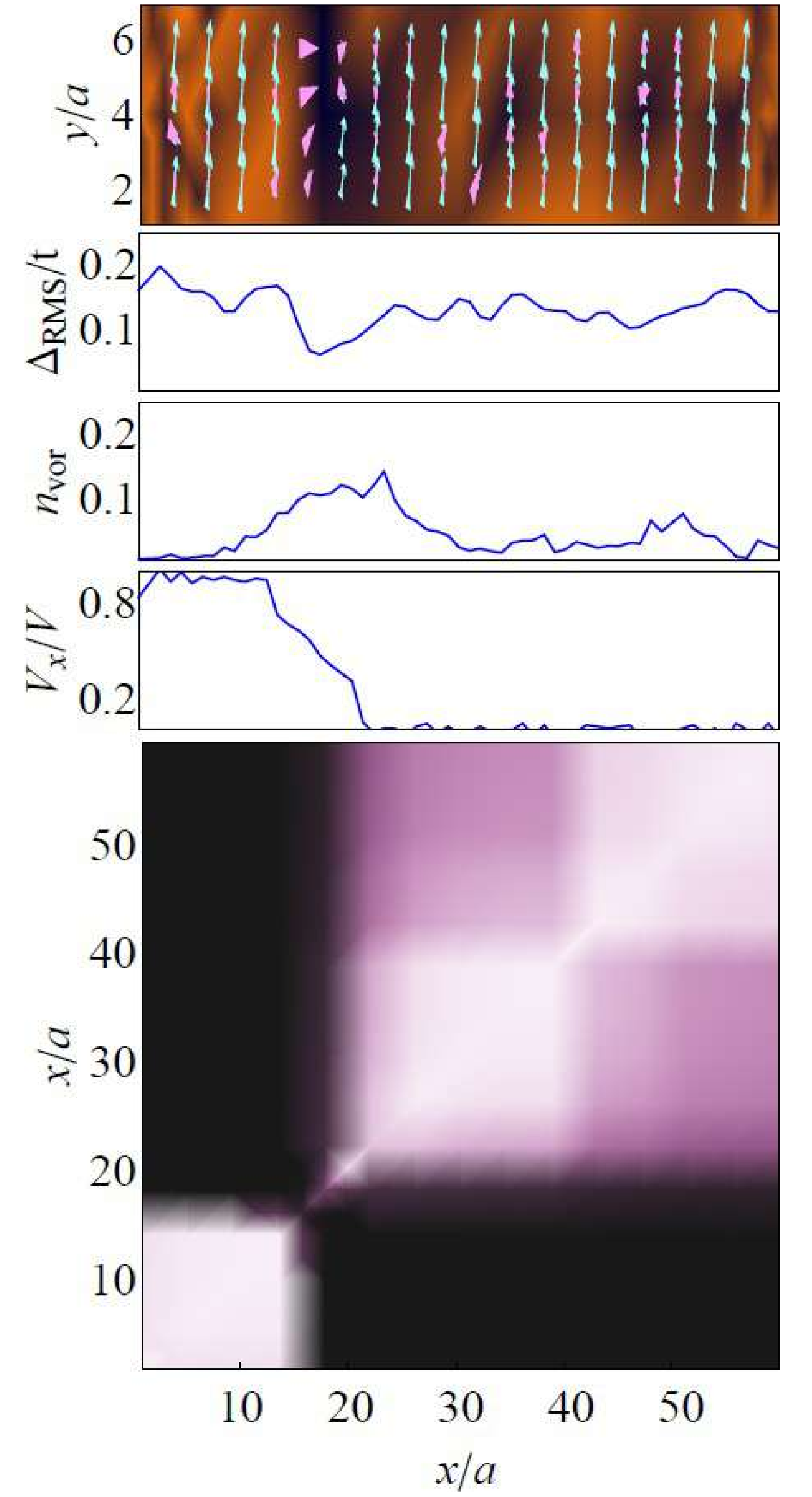
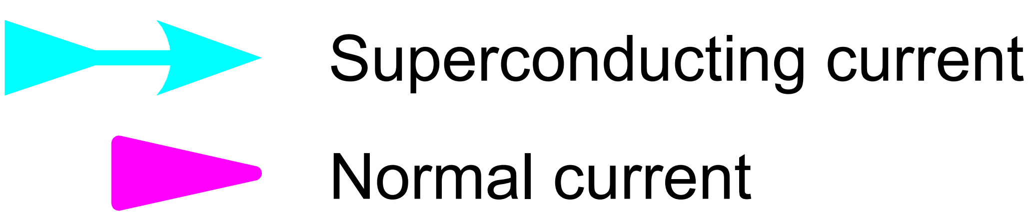
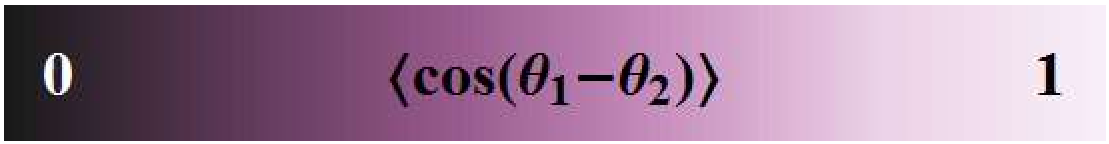


