Supercurrent through grain boundaries in the presence of strong correlations

Kolloquium zur gleichnamigen Masterarbeit

F. Alexander Wolf

Universität Augsburg

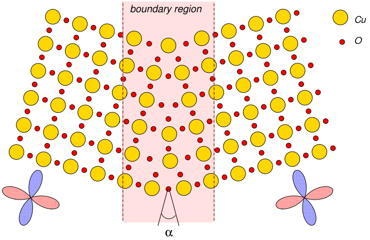
12 July 2011

Contents

Experimental fact

Exponential reduction of critical supercurrent j_c w.r.t. increasing grain boundary misalignment angle

see e.g. review by Hilgenkamp and Mannhart, RMP (2002)



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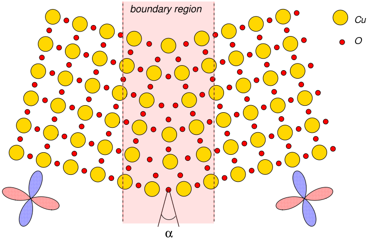

Practical motivation

- Largest application of conventional superconductors in the form of superconducting wires for magnets (e.g. in magnetic resonance imaging machines)
- High-temperature superconductors not usable for this purpose due to exponential reduction of current at GBs

Theoretical motivation

Microscopic modeling of current suppression already by

Graser, Hirschfeld, Kopp, Gutser, Andersen, and Mannhart, Nat. Phys. (2010)

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Reason for suppresion

charge fluctuations (not e.g. suppression of tunneling amplitude)

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Speculation: strong correlations responsible?

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Main question of this thesis

Is it possible to model the suppression with a simple approach to strong correlations, the Gutzwiller approximation? If yes, what are the results?

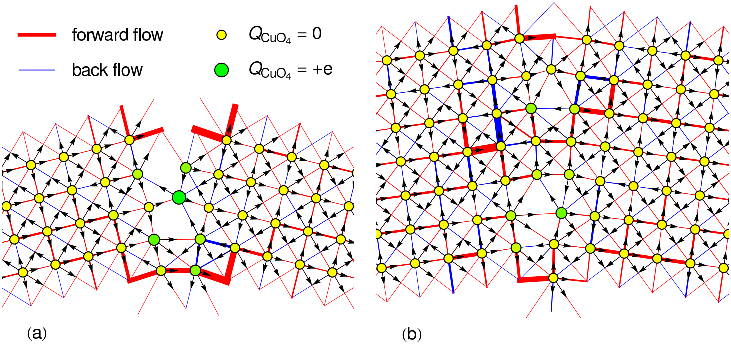
What could happen?

- Qualitatively: Decay still exponential or stronger?
- Quantitatively: Reduction in which order of magnitude (augmentation not likely)?

Overview of model system

Graser, Hirschfeld, Kopp, Gutser, Andersen, and Mannhart, Nat. Phys. (2010)

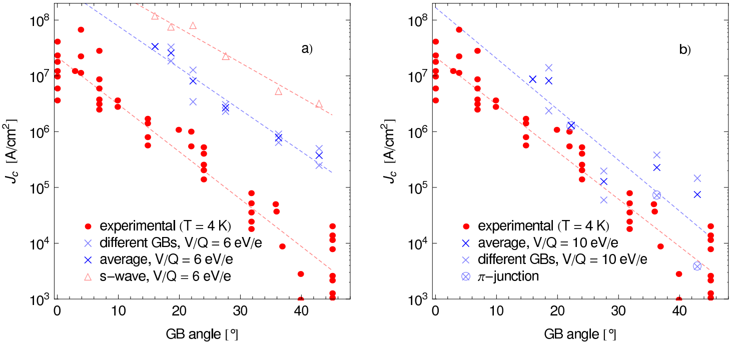
Current transport pattern



Overview of model system

Graser, Hirschfeld, Kopp, Gutser, Andersen, and Mannhart, Nat. Phys. (2010)

