Quasiclassical circuit theory of spin transport in superconducting heterostructures

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Outline

- Some history of superconductor-ferromagnet heterostructures
- Quasiclassical Greens functions and boundary conditions
- Quantum Circuit Theory
- Spectral properties of SF bilayers
- (Spin-)Thermoelectric effects in SF



Critical current oscillations

Fulde, Ferrell (1964), Larkin, Ovchinnikov (1964)
 Superconductor with exchange field H_{ex} → inhomogeneous order parameter

 $\Delta(x) = \Delta \cos(q_{ex}x) \qquad q_{ex} = \frac{\hbar v_F}{2H_e}$

 Buzdin, Bulaevskii, Panyukov (1982)
 Critical current of an SFS Josphson junction oscillates!

$$I_c = I_c^0 e^{-q_{ex}d_F} \cos(q_{ex}d_F)$$

 Buzdin and Kuprianov (1990); Radovic *et al.* (1991) Critical temperature of SFS oscillates as function F-thickness (Exp. observed by Jiang et al. and Mercaldo et al 1995,...)



History of SF (some aspects...)

 Buzdin, Bulaevskii, Panyukov (1982) Critical current of an SFS Josephson junction oscillates!

$$I_c = I_c^0 e^{-q_{ex}d_F} \cos(q_{ex}d_F)$$

$$q_{ex} = \frac{\hbar v_F}{2H_{ex}}$$

 Buzdin and Kuprianov (1990); Radovic *et al.* (1991) Critical temperature of SFS oscillates as function F-thickness (Exp. observed by Jiang et al. and Mercaldo et al 1995,...)



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(Some) Experimental progress since 2000



Quasiclassical Theory & Boundary Conditions

The quasiclassical theory of inhomogeneous superconductors

General superconductors: Gorkov equations for matrix Greens function [Note: GF is in general a matrix in Nambu-Keldysh-Spin-....-Space]

 $\Psi = \left(\psi_{\uparrow}, \psi_{\downarrow}, \psi_{\downarrow}^{\dagger}, -\psi_{\uparrow}^{\dagger} \right)$ [Gorkov (1957), Abrikosov (1958)]

$$\breve{G}(x,x') = -i \left\langle \mathcal{T} \Psi(x) \Psi^{\dagger}(x') \right\rangle \approx \breve{G}(x,x) e^{ik_F(x-x')}$$

Contains full microscopic oscillations on scale of Fermi wavelength



Usually unnecessary amount of information!

Realistic case: impurities, microscopic imperfections lead to random elastic scattering \rightarrow all interference effects ~exp(ik_Fx) are washed out

The quasiclassical theory of inhomogeneous superconductors

$$\begin{array}{ll} \hline \mbox{Transport-like equation for the qc Greensfunction} & \hline \mbox{$\frac{\vec{p}^2}{2m} - \epsilon_F = \frac{\vec{p}_F^2}{2m} - i\frac{\vec{p}_F}{m}\vec{\nabla} - \epsilon_F = -i\vec{v}_F\vec{\nabla}$}\\ \hline & \left[\underbrace{-i\partial_t}_{\varepsilon} + i\vec{v}_F\vec{\nabla} + \breve{\Sigma}(\vec{x}, \mathcal{E}), \breve{G}(\vec{v}_F, \vec{x}, \mathcal{E})}_{\varepsilon} \right] = 0 & \vec{j} = e^2N_0 \int d\mathcal{E} \left\langle {\rm tr}\hat{\tau}_3\breve{G}_K(\vec{v}_F, \vec{x}, \mathcal{E}) \right\rangle_{v_F}$\\ \hline \mbox{[Eilenberger (1968); Larkin, Ovchinnikov (1968)]} & {\rm current density} \\ \hline \mbox{Normalization condition} & \boxed{\vec{G}(\vec{v}_F, \vec{x}, t, t')^2 = \vec{1}} & {\rm angular average} \\ \hline \mbox{Selfenergy contributions (phonons, impurities, Coulomb,...)} \\ \hline \mbox{E.g.} & \breve{\Sigma}_{ph}(\vec{x}) = \breve{\Delta}(\vec{x}) = \lambda \int d\mathcal{E} \left\langle \breve{G}(x, v_F, \mathcal{E}) \right\rangle_{off-diag} & \breve{\Sigma}_{imp}(\vec{x}, \mathcal{E}) = \frac{1}{2\tau} \left\langle \breve{G} \right\rangle_{\vec{v}_F} \\ \hline \mbox{Pairing potential} & Elastic impurity scattering \\ \hline \mbox{Diffusive approximation} & [Usadel 1970] & l = v_F \tau \ll \frac{V_F}{\Delta_{\vec{\xi}s}}, \frac{kT}{\xi_F} \\ \hline \mbox{G}(\vec{v}_F, \vec{x}) = \breve{G}(\vec{x}) + \vec{v}_F \vec{\breve{G}}(\vec{x}) + \dots \\ \hline \mbox{Usadel equation (quantum diffusion equation)} & D = v_F^2 \tau / 3 \\ \hline \mbox{D} \partial_x \breve{G}(x) \partial_x \breve{G}(x) = \left[-iE\hat{\tau}_3 + \hat{\Delta} + \hat{\Sigma}', \vec{G}(x) \right] & \vec{j} = e^2N_0 D \int d\mathcal{E} {\rm tr}\hat{\tau}_3 \breve{G}(\vec{x}) \vec{\nabla} \breve{G}(\vec{x})_K \\ \hline \mbox{current density} \\ \hline \mbox{Cur$$

