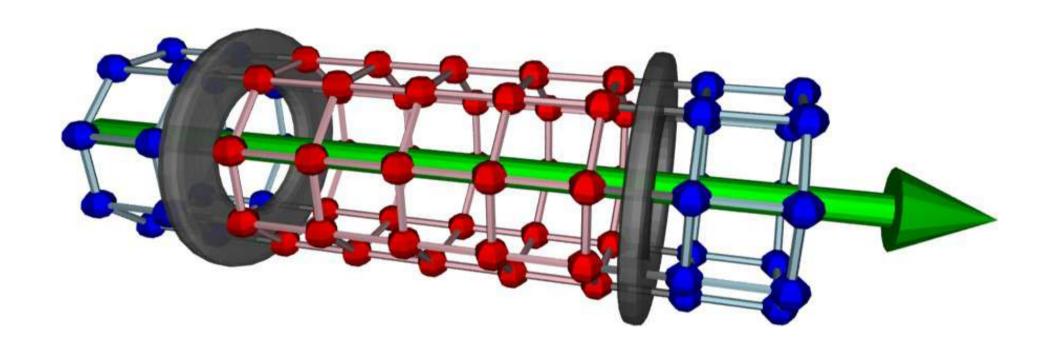
An *ab initio* study of the Little-Parks effect