Half flux quantum normal state



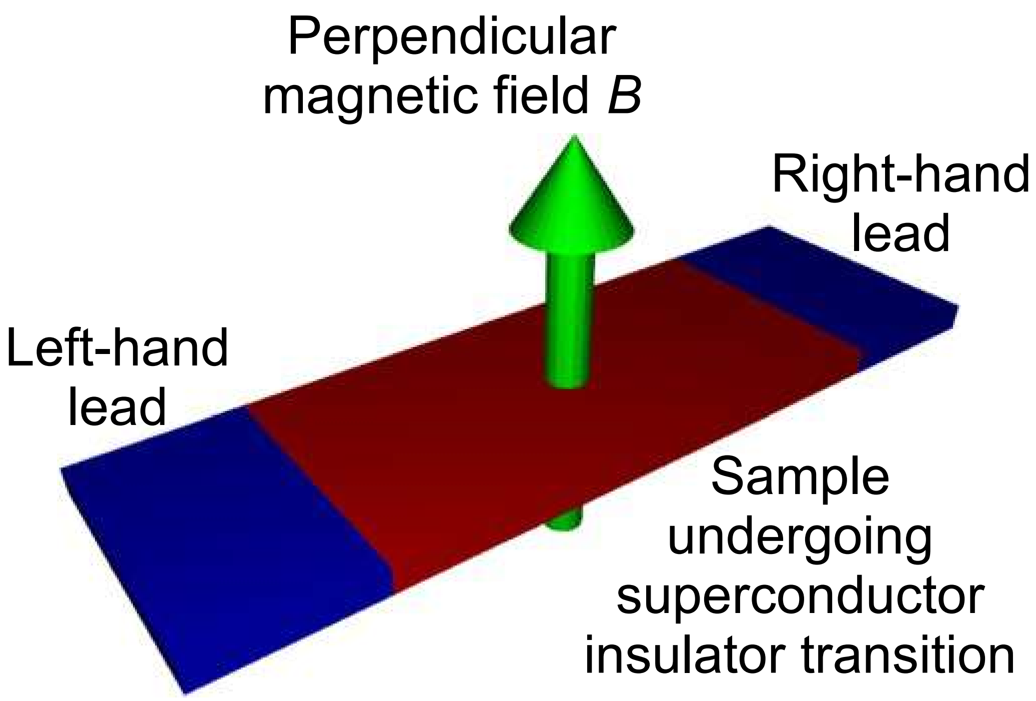


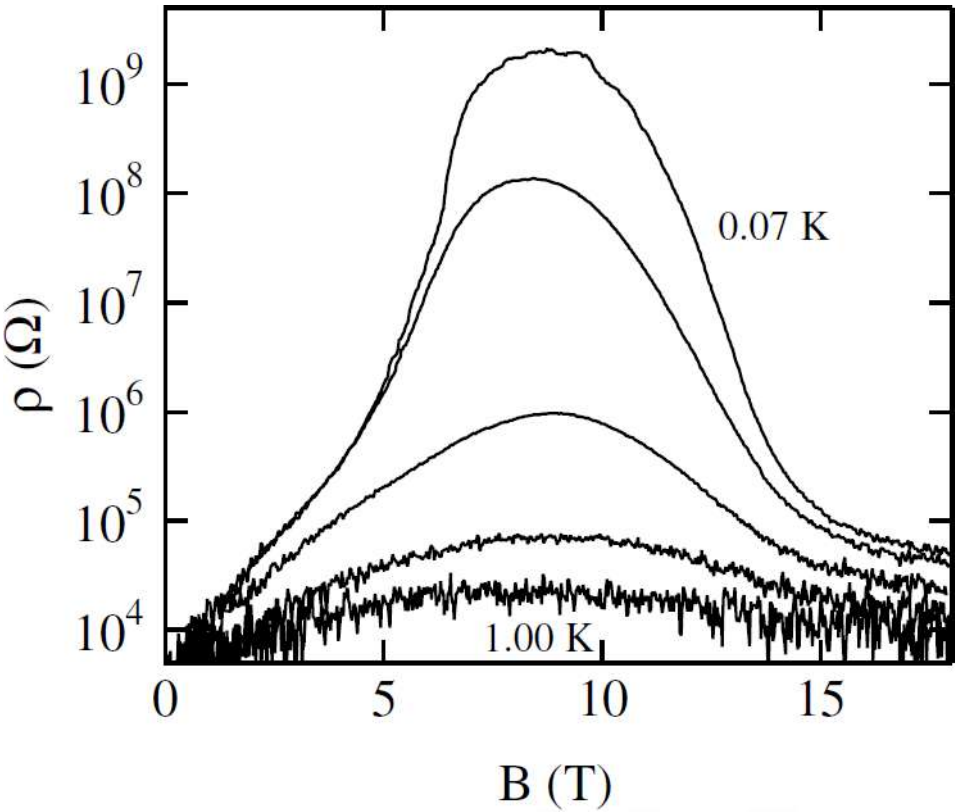