The quasiclassical theory and the boundary condition problem

[Eilenberger (1968), Larkin & Ovchinnikov (1968)]

 $\rho^{ik_F(x-x')}$

Principle of quasiclassics: integrate out "fast oscillations"

Equation reduced to envelope functions:

$$\breve{G}(x,x') \approx \breve{G}(x,x)e^{ik_F(x-x')}$$



Envelope functions (quasiclassical Green's functions) have jumps at atomically sharp interfaces, which cannot be derived within the quasiclassical theory

Need for separately derived boundary conditions!

HISTORY OF BOUNDARY CONDITIONS IN THE QUASICLASSICAL THEORY

- Zaitsev (1984): boundary conditions for ballistic interfaces
 - spin-degenerate interface, only transmission probabilities
 - complicated non-linear equations
- Rainer, Sauls, Millis (1988): spin-active interface, ballistic
 - general scattering matrix, complicated non-linear equations
- Kupriyanov, Lukichev (1988): diffusive case
 - Only small transmission
 - One parameter: tunnel conductance
- Nazarov (1999): diffusive case
 - arbitrary transmission, spin-degenerate
- More aspects: Zaikin, Shelankov, Eschrig,....

$$G_T = 2G_Q \sum T_n$$

Circuit theory formulation of the diffusive theory and the boundary condition

Matrix current
(unit area)
$$I(x) = -\sigma \breve{G}(x) \partial_x \breve{G}(x)$$
Conductivity $\sigma = e^2 N_0 D$ Usadel equation $\partial_x \breve{I}(x) = -\frac{\sigma}{D} \Big[-iE\hat{\tau}_3 + \hat{\Delta} + \hat{\Sigma}, \breve{G}(x) \Big]$ Characteristic length
 $\xi = \sqrt{\frac{\hbar D}{Max(E, \Delta, \Sigma)}}$ Close to an interface: $\breve{I}_{L,R} = -\sigma \breve{G} \partial_x \breve{G} \Big|_{L,R}$ \breve{G}_L Scattering region = non-quasiclassical description
(scattering matrix S) \breve{G}_L \breve{I}_{LR}

Nazarov (1999): for a spin-independent scattering matrix S

$$\widetilde{I}_{LR} = \frac{2e^2}{h} \sum_{n} \frac{T_n \left[\widetilde{G}_L, \widetilde{G}_R \right]}{4 + T_n \left(\left\{ \widetilde{G}_L, \widetilde{G}_R \right\} - 2 \right)} \stackrel{T_n \ll 1}{\approx} \frac{G_T}{2} \left[\widetilde{G}_L, \widetilde{G}_R \right]$$

Boundary condition:

$$\breve{I}_L = \breve{I}_{LR} = \breve{I}_R \quad o$$

$$\left[\begin{smallmatrix} r_R \\ R \end{smallmatrix}
ight]$$
 depends on transmission eigenvalues $\left\{ T_n
ight\}$

 $\ll \xi$

SF-Heterostructures: need for a spin-dependent boundary conditions!

The problem of spin-dependence (or energy) of the boundary scattering:

Isotropic GF (Usadel, diffusive regions)

 $\check{G}(x,E)$

= Matrix in Keldysh-Nambu-Spin space General scattering matrix (across the interface)

$$\hat{S}(E) = \begin{pmatrix} r & t \\ t' & r' \end{pmatrix}$$

= Matrix in Nambu-Spin space

If: $\hat{S}(E) \sim \overline{S} \otimes \sigma_0$ (spin- & energy-independent)

Then:
$$\left[\breve{G}(x,E), \hat{S}\right] = 0 \rightarrow$$
 extreme simplification!