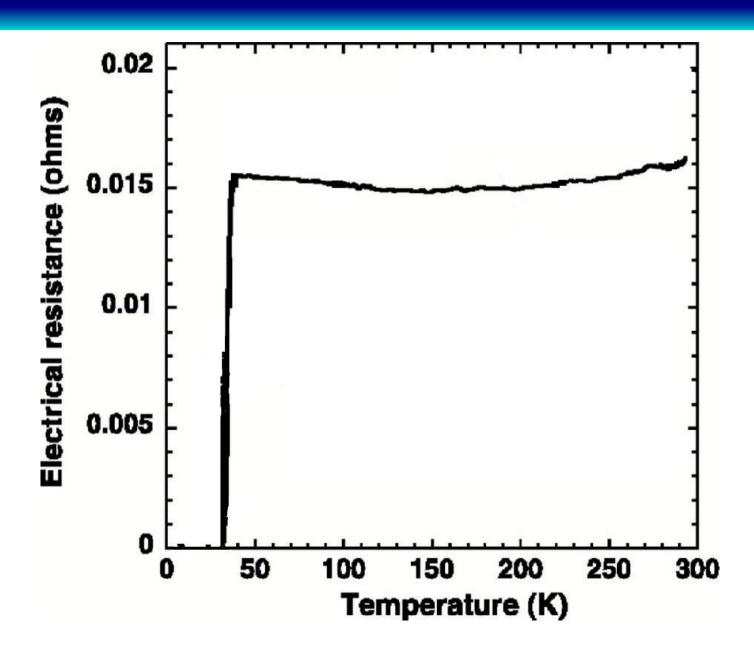


Gareth Conduit, Yigal Meir

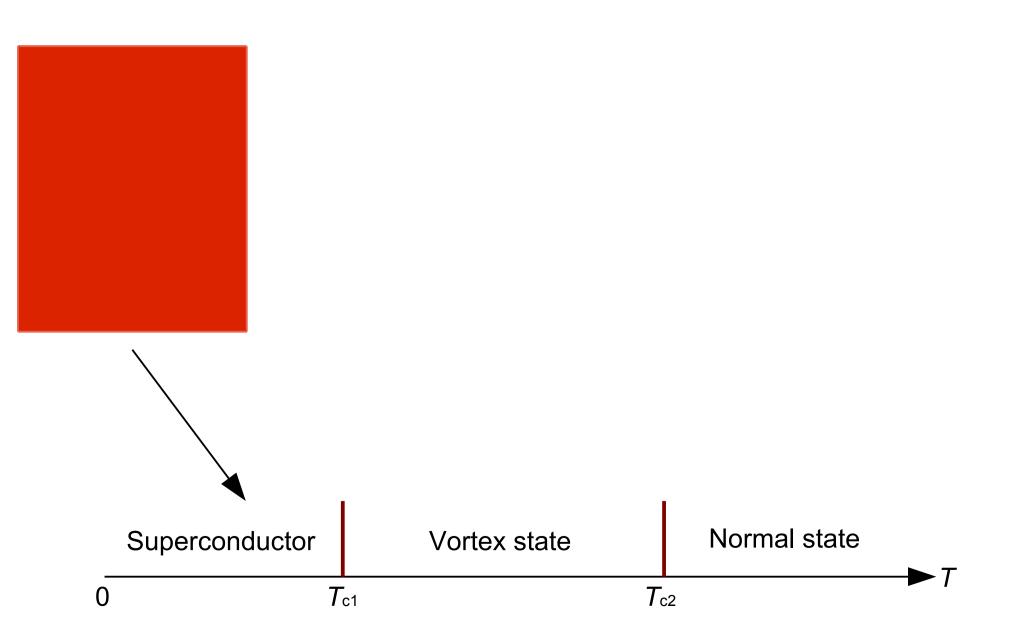
Ben Gurion University

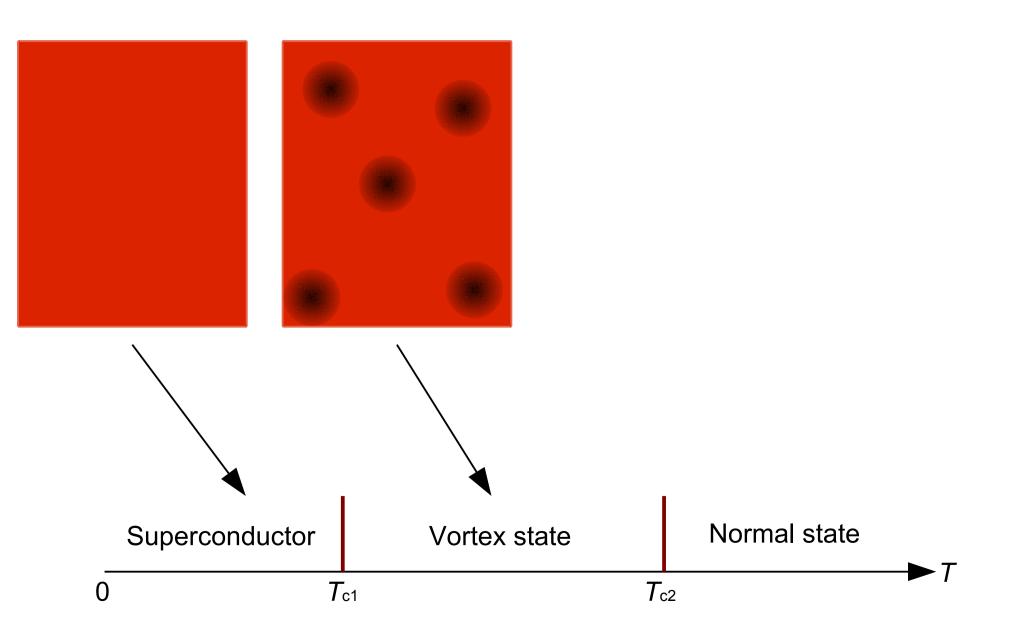
arXiv:1102.1604

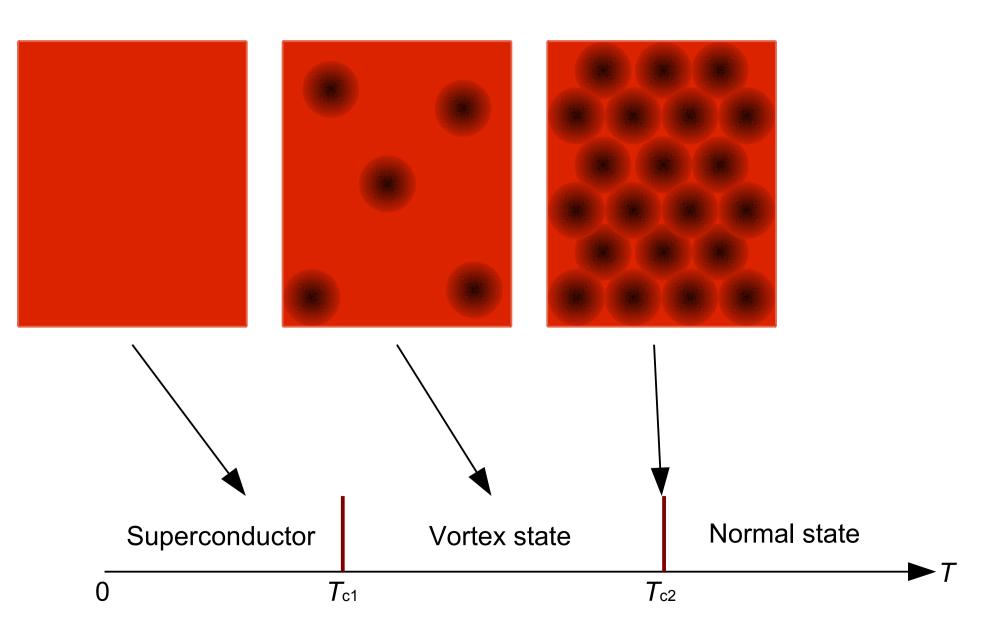
BCS superconductivity

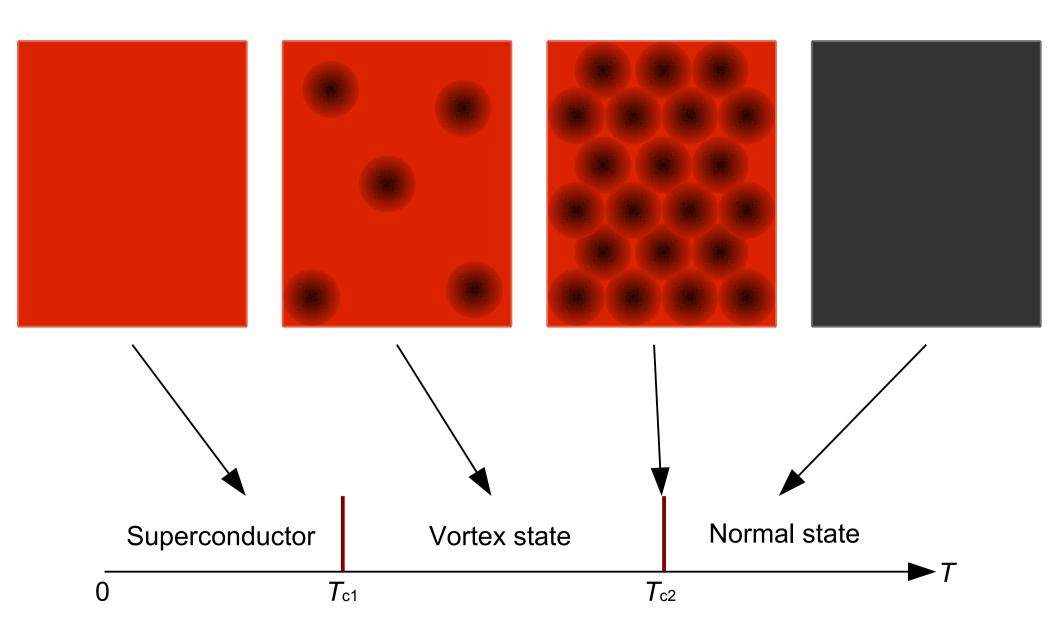


Monteverde et al., Science 292, 75 (2001)

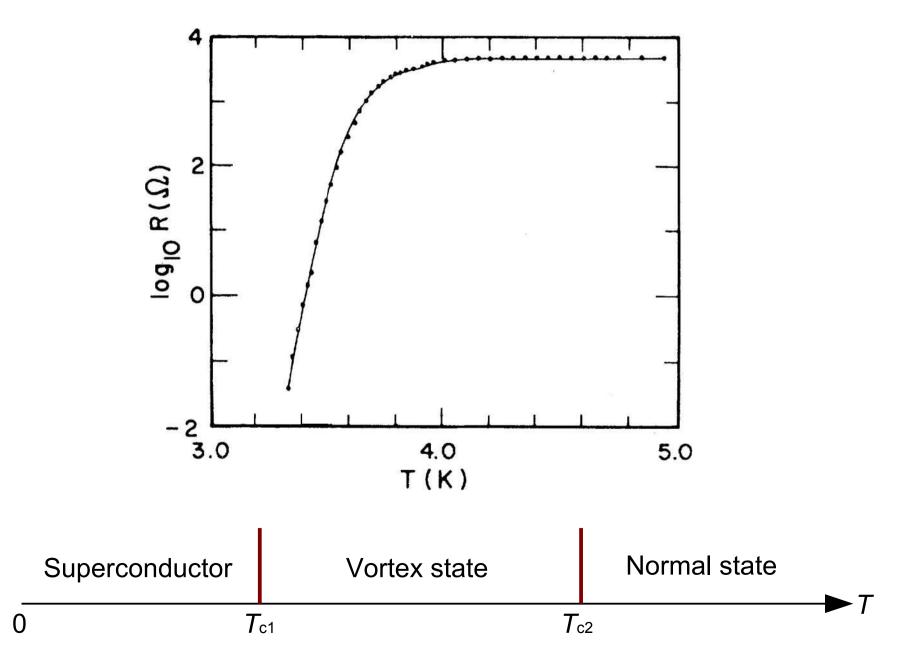






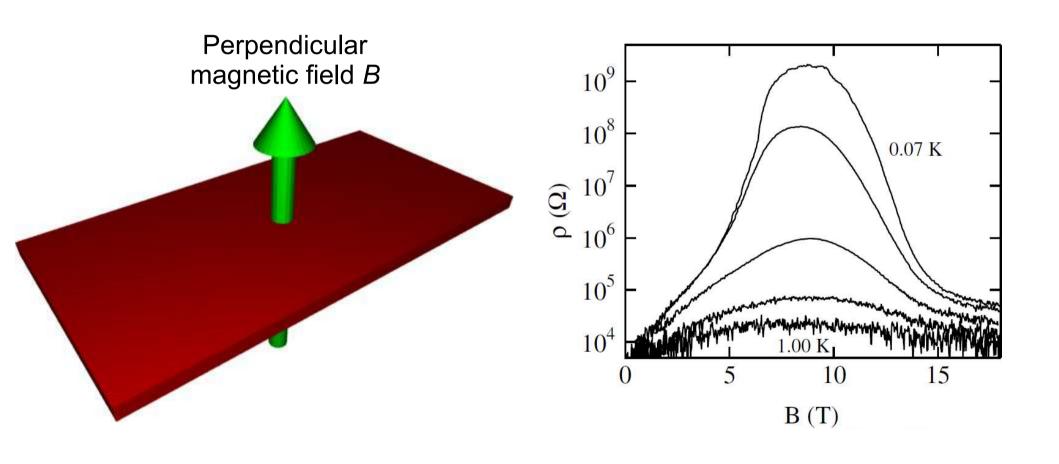


KT transition conductivity

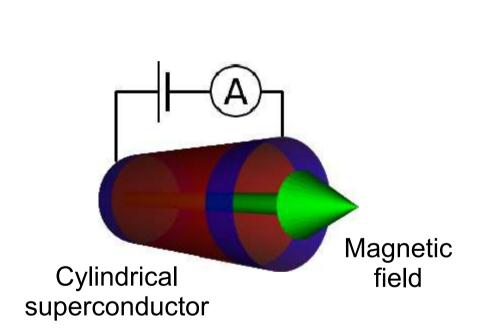


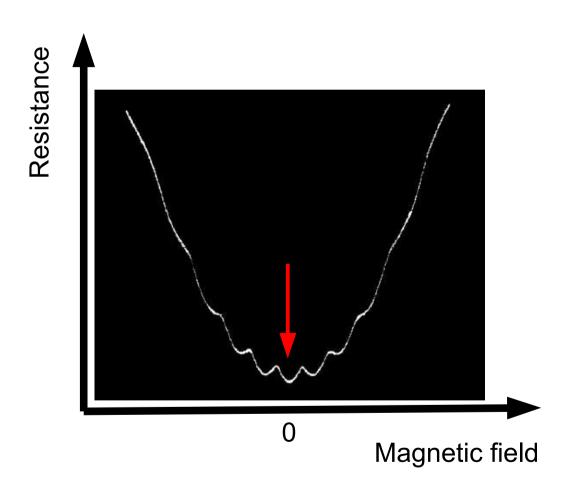
Transition in highly disordered systems

Magnetoresistance peak [Sambandamurthy 04]

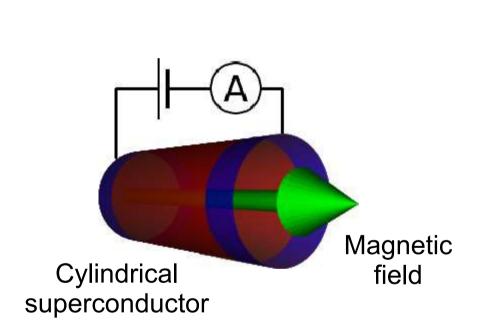


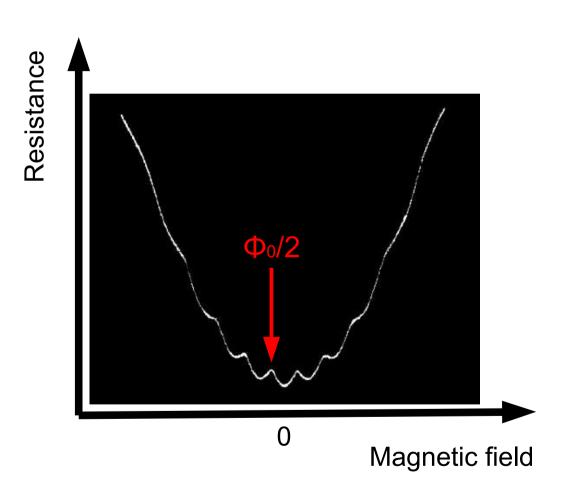
 Cylindrical superconductor held at transition temperature and zero threading flux [Little & Parks, PRL 1962]