Magnetoresistance peak

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





Magnetoresistance peak

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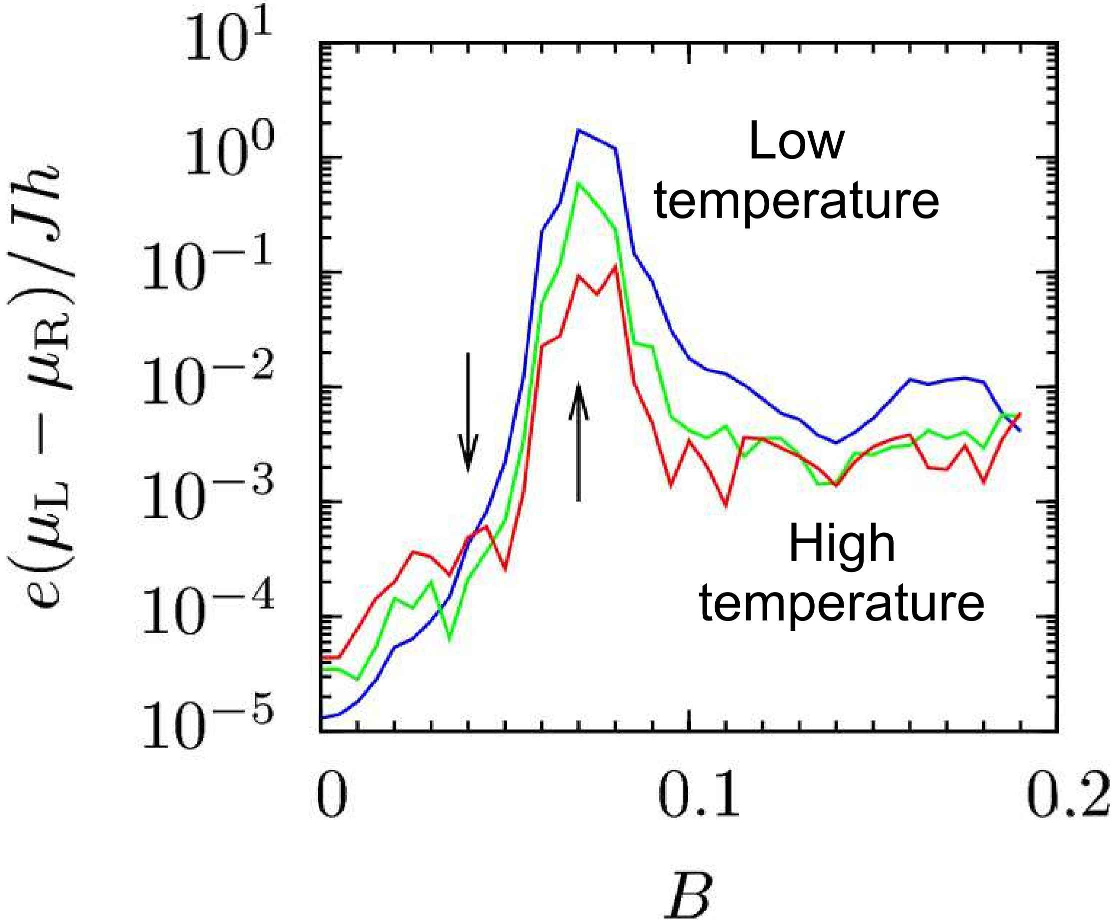