Results for the angle dependence of the critical current



Contents

RVB groundstate for cuprate superconductors

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$$H_{\text{Hubbard}} = -\sum_{\langle ij\rangle s} t_{ij}(c_{is}^\dagger c_{js} + \text{h.c.}) + U\sum_i (\hat{n}_{i\uparrow} - \tfrac{1}{2})(\hat{n}_{i\downarrow} - \tfrac{1}{2})$$

Proposition for superconducting groundstate of cuprates Anderson, Science (1987)

$$|\psi\rangle \equiv |\text{RVB}\rangle \equiv \mathcal{P}|\psi\rangle_0 \quad \text{where} \quad |\psi_0\rangle \equiv |\text{BCS}\rangle \equiv \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger)|\text{vac}\rangle$$

$$\mathcal{P} \equiv \prod_i (1 - \hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$$

Focus on the t-J-model in this thesis

RVB groundstate for cuprate superconductors

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Focus on the t-J-model in this thesis

$$H = -\sum_{(ij)s} t_{ij}(c^\dagger_{is}c_{js} + \text{h.c.}) + J\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Gutzwiller approximation for homogeneous systems

Evaluation of $|\psi\rangle \equiv |\text{RVB}\rangle \equiv \mathcal{P}|\psi\rangle_0$ using the Gutzwiller approximation (i.e. the assumption of complete statistical independence of site populations)

Gutzwiller, Phys. Rev. (1965)

Idea of Zhang, Gros, Rice, and Shiba, Supercond. Sci. Technol. (1988)

Employ Gutzwiller approximation for the RVB state in the derivation of an effective one-particle hamiltonian for the *t*-*J*-model

For that use expressions obtained in the thermodynamic limit

$$\langle c_{is}^\dagger c_{js}\rangle \overset{\text{Gutzw.}}{\simeq} g^t(n)\langle c_{is}^\dagger c_{js}\rangle_0 \quad , \qquad g^t(n) \equiv \frac{2(1-n)}{2-n}$$

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle \overset{\text{Gutzw.}}{\simeq} g^J(n)\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle_0 \quad , \qquad g^J(n) \equiv \frac{4}{(2-n)^2}$$

Gutzwiller approximation for inhomogeneous systems

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Wang, Wang, Chen, and Zhang, Phys. Rev. B (2006) extended formalism to inhomogeneous systems

$$\mathcal{P} \equiv \prod_i \mathcal{P}_i \quad \text{where} \quad \mathcal{P}_i \equiv y_i^{\hat{n}_i}(1 - D_i) \quad \text{where} \quad D_i \equiv \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

This projection operator leads to the renormalization

$$g_{ij}^t \equiv g_i^t g_j^t \quad \text{where} \quad g_i^t \equiv \sqrt{\frac{2(1-n_i)}{(2-n_i)}}$$

$$g_{ij}^J \equiv g_i^J g_j^J \quad \text{where} \quad g_i^J \equiv \frac{2}{2-n_i}$$

But: What to use for the description of electron doped systems?

Gutzwiller approx. for strongly inhom. systems

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Wolf, Graser, Loder, and Kopp, arXiv:1106.5759 (2011)

$$g_i^t \equiv \sqrt{\frac{2|1-n_i|}{|1-n_i|+1}}$$

$$g_i^J \equiv \frac{2}{|1-n_i|+1}$$

Gutzwiller approx. for strongly inhom. systems

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$$g_i^t \equiv \sqrt{\frac{2|1-n_i|}{|1-n_i|+1}} \equiv \begin{cases} \sqrt{\frac{2(1-n_i)}{(2-n_i)}} & \text{if} \quad n_i \leq 1 \\ \sqrt{\frac{2(n_i-1)}{n_i}} & \text{if} \quad n_i > 1 \end{cases}$$

$$g_i^J \equiv \frac{2}{|1-n_i|+1} \equiv \begin{cases} \frac{2}{2-n_i} & \text{if} \quad n_i \leq 1 \\ \frac{2}{n_i} & \text{if} \quad n_i > 1 \end{cases}$$