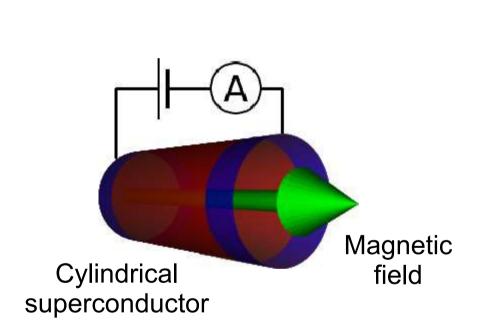


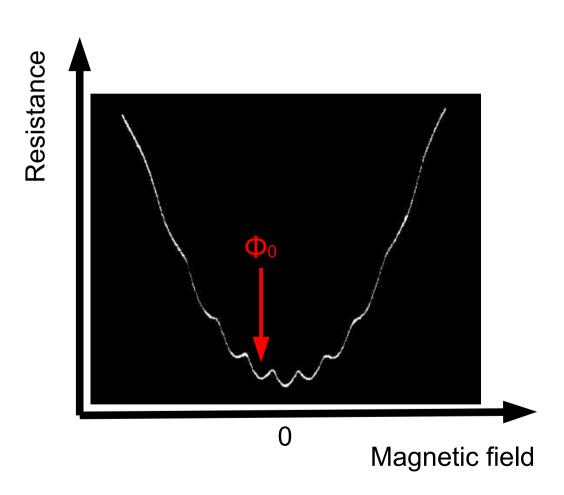
 Cylindrical superconductor held at transition temperature and threading flux is increased [Little & Parks, PRL 1962]



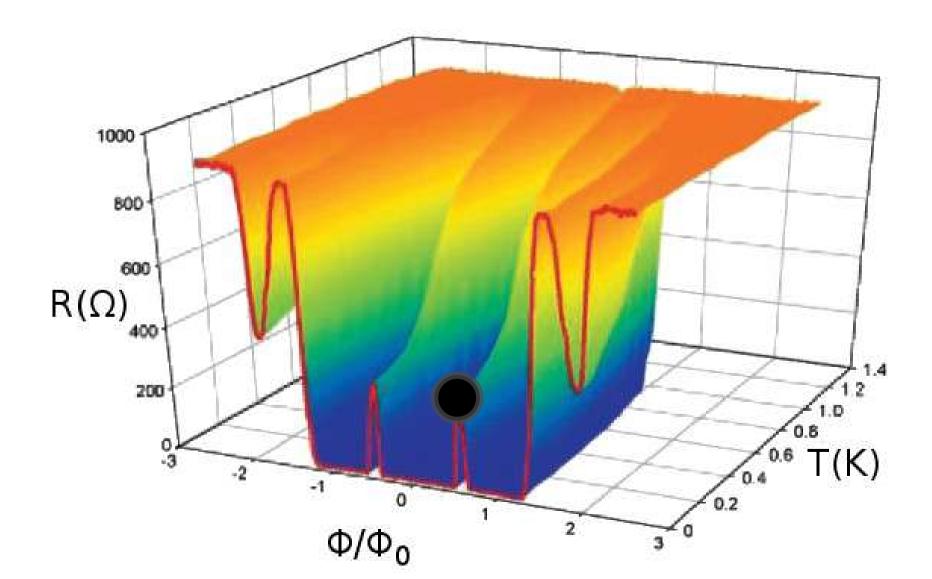


 Cylindrical superconductor held at transition temperature and threading flux is increased [Little & Parks, PRL 1962]





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



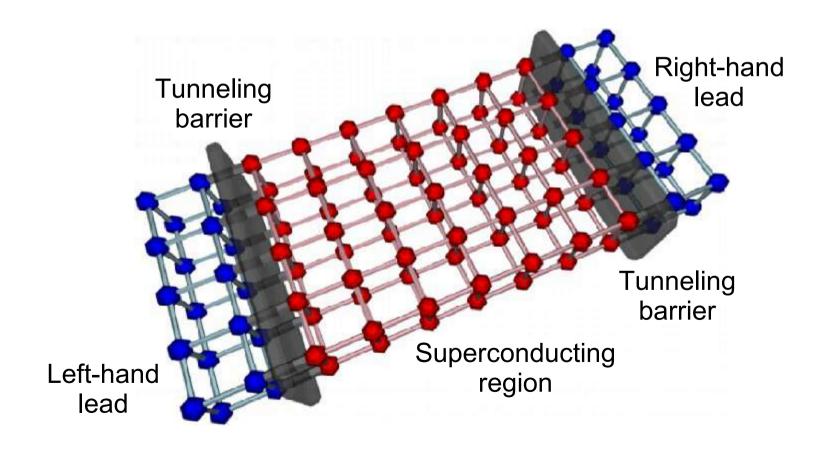
Strategy to study superconductors

- 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]

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



Decoupling the interactions

Negative U Hubbard model

$$\hat{H}_{\text{Hubbard}} = \sum_{i,\sigma} \epsilon_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{i} U_{i} c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i\downarrow} c_{i\uparrow}$$
$$- \sum_{\langle i,j \rangle, \sigma} \left(t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + t_{ij}^{*} c_{j\sigma}^{\dagger} c_{i\sigma} \right)$$

Decouple Hamiltonian in density and Cooper pair channels

$$\hat{\mathcal{H}}_{BdG} = \sum_{i,\sigma} (\epsilon_i + \rho_i) c_{i\sigma}^{\dagger} c_{i\sigma} - \sum_{\langle i,j \rangle, \sigma} \left(t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + t_{ij}^* c_{j\sigma}^{\dagger} c_{i\sigma} \right) + \sum_{i} \left(\Delta_i c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} + \bar{\Delta}_i c_{i\downarrow} c_{i\uparrow} \right) + \sum_{i} \frac{|\Delta_i|^2 + \rho_i^2}{U_i}$$

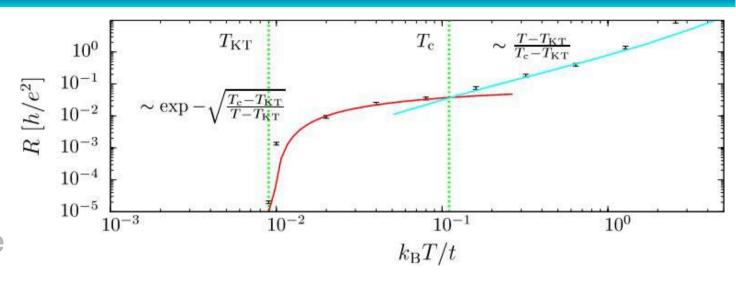
Accelerated Metropolis sampling

To perform thermal sum calculate

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

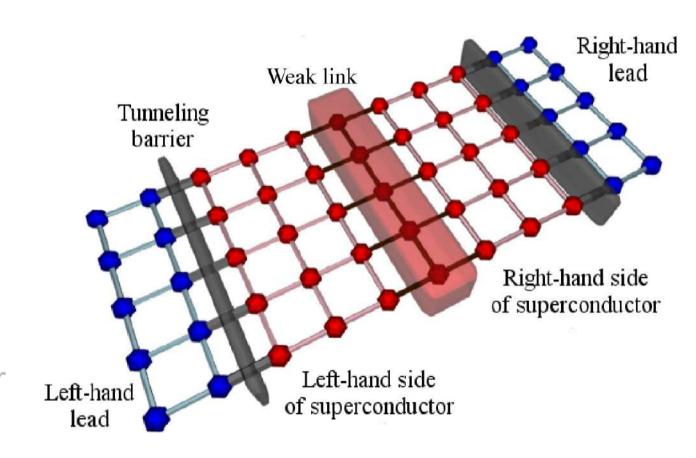
- Propose new configuration of Δ and ρ , accept with probability $\exp(\beta E[\Delta_{\text{old}}, \rho_{\text{old}}] \beta E[\Delta_{\text{new}}, \rho_{\text{new}}])$
- Calculating $E[\Delta, \rho]$ costs $O(N^4)$, where N is the number of sites
- New method calculates $E[\Delta, \rho] E[\Delta + \delta \Delta, \rho + \delta \rho]$ using a order M Chebyshev expansion [Weisse 09] in $O(N^{1.9}M^{2/3})$ time

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

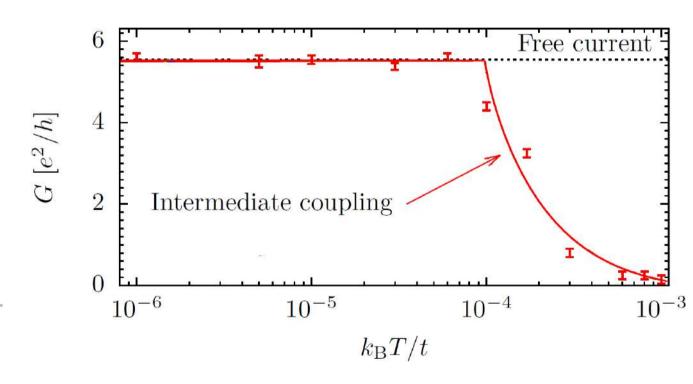


Halperin & Nelson, J. Low Temp. Phys 1979 Ambegaokar *et al.*, PRB 1980

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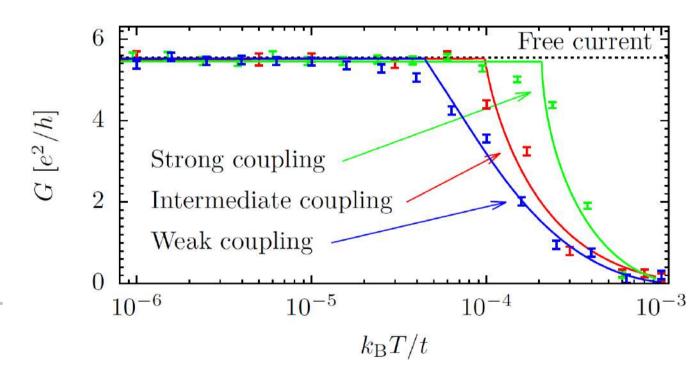