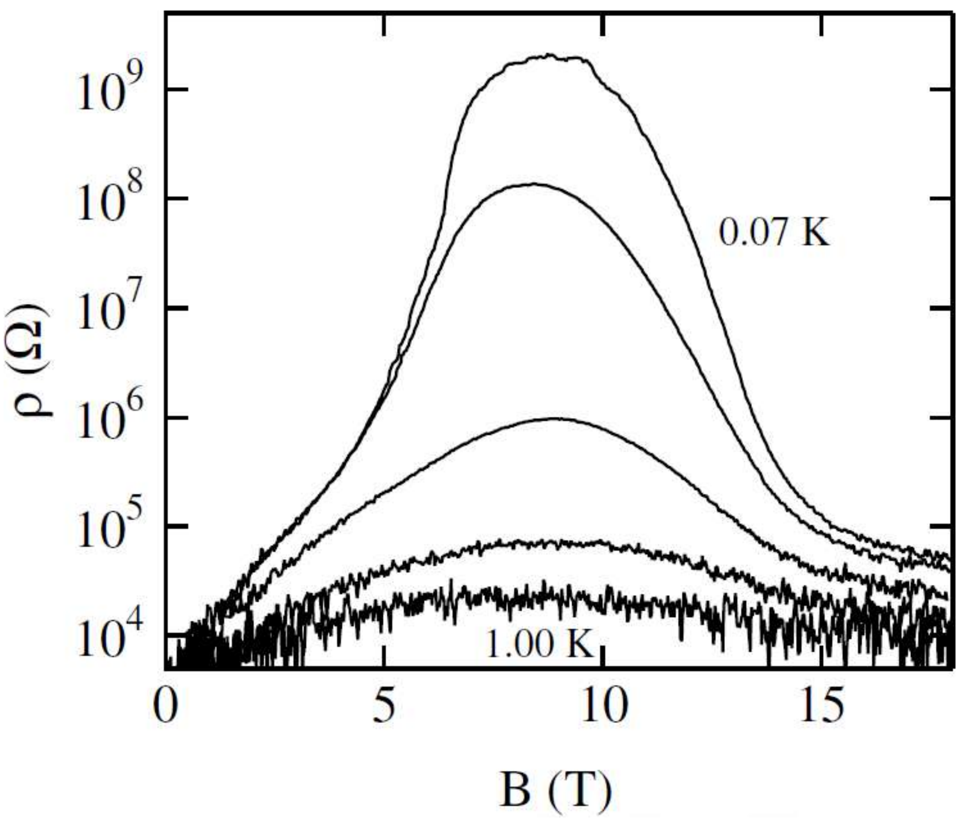
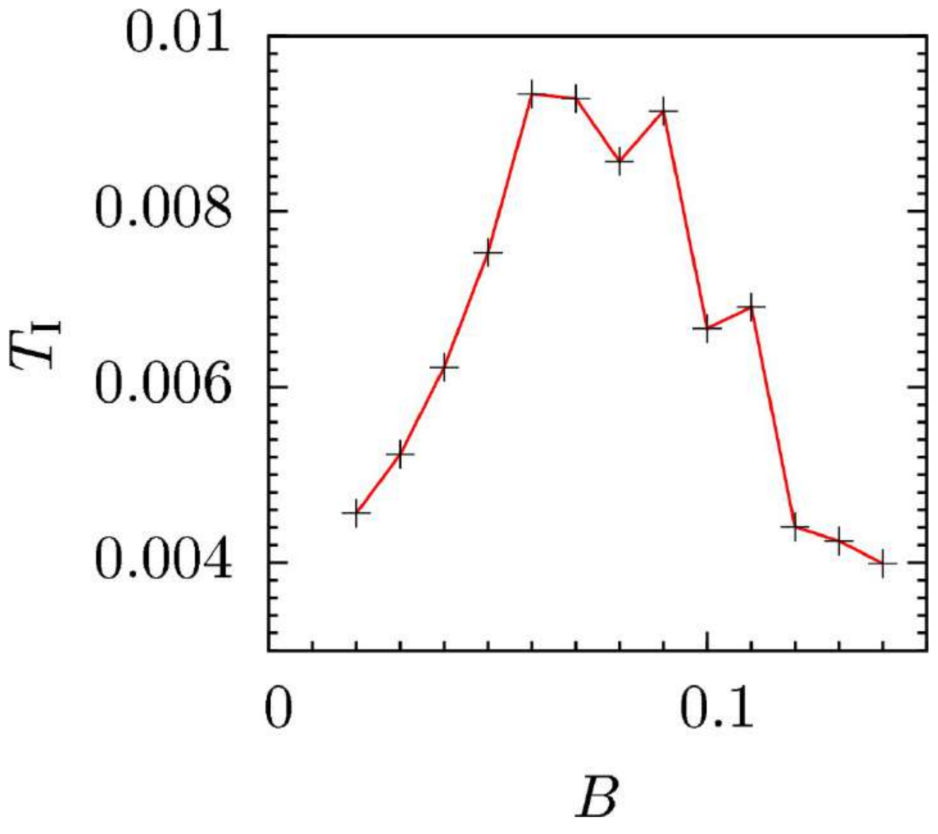
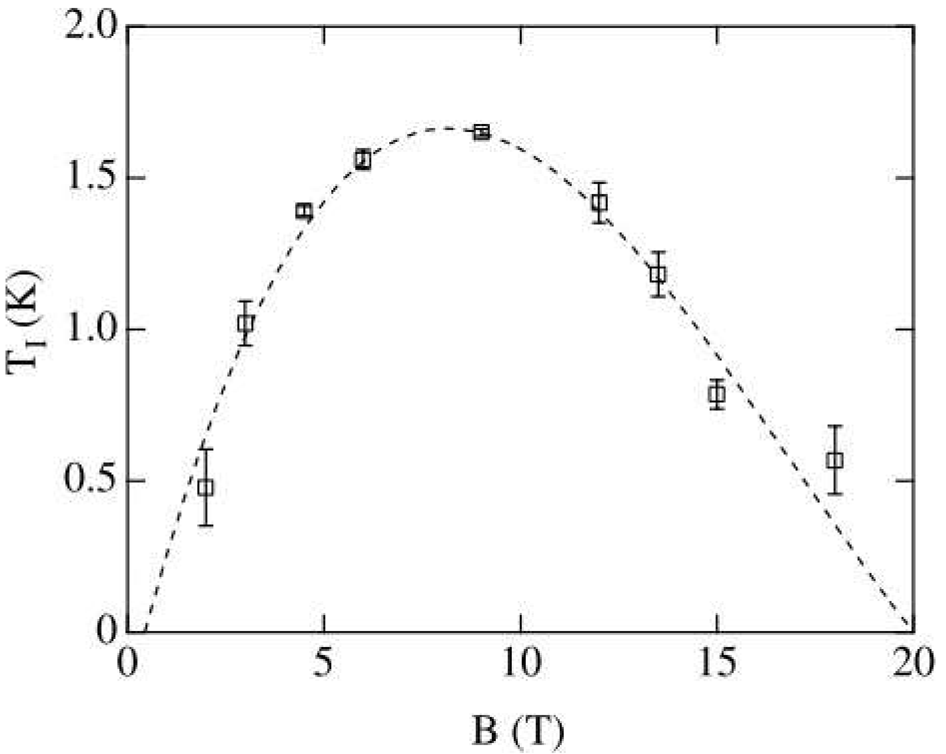