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$$g_i^J \equiv \frac{2}{|1-n_i|+1} \equiv \begin{cases} \frac{2}{2-n_i} & \text{if} \quad n_i \leq 1 \\ \frac{2}{n_i} & \text{if} \quad n_i > 1 \end{cases}$$

This corresponds to the projection operator:

$$\mathcal{P} \equiv \prod_i \mathcal{P}_i \quad \text{where} \quad \mathcal{P}_i \equiv \begin{cases} \mathcal{P}_i^d \equiv y_i^{\hat{n}_i}(1-D_i) & \text{if} \quad n_i \leq 1 \\ \mathcal{P}_i^h \equiv y_i^{\hat{n}_i}(1-E_i) & \text{if} \quad n_i > 1 \end{cases}$$

Application to GB

$$H_{\mathrm{GB}} = -\sum_{ijs} (g^t_{ij} t_{ij} + \chi^*_{ij}) c^\dagger_{is} c_{js}$$
$$- \sum_{ij} (\Delta_{ij} c^\dagger_{j\uparrow} c^\dagger_{i\downarrow} + \text{h.c.}) - \sum_i \mu_i \hat{n}_i$$

with $\Delta_{ij} \equiv (\frac{3}{4} g^J_{ij} + \frac{1}{4}) J_{ij} \widetilde{\Delta}_{ij},$

$\chi_{ij} \equiv (\frac{3}{4} g^J_{ij} - \frac{1}{4}) J_{ij} \widetilde{\chi}_{ij},$

Application to GB

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$$H_{\text{GB}} = -\sum_{ijs}(g^t_{ij}t_{ij} + \chi^*_{ij})c^\dagger_{is}c_{js} - \sum_{ij}(\Delta_{ij}c^\dagger_{j\uparrow}c^\dagger_{i\downarrow} + \text{h.c.}) - \sum_i \mu_i\hat{n}_i$$

$$\text{with}\quad \Delta_{ij} \equiv (\tfrac{3}{4}g^J_{ij} + \tfrac{1}{4})J_{ij}\widetilde{\Delta}_{ij},\qquad \chi_{ij} \equiv (\tfrac{3}{4}g^J_{ij} - \tfrac{1}{4})J_{ij}\widetilde{\chi}_{ij},$$

where $\widetilde{\Delta}_{ij} \equiv \frac{1}{2}(\langle c_{i\downarrow}c_{j\uparrow}\rangle + \langle c_{j\downarrow}c_{i\uparrow}\rangle)$, $\widetilde{\chi}_{ij} \equiv \frac{1}{2}(\langle c^\dagger_{i\uparrow}c_{j\uparrow}\rangle + \langle c^\dagger_{i\downarrow}c_{j\downarrow}\rangle)$, $\mu_i \equiv \mu - \varepsilon_i$, and

$$g^t_i \equiv \sqrt{\frac{2|1-n_i|}{|1-n_i|+1}} \quad\text{and}\quad g^J_i \equiv \frac{2}{|1-n_i|+1}$$

Solved self-consistently using the Bogoliubov - de Gennes formalism.