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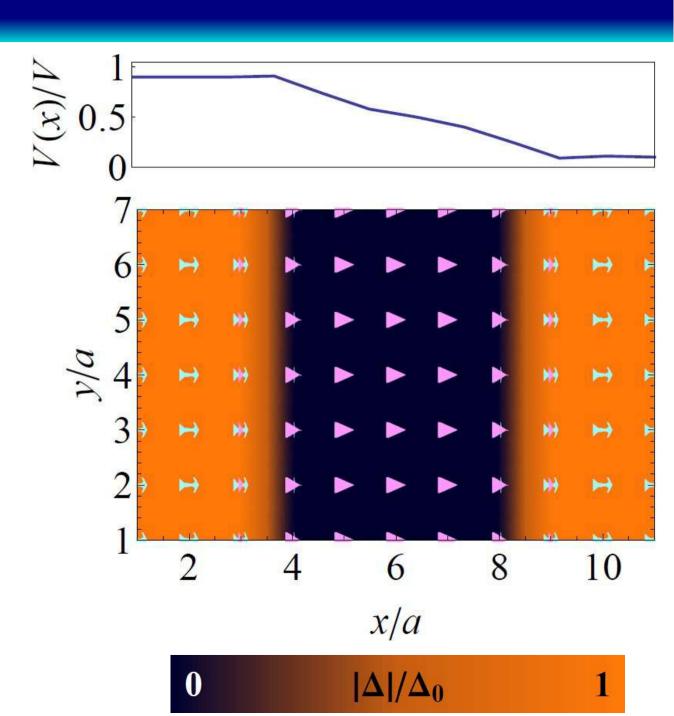


Ambegaokar & Baratoff, PRL 10, 486 (1963)

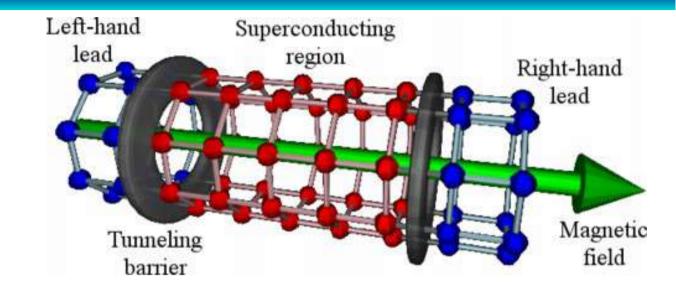
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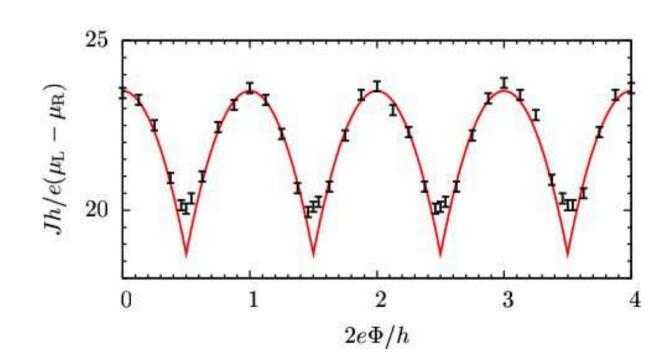


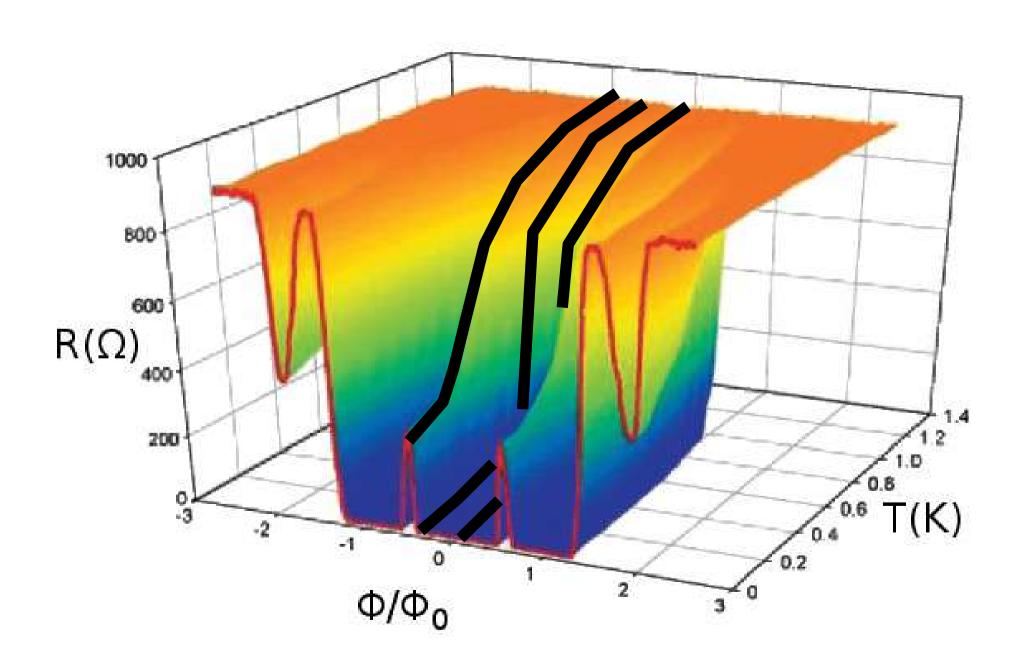
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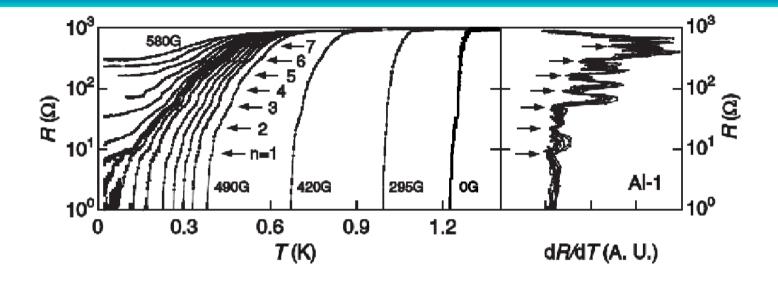
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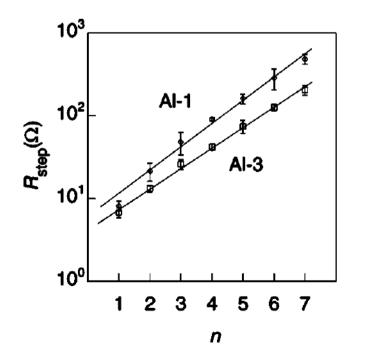


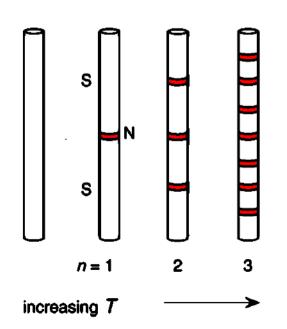




Quantum phase transition hypothesis

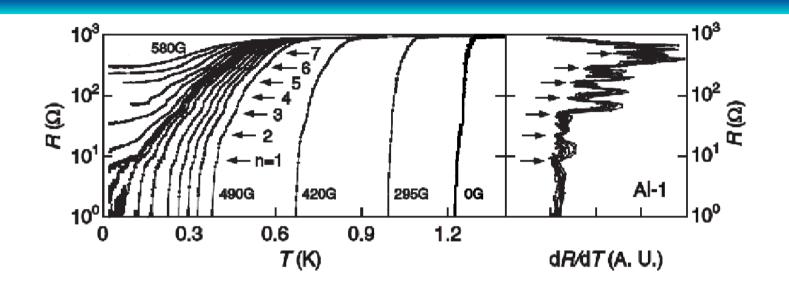


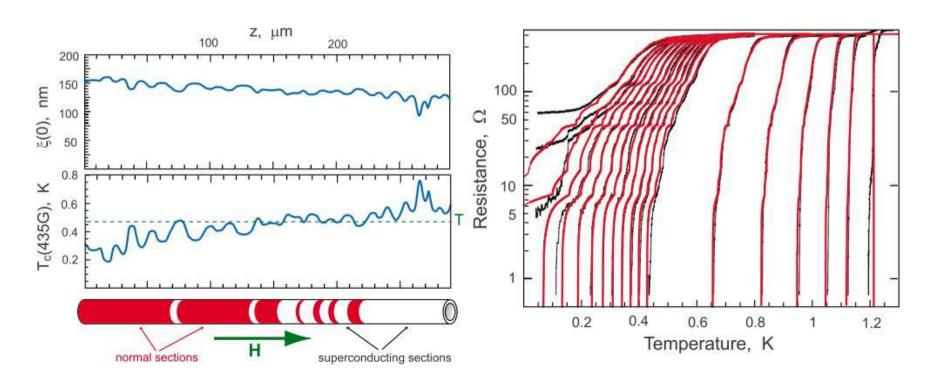




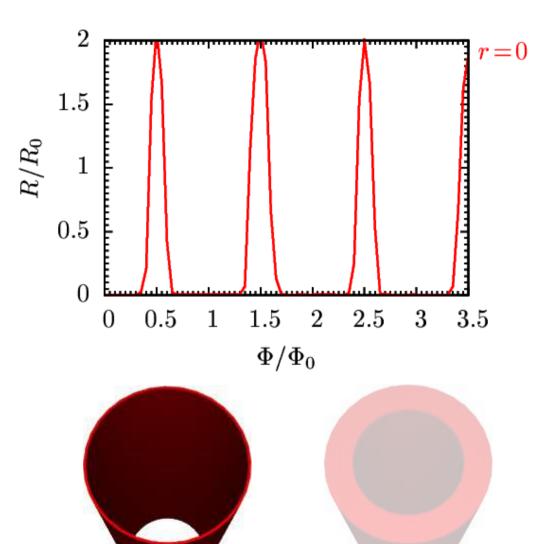
Dao & Chibotaru, PRB (2009)