Clues: activated transport

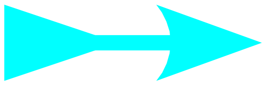
- Activated transport $\rho = \rho_0 e^{T_I/T}$

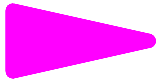




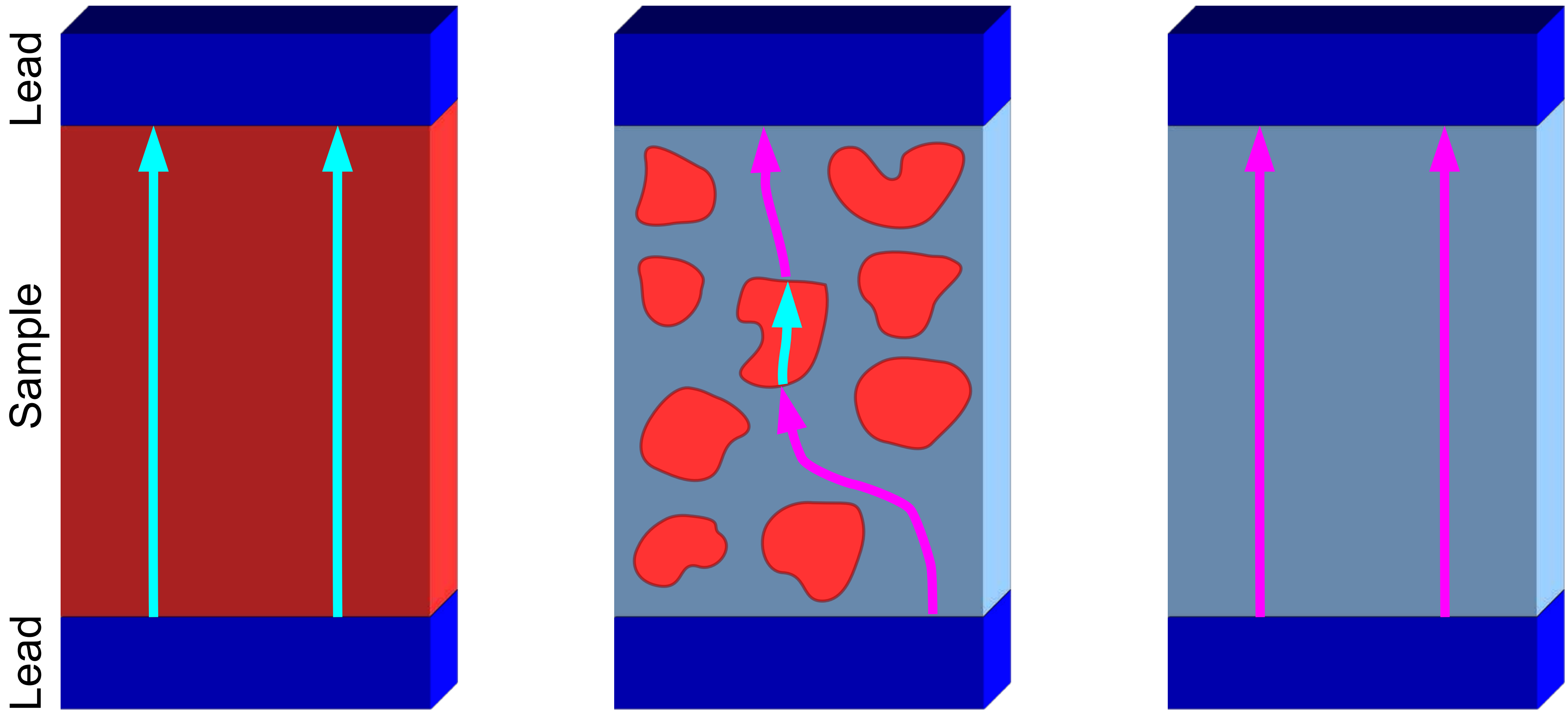
Clues: current maps

- Weak links across superconducting puddles


Superconducting current


Normal current

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