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

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BCS superconductivity in MgB$_2$

Monteverde et al., Science 292, 75 (2001)
BCS superconductivity
Kosterlitz Thouless transition

- Superconductor
- Vortex state
- Normal state

Temperature ($T$) scale:
- 0
- $T_{c1}$
- $T_{c2}$
Kosterlitz Thouless transition

Superconductor | Vortex state | Normal state

0 \quad T_{c1} \quad T_{c2} \quad T
Kosterlitz Thouless transition

Superconductor

Vortex state

Normal state

0

$T_{c1}$

$T_{c2}$

$T$
Kosterlitz Thouless transition

Superconductor \rightarrow Vortex state \rightarrow Normal state

0 \quad T_{c1} \quad T_{c2} \quad T
KT transition conductivity

The graph illustrates the log-log plot of $\log_{10} R(\Omega)$ vs. $T$ (K) with transition points $T_{c1}$ and $T_{c2}$. The states are defined as:

- **Superconductor**
- **Vortex state**
- **Normal state**
KT transition conductivity

$V \propto J^\gamma$

Superconductor $\rightarrow$ Vortex state $\rightarrow$ Normal state

$T > 3.8 \text{ K}$

$T = 3.3 \text{ K} = T_c$

$T = 3.4 \text{ K}$

$T = 3.0 \text{ K}$

$T = 2.6 \text{ K}$

$\log_{10} I (\mu \text{A})$

$\log_{10} R (\Omega)$

$T (\text{K})$
Transition in highly disordered systems

- Magnetoresistance peak [Sambandamurthy 04]

Perpendicular magnetic field $B$
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]
Little-Parks in a large diameter cylinder

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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]

\[ J = \frac{ie}{2h} \int d\epsilon \left[ \text{Tr} \left\{ (f_L(\epsilon)\Gamma^L - f_R(\epsilon)\Gamma^R) \left( G_e^{r\sigma} - G_e^{a\sigma} \right) \right\} + \text{Tr} \left\{ (\Gamma^L - \Gamma^R)G_e^{S\sigma} \right\} \right] \]
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 in density and Cooper pair channels

$$\rho_{i\sigma} = - |U_i| c_{i\sigma}^\dagger c_{i\sigma} \quad \Delta_i = |U_i| c_{i\downarrow} c_{i\uparrow}$$

- Hamiltonian now contains single-body operators

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

$$+ \sum_i \left( \Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \Delta_i c_{i\downarrow} c_{i\uparrow} \right) + \sum_i \frac{|\Delta_i|^2 + \rho_i^2}{U_i}$$
Diagonalizing the Hamiltonian

- Hamiltonian now contains single-body operators

\[
\hat{H}_{\text{BdG}} = \sum_{i, \sigma} (\epsilon_i + \rho_i) c_{i\sigma}^\dagger c_{i\sigma} - \sum_{\langle i, j \rangle, \sigma} (t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + t_{ij}^* c_{j\sigma}^\dagger c_{i\sigma}) \\
+ \sum_i \left( \epsilon_{i\uparrow} c_{i\uparrow}^\dagger c_{i\downarrow} + \epsilon_{i\downarrow} c_{i\downarrow}^\dagger c_{i\uparrow} \right) + \sum_i \frac{|\Delta_i|^2 + \rho_i^2}{U_i}
\]

- Energy eigenstates can be found from diagonalization of

\[
\hat{H}_{\text{Bgg}} = \frac{|\Delta|^2 + \rho^2}{U} + \left( \begin{array}{cc} c_{\uparrow}^\dagger & c_{\downarrow} \end{array} \right) \left( \begin{array}{cc} \epsilon + \rho & \frac{\Delta}{\Delta} \\ \frac{\Delta}{\Delta} & -(\epsilon + \rho) \end{array} \right) \left( \begin{array}{c} c_{\uparrow} \\\ c_{\downarrow} \end{array} \right) + \epsilon + \rho
\]
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 \( \Delta \) and \( \rho \), accept with probability
  \[
  \exp \left( \beta E[\Delta_{\text{old}}, \rho_{\text{old}}] - \beta E[\Delta_{\text{new}}, \rho_{\text{new}}] \right)
  \]

- 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

Ambegaokar et al., PRB 1980
Verification

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Ambegaokar & Baratoff, PRL 10, 486 (1963)
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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
Little-Parks in a small diameter cylinder

Theory:

\[ \frac{R}{R_0} \]

Experiment:

\[ R(\Omega) \]

\[ \frac{\Phi}{\Phi_0} \]

\[ r = 0 \]
Little-Parks in a small diameter cylinder

Theory:

\[ \frac{R}{R_0} \]

\[ \Phi / \Phi_0 \]

\[ r = 0 \]

\[ r = \alpha \]

Experiment:

\[ R(\Omega) \]

\[ \Phi / \Phi_0 \]

\[ T(K) \]
Variation with diameter

\[
\frac{\Phi}{\Phi_0}
\]

\[
d/\xi_0
\]
Little-Parks in a small diameter cylinder

Experiment:

Theory:
Little-Parks in a small diameter cylinder

Experiment:

Theory:
Evidence of phase reconstruction

- **Experiment:**

- **Theory:**
Completely superconducting

Superconducting current

Normal current

\[ \langle \cos(\theta_1 - \theta_2) \rangle \]
Two superconducting regions

Superconducting current

Normal current

\[ \langle \cos(\theta_1 - \theta_2) \rangle \]
Three superconducting regions

Superconducting current

Normal current

\[ \langle \cos(\theta_1 - \theta_2) \rangle \]
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 \( \rho = \rho_0 e^{T_i/T} \)
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