Mean-field BCS transition hypothesis

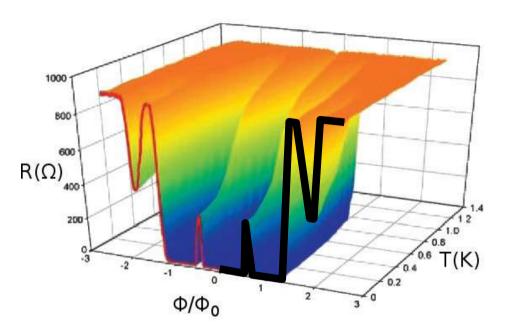




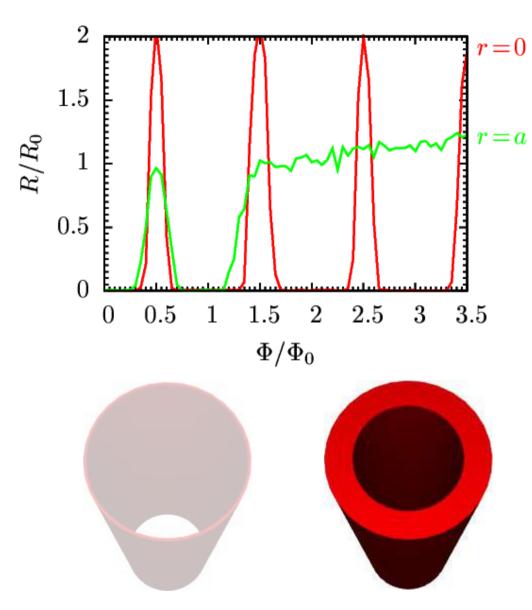
Theory:



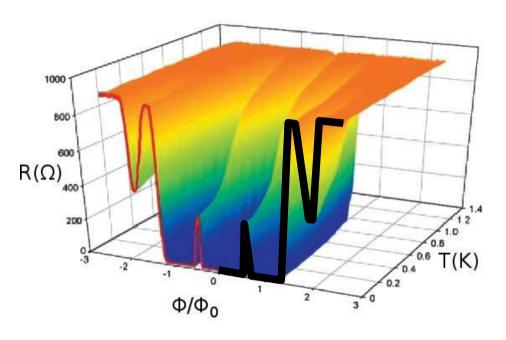
Experiment:

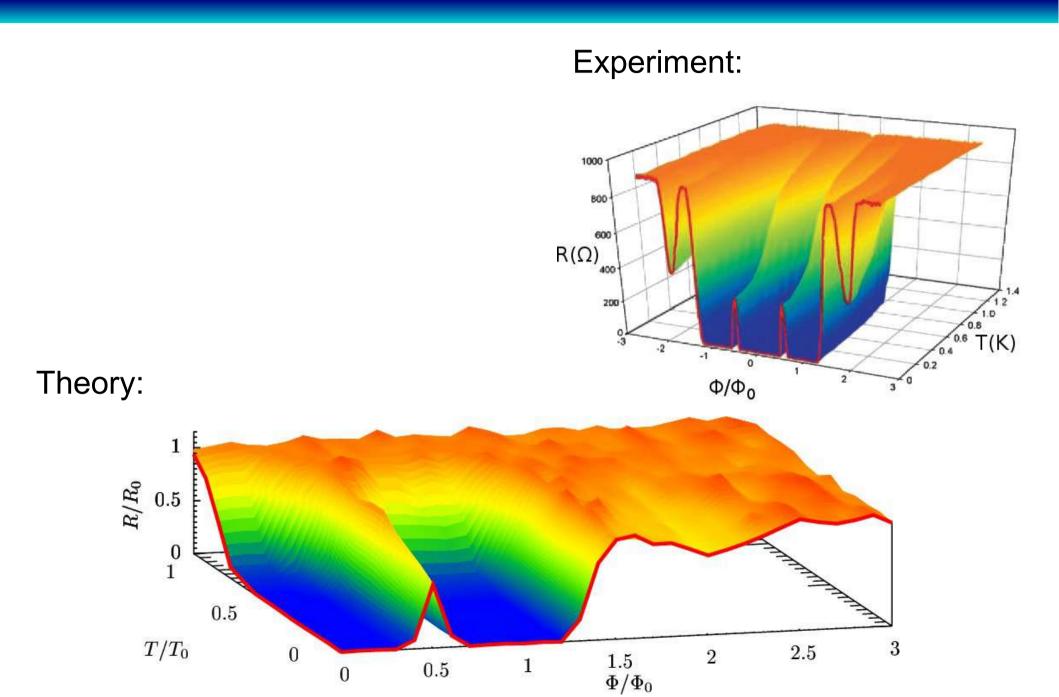


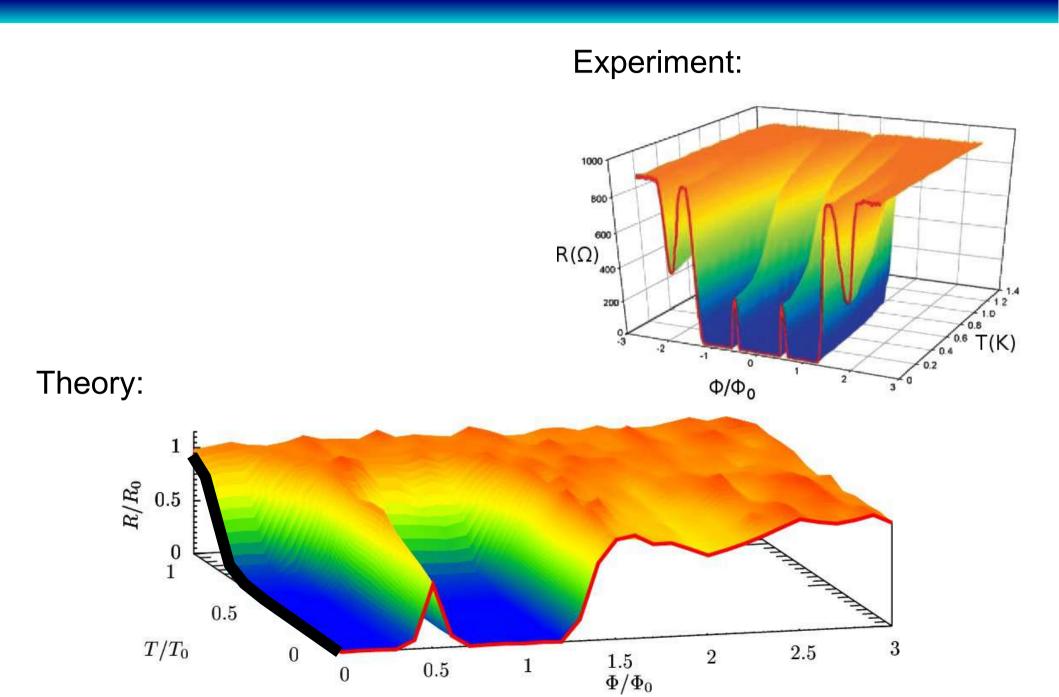
Theory:



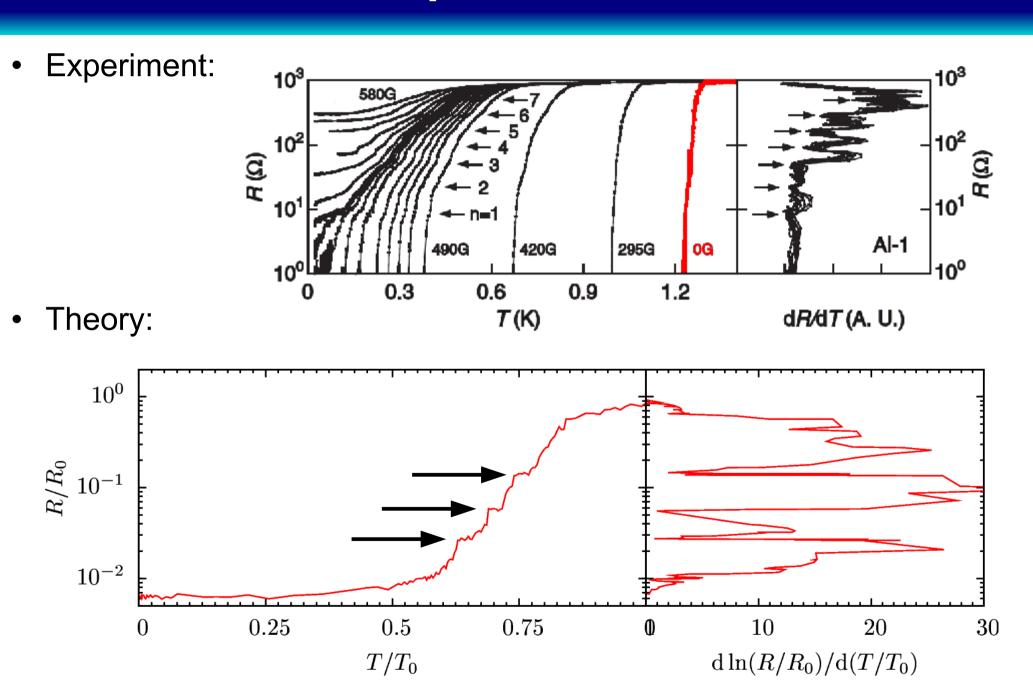
Experiment:



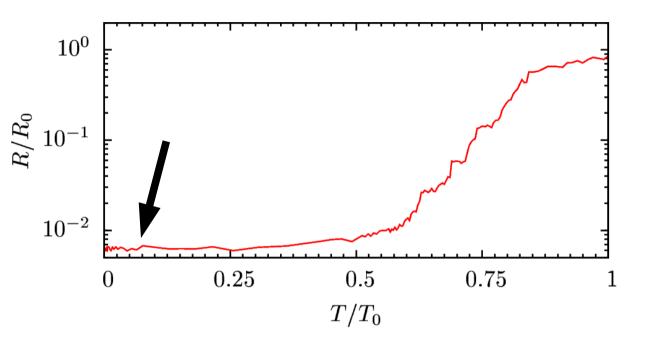




Evidence of phase reconstruction

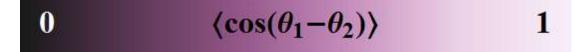


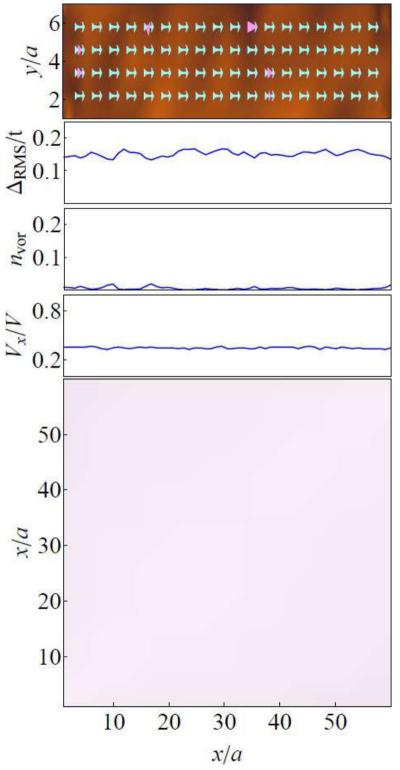
Completely superconducting



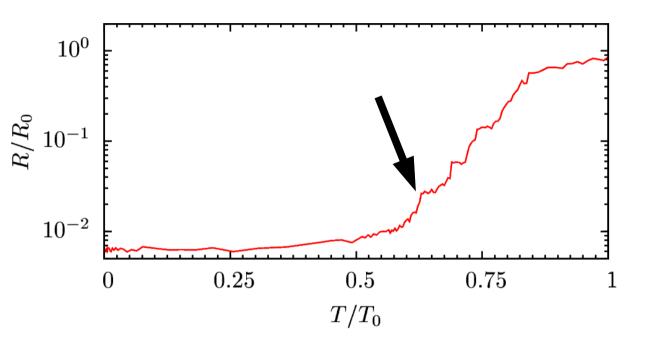






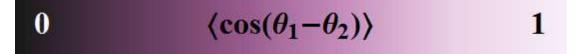


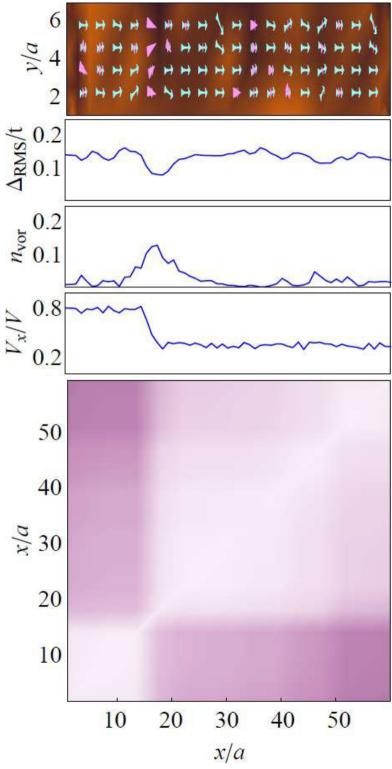
Two superconducting regions



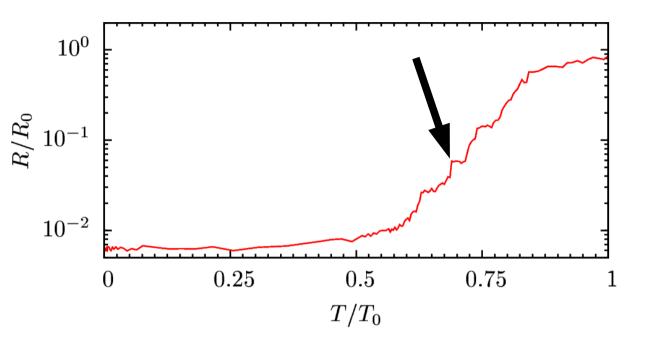






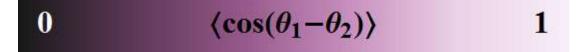


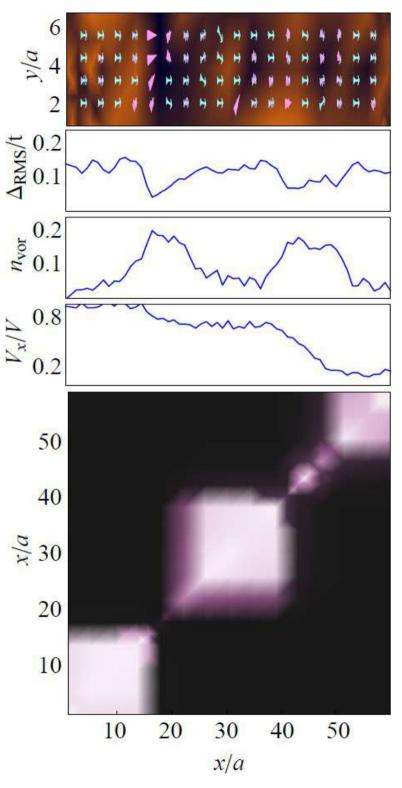
Three superconducting regions



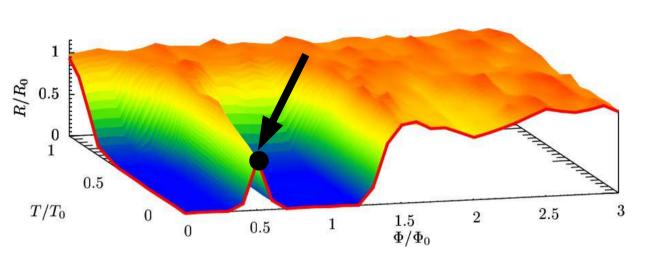






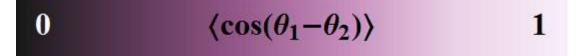


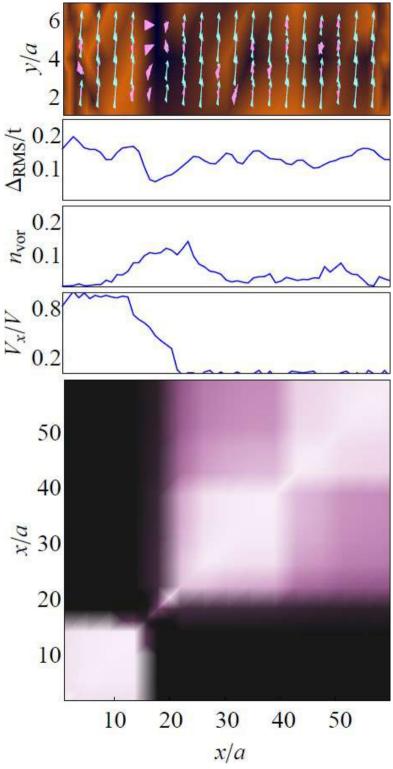
Half flux quantum normal state





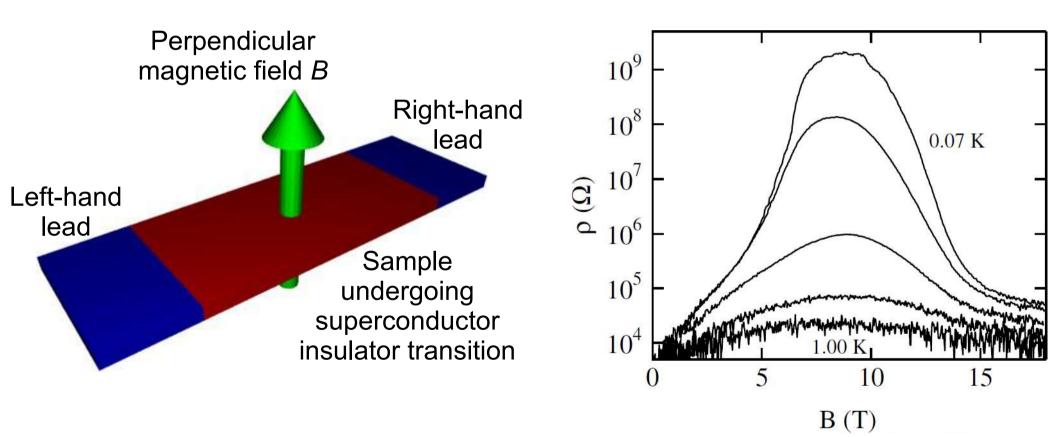






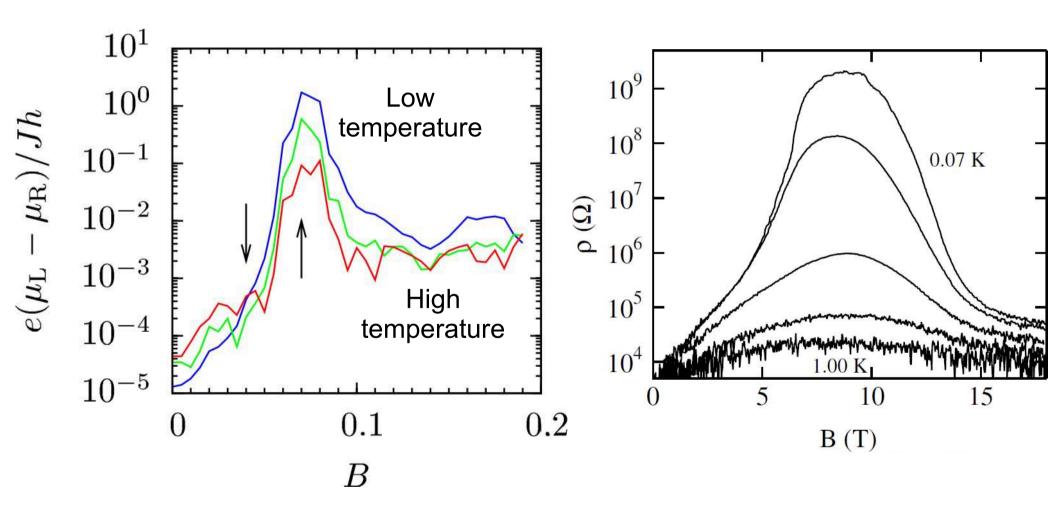
Magnetoresistance peak

 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: current maps

Weak links across superconducting puddles

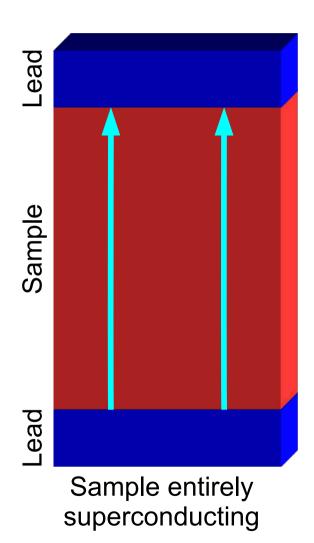




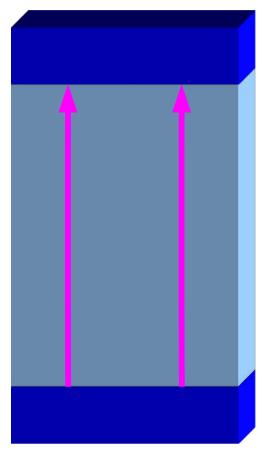




Working hypothesis



Superconducting puddles have a charging energy and a tunneling barrier

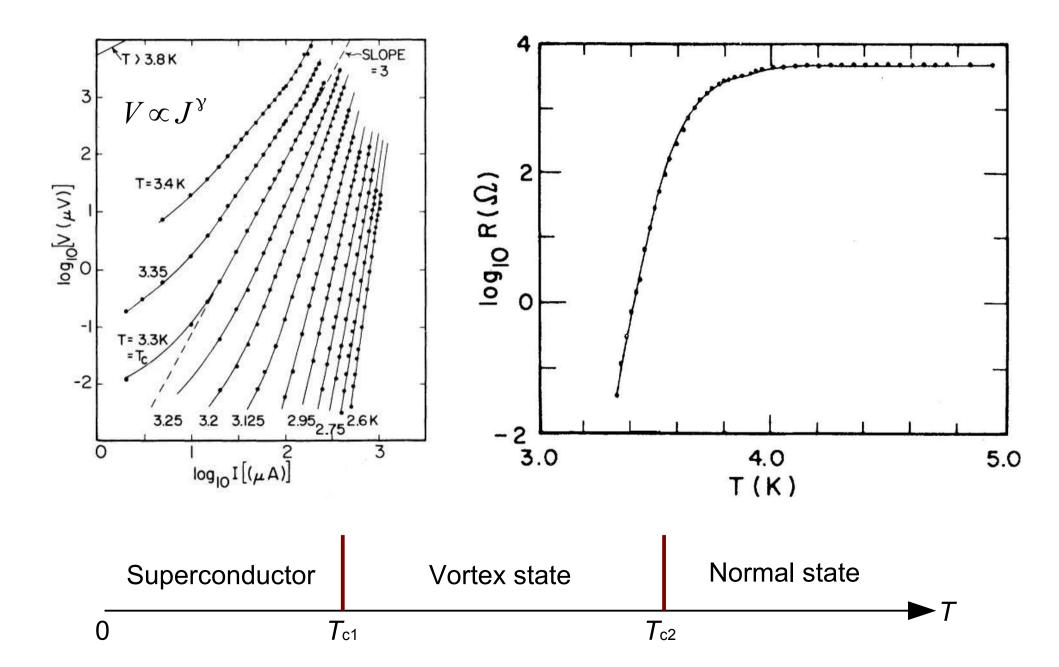


Sample entirely normal

Summary & future prospects

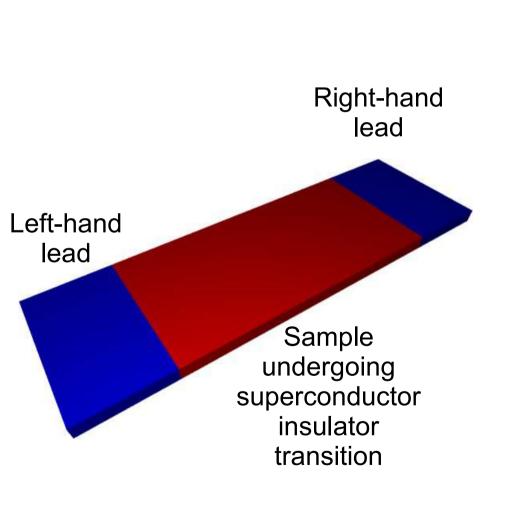
- Developed new formalism that includes thermal phase fluctuations to calculate and probe transport in superconductors
- New numerical techniques permit access to large systems
- Tested formalism against a series of well established results
- Shown that superconductor-insulator transition in small diameter 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

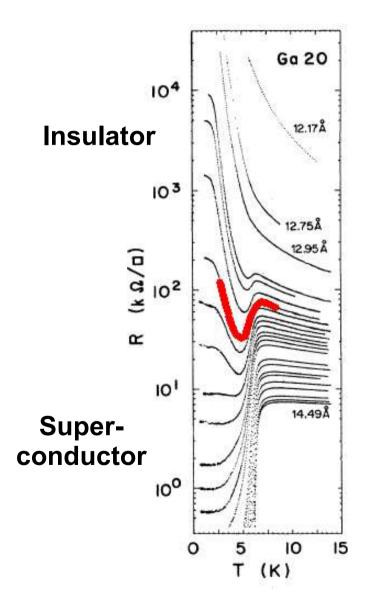
KT transition conductivity



Superconductor-insulator transition

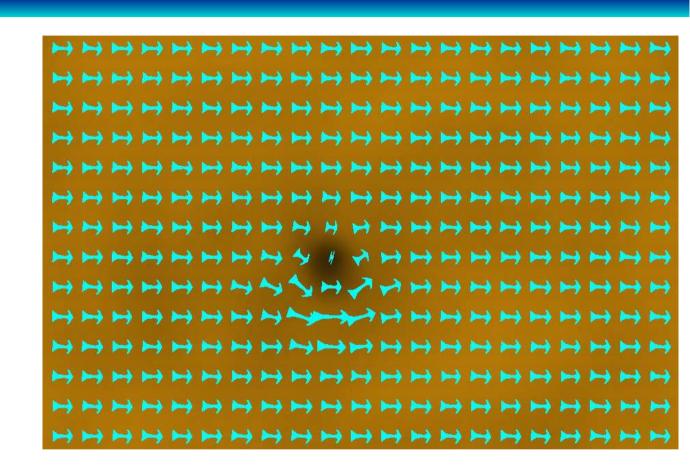
Non-monotonic R-T curves [Jaeger 89, Baturina 07]