Consequence: e.g. only $T_n = \text{Eigenvalues}[t^{\dagger}t]$ enter the BC (Nazarov `99)

The way to spin-dependent boundary conditions in the diffusive case:

 $\delta \varphi = \arg r_{\uparrow} - \arg r_{\downarrow}$ Generalization of the Nazarov-BC to weak spin dependence: Spin-dependent interfacial phase shifts Spin-polarization conductance $G_{\phi} = G_O \sum \delta \varphi_n$ $G_P = G_O \sum \left(T_{n\uparrow} - T_{n\downarrow} \right)$ \rightarrow Spin-polarized current \rightarrow Induced exchange splitting Huertas-Hernando, Nazarov, Belzig (2002) Taking into account strongly polarized magnetic insulators $G_{\phi 2} = G_Q \sum_n \delta \varphi_n^2 \qquad G_{\phi 3} = G_Q \sum_n \delta \varphi_n^3 \qquad G_{\phi 4} = \cdots$ $\Rightarrow \text{ pair-breaking} \qquad \text{Cottet, Huertas-Hernando, Belzig, Nazarov (2009)}$ Barriers with constant spin polarization (per channel) $\hat{S}(E) = S \otimes \sigma_0 + S' \otimes \vec{m}\vec{\sigma} \rightarrow$ all details of S and m enter! Machon, Belzig (2015) Fully general spin-dependent BC

(including arbitrary polarization, textures, and spin-mixing)

 $\hat{S}(E) = \begin{pmatrix} \overline{r}(\vec{m}_L) & \overline{t}(\vec{m}) \\ \overline{t}'(\vec{m}) & \overline{r}'(\vec{m}_R) \end{pmatrix} \rightarrow \text{all details of S and all m's enter!}$ Eschrig, Cottet, Belzig, Linder (2015)

Quantum Circuit Theory

Classical circuit theory

- Description by full Poisson equations is very complicated and ineffective
- **Conserved** static currents flow between contacts with fixed voltages
- No current through boundaries





The problem is drastically simplified by mapping onto a **discretized** structure with elements

- Network of nodes and connectors (resistors)
- Contacts to outer world: voltages in terminals are fixed
- The voltages on the nodes have to be determined by set of rules

Circuit theory and Kirchhoff rules

Conservations laws can be cast into two rules for an electric circuit composed of discrete elements

- Rule 1: The current in each node is conserved (node rule)
- Rule 2: The sum of all voltage differences around a closed loop is zero (loop rule)

At connections to the outer world, the voltages are fixed. The rules completely determine all **internal voltages and currents.**

In addition we need the microscopic description of the connector: **Ohms law**

$$I = \left(U_1 - U_2\right) / R$$

Remarkable consequence: all conductance properties of arbitrarily complicated networks are fully determined by the set of Kirchhoff Rules!



Nazarov 94-

Quantum Circuit theory

related to the gradient of a "matrix voltage" $\,\,\hat{g}\,$

We use the matrix current: $\hat{I}(x) = -\sigma \hat{g} \frac{\partial}{\partial x} \hat{g}$ Electrical current:

$$I = Tr\hat{\tau}_{K}\hat{I}$$

The matrix current obeys a "conservation" law (up to decoherence)



The matrix current conservation law is the basis of a circuit theory! We can construct a network of connectors (with matrix voltage drop) and nodes (with matrix voltages)

[Usadel 70]

Quantum Kirchhoff rules (without decoherence)

Principle: Consider a quantum electric circuit as composed of discrete elements with unknown matrix voltages

Rule 1: The matrix current in each node is conserved

$$\sum_{i} \hat{I}_{i} = 0$$

Rule 2: The **matrix** voltages obey the normalization

$$\hat{g}_i^2 = \hat{1}$$

In addition we need the description of the connector: Quantum Ohms law

$$\hat{I}_{12} = \frac{e}{\hbar} \sum_{n} \frac{T_n [\hat{g}_1, \hat{g}_2]}{4 + T_n (\{\hat{g}_1, \hat{g}_2\} - 2)}$$

T_n: Transmission probabilities, determined by the microscopic details Nonlinear functional relation between matrix voltages $\{T_i\}$

Derivation requires a microscopic theory of the interface.