Contents

System parameters

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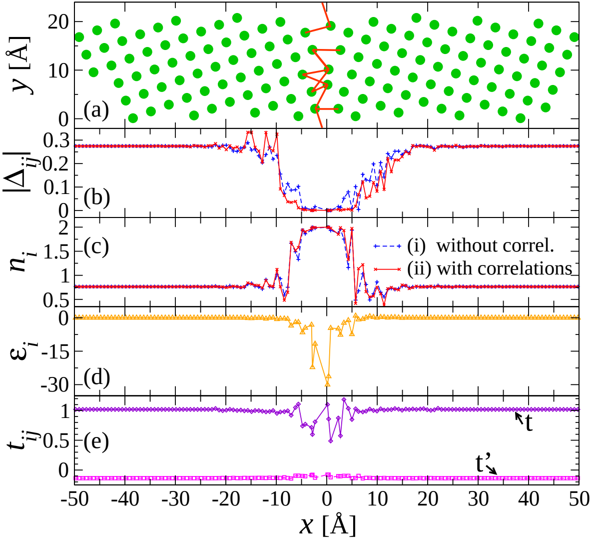
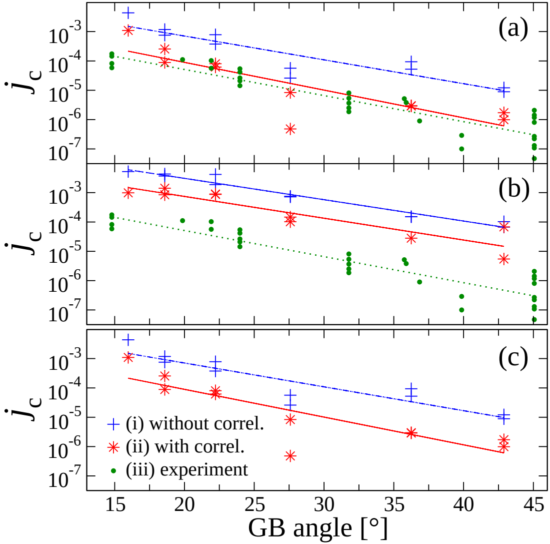
Wolf, Graser, Loder, and Kopp, arXiv:1106.5759 (2011)



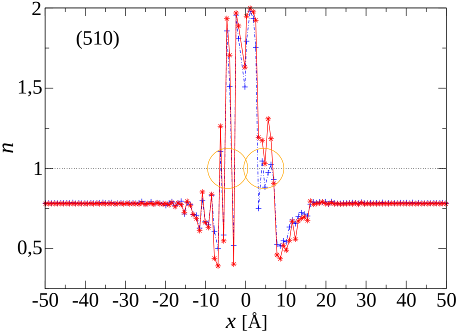
Supercurrent through grain boundaries

Wolf, Graser, Loder, and Kopp, arXiv:1106.5759 (2011)

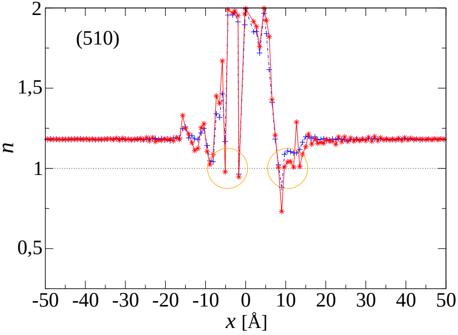


Density distribution

hole-doped

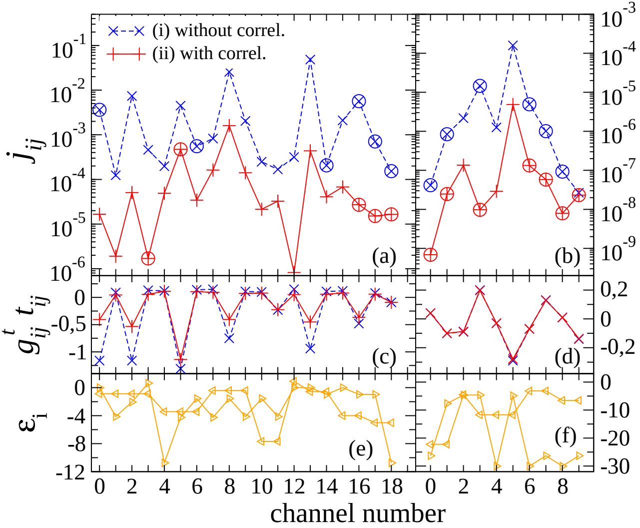


electron-doped



Mechanism for current transport

Wolf, Graser, Loder, and Kopp, arXiv:1106.5759 (2011)



Summary

First Part – Theoretical methods

- Review of Gutzwiller approximation as employed within the BdG formalism
- Presentation of a particle-hole symmetric form of Gutzwiller factors

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Thank you for your attention!