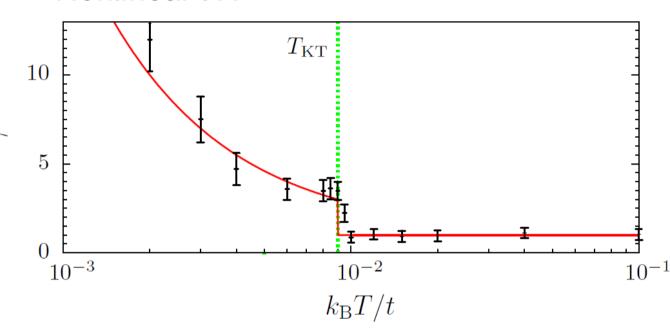


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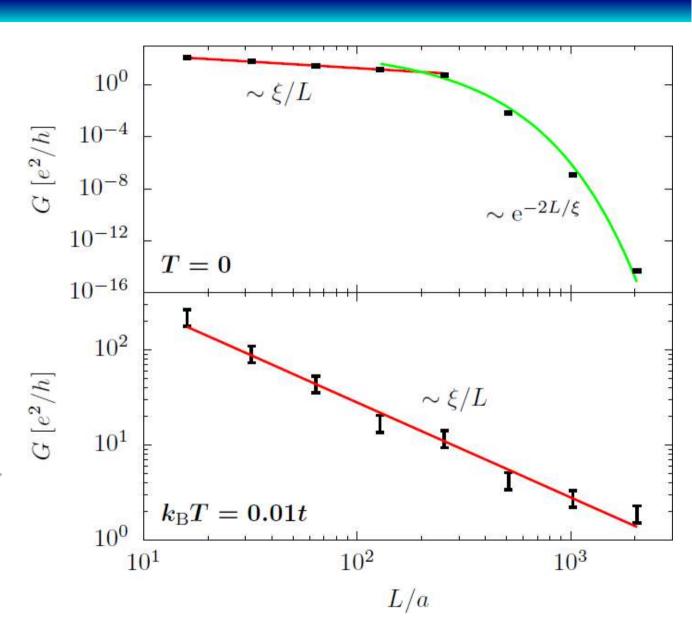


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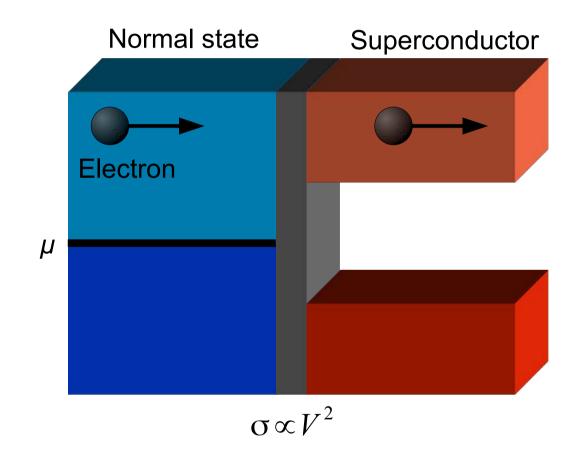




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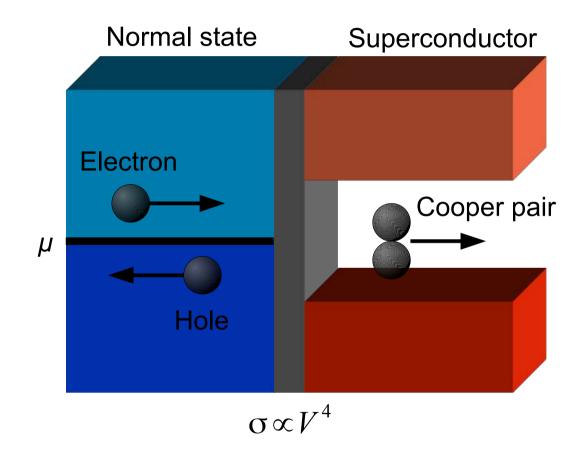


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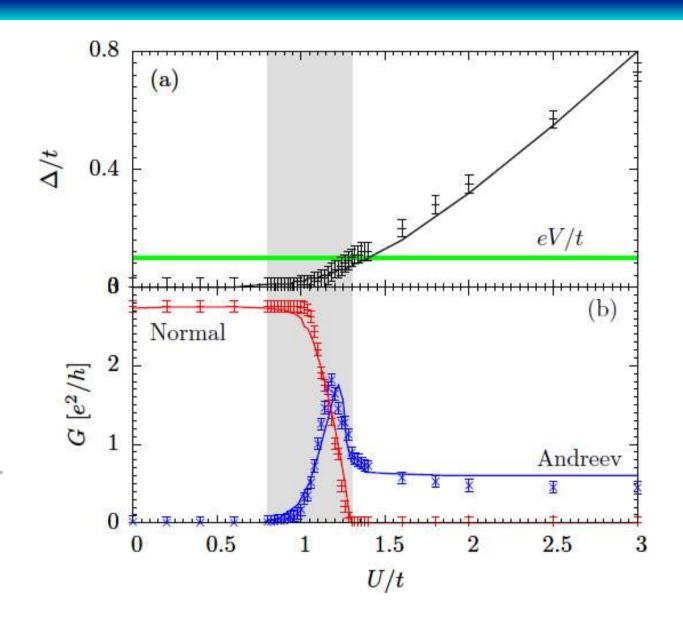
Andreev, JETP 19, 1228 (1964)

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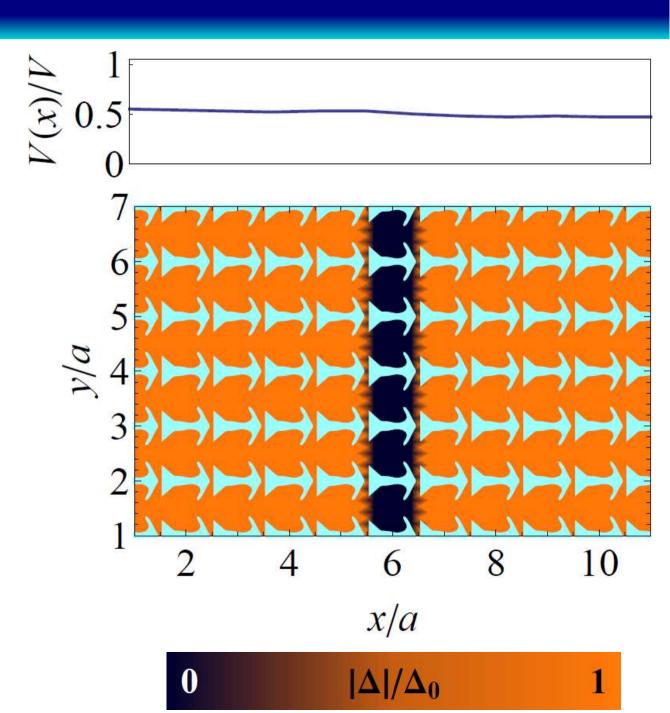
Andreev, JETP 19, 1228 (1964)

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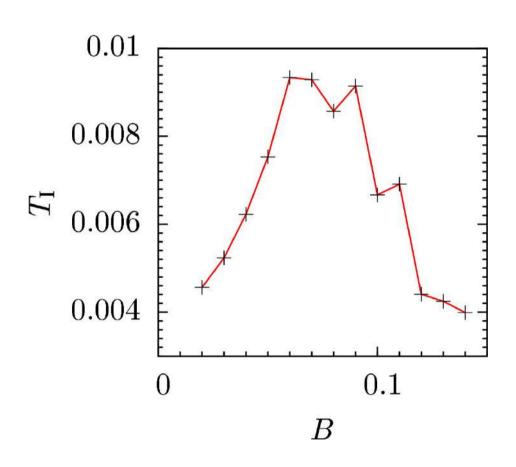
Blonder, Tinkham & Klapwijk, Phys. Rev. B 25, 4515 (1982)

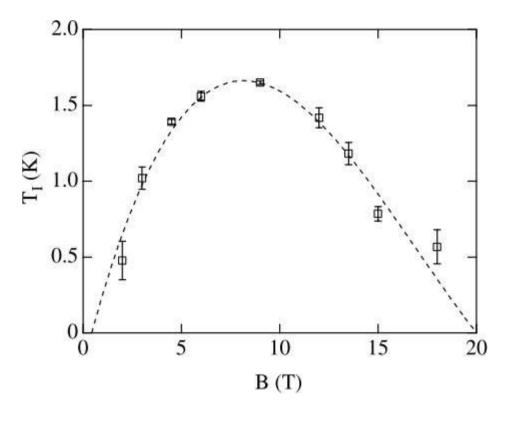
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Clues: activated transport

• Activated transport $\rho = \rho_0 e^{T_1/T}$





Model one-dimensional systems