Leads: connected to circuit with some connector and a fixed Green's function (determine type of contact: normal metal, superconductor,....





Electron-hole (de)coherence

Decoherence can be taken into account analogously to a leakage current

$$-\frac{\partial}{\partial x}\hat{I}(x) = \left[-iE\hat{\tau}_3, \hat{g}(x)\right]$$

 $\hat{I}_{1} + \hat{I}_{2} + \hat{I}_{leakage} = 0$ discretization $\hat{I}_{leakage} = \frac{G_{Q}}{\delta} \left[-iE\hat{\tau}_{3}, \hat{g}_{c} \right]$ ne

Quantum mechanical decoherence has the same form as a **leakage current.** No charge is lost, only coherence!

Other contributions (from self energies)

- superconductor (Δ) = source of coherence
- spin-flip scattering = loss of spin coherence
- Zeeman field/exchange = spin-dependent energy shift

Quantum circuit theory:

- Quantum Kirchhoff rules
- Matrix voltages and matrix currents
- Dephasing as leakage of coherence





Spin-dependent Quantum Circuit Theory (boundary condition)

$$\frac{Connectors (contacts)}{\hat{I}_{1\to c}}(\varepsilon) = \frac{G_T}{2} \left[\hat{G}_1, \hat{G}_c \right] + \frac{G_P}{2} \left[\left\{ \hat{\kappa}, \hat{G}_1 \right\}, \hat{G}_c \right] - i \frac{G_\phi}{2} \left[\hat{\kappa}, \hat{G}_c \right] \\$$
Standard tunneling conductance
$$G_T = G_Q \sum_n \left(T_{n\uparrow} + T_{n\downarrow} \right) \\
\Rightarrow \text{ Usual charge current} \\$$
Spin-polarization conductance
$$G_P = G_Q \sum_n \left(T_{n\uparrow} - T_{n\downarrow} \right) \\
\Rightarrow \text{ Spin-polarized current} \\$$
Spin-dependent interfacial phase shifts
$$G_\phi = G_Q \sum_n \delta \phi_n \\
\Rightarrow \text{ Induced exchange splitting} \\$$
To

Huertas-Hernando, Belzig, Nazarov, PRL (2001) Cottet, Huertas-Hernando, Belzig, Nazarov, PRB (2009) Machon, Eschrig, Belzig, PRL (2013) Nodes (finite dwell time):

Leakage of coherence $\hat{I}_{L}(\varepsilon) = -iG_{Q}\frac{\varepsilon}{\delta}\left[\hat{\tau}_{3},\hat{G}_{c}\right]$



Some effects of the spin-dependent boundary conditions on the density of states

The density of states in a proximity metal with magnetic contacts



[Machon, Eschrig, Belzig, Phys. Rev. Lett. **110**, 047002 (2013)]

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How does the calculation look like in practice?

Spin-dependent the density of states in N



100% spin-polarized energy bands*!

Spincaloritronics with an SF-heterostructure: Spinthermoelectric "transistor" structure







[Machon, Eschrig, Belzig, New J. Phys. 16, 073002 (2014)]

Non-local caloritronics with an SF-heterostructure:



Local thermoelectric response

Nonlocal thermoelectric response

Ballistic limit: identifying the different processes



3-TERMINAL SYSTEM





- Similar behaviour, larger magnitude in clean case
- Maximal nonlocal thermopower small exchange splitting (comparable to E_{th})
- Maximal for large polarization
- Sign change, more pronounced in clean limit

ONSAGER SYMMETRY



Conclusion/Summary

Quantum circuit theory of spin transport

- Circuit theory: nodes, connectors, leads
- Quantum Kirchhoff rules (Matrix current conservation)
- Spin-dependent boundary conditions/connector

Spin effects on proximity effect

- Spin-mixing in superconductors
- Superconducting proximity spin-split density of states due to a ferromagnetic insulator

Thermoelectricity:

- Spin-splitting + spin-polarized tunneling →large Seebeck effect
- Maximizing thermoelectric efficiency in a N-SFI-N transistor heterostructures
- Non-local Seebeck effect

General reference for QCT: Yu.V. Nazarov, arxiv:1999 Further references: Machon, Eschrig, Belzig, Phys. Rev. Lett. **110**, 047002 (2013) Machon, Eschrig, Belzig, New J. Phys. **16**, 073002 (2014) Machon, Belzig , arxiv 02/2015 Eschrig, Cottet, Belzig, Linder arxiv 04/2015

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