Correlation effects in superconducting quantum dot systems

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11. 1. 2018, Uni Regensburg
Introduction

single-level quantum dot connected to two superconducting (sc) BCS leads:

- ideal system for studying the interplay of electronic correlations and superconducting order
- proximity effect: Cooper pairs from the superconductor leak into the quantum dot, opening a gap in the DoS (induced pairing)
- multiple Andreev reflections on the opposite interfaces give rise to discrete subgap states (Andreev bound states)
- Josephson current can flow between the superconducting electrodes
- presence of a third normal (non-sc) electrode populates the gap with finite DoS, gives control over the Kondo effect
- experimental and theoretical results show that system can undergo a quantum phase transition from spin-singlet (BCS or Kondo) ground state to spin-doublet ground state: $0 - \pi$ transition known from SFS junctions

- What does it mean “single-level”?
  level spacing: (like a particle in a box)
  $\delta E \sim \frac{500\text{meV}}{L[\text{nm}]}$ for short carbon nanotube
  is the dominant energy scale
- long sc nanotubes/nanowires: different physics (e.g. Majorana fermions)
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- **theoretical description**: single-impurity Anderson model (SIAM) + BCS
  - analytic solvers: Hartree-Fock, NCA, 2nd order PT...
  - heavy numerics: ED, NRG, fRG, QMCs...

- **experimental realization**:
  - carbon nanotube
  - InAs/InSb nanowire
  - $C_{60}$ molecule in break junction
  - self-assembled SiGe quantum dots

PRB 88, 045101 (2013). Nature 442, 667 (2006).

- **applications**:
  - quantum computing: Andreev qubits: Science 349, 1199 (2015). (CNT)
  - single-molecule SQUIDs: Nat. Nano. 1, 53 (2006). (InAs nanowire)
  - Cooper pair splitters: Nature 461 960 (2009). (InAs nanowire)
  - ...
Introduction

Andreev bound states and the $0 - \pi$ transition

- Electron with energy $E < \Delta$ incident on the QD-S interface penetrates into sc, creates a Cooper pair and is reflected back as a hole - Andreev reflection

- Multiple Andreev reflections lead to the formation of Andreev bound states within the sc gap

Exp.: evolution of ABS with gate voltage

Nat. Nano. 9, 79 (2014).

- Crossing of ABS at the Fermi energy marks QPT from spin-singlet 0-phase to spin-doublet $\pi$-phase.

- ABS are current-carrying states

- The Josephson current jumps from positive to negative values at $0 - \pi$ transition - can be observed in current-phase relations.
Observables depend only on the phase difference $\Phi = \Phi_L - \Phi_R$ between the sc leads, not on the absolute values of the two phases.

Result: gauge invariance under $\Phi_{L,R} \to \Phi_{L,R} + \Phi_{sh}$ with important consequences.

A. Kadlecová, M. Žonda, T. Novotný, Phys. Rev. B 95, 195114 (2017).
Introduction
description of the model

- \( \varepsilon \) - on-site energy level
- \( U \) - on-site Coulomb interaction
- \( \Delta_\alpha \) - superconducting gap (we assume \( \Delta_L = \Delta_R = \Delta \))
- \( \Phi_\alpha \) - order parameter phase
- \( \Gamma_\alpha \) - tunneling rate (dot-lead coupling)

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the modified single-impurity Anderson model

\[ \mathcal{H} = \mathcal{H}_{\text{dot}} + \sum_{\alpha=R,L,N} (\mathcal{H}_{\text{lead}}^{\alpha} + \mathcal{H}_{c}^{\alpha}) \]

- quantum dot (single-level):
  \[ \mathcal{H}_{\text{dot}} = \sum_{\sigma} \varepsilon_{\sigma} d_{\sigma}^\dagger d_{\sigma} + Ud_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow} \quad \varepsilon_{\sigma} = \varepsilon + \sigma B \]

- leads:
  \[ \mathcal{H}_{\text{lead}}^{\alpha} = \sum_{k\sigma} \varepsilon_{\sigma}(k)c_{\alpha,k\sigma}^\dagger c_{\alpha,k\sigma} - \Delta_{\alpha} \sum_{k}(e^{i\phi_{\alpha}} c_{\alpha,k\uparrow}^\dagger c_{\alpha,-k\downarrow}^\dagger + \text{H.c.}) \quad \alpha = R, L, N \]

- couplings:
  \[ \mathcal{H}_{c}^{\alpha} = -t_{\alpha} \sum_{k\sigma}(c_{\alpha,k\sigma}^\dagger d_{\sigma} + \text{H.c.}) \quad \Gamma_{\alpha} = 2\pi \rho_{\alpha}|t_{\alpha}|^2 \quad \text{tunneling rate} \]

- reliable description of the system: numerically exact calculations (NRG, QMC) show good agreement with experiment (ABS frequencies, Josephson current)
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Methods  Nambu Green function and Hartree-Fock approximation

- Nambu spinor: \[ \Psi(\tau) = \begin{pmatrix} d_{\uparrow}(\tau) \\ d_{\downarrow}(\tau) \end{pmatrix} \]

- Nambu Green function: \[ \hat{G}(\tau) = -\langle T_{\tau} [\Psi(\tau)\Psi(0)^\dagger]\rangle \]

- $2 \times 2$ matrix with normal (diagonal) and anomalous (off-diagonal) components

\[ \hat{G} = -\begin{pmatrix} \langle d_{\uparrow} d_{\uparrow}^\dagger \rangle & \langle d_{\uparrow} d_{\downarrow} \rangle \\ \langle d_{\downarrow} d_{\uparrow}^\dagger \rangle & \langle d_{\downarrow} d_{\downarrow} \rangle \end{pmatrix} \equiv \begin{pmatrix} G_n & G_a \\ G_a^\ast & G_n^\ast \end{pmatrix} = \begin{pmatrix} \rightarrow & \rightarrow \\ \rightarrow & \rightarrow \end{pmatrix} \]

- Equilibrium physics: Matsubara frequencies $\omega_n = (2n + 1)\pi/\beta$

Hartree-Fock approximation (spin-symmetric)

- Static mean-field, simplest way how to study Coulomb interaction effects

- Static self-energies: $\Sigma_{HF} = U\langle G_n \rangle$, $S_{HF} = U\langle G_a \rangle$

- Self-consistent equations:

\[ \Sigma_{HF} = \frac{U}{\beta} \sum_n G_n(i\omega_n, \Sigma_{HF}, S_{HF}), \quad S_{HF} = \frac{U}{\beta} \sum_n G_a(i\omega_n, \Sigma_{HF}, S_{HF}) \]

- Straightforward continuation to the real axis \[ \rightarrow G_n(\omega + i0), \; G_a(\omega + i0) \]
  (important for calculating ABS frequencies)
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- straightforward continuation to the real axis \( \rightarrow G_n(\omega + i0), \quad G_a(\omega + i0) \)
  (important for calculating ABS frequencies)
**Methods**

- first step beyond Hartree-Fock approximation
- **dynamical self-energy**: \( \hat{\Sigma}(i\omega_n) = \hat{\Sigma}_{HF}^{1} + \hat{\Sigma}_{HF}^{(2)}(i\omega_n) \), input: HF propagators

\[
\hat{\Sigma} = \begin{array}{c}
\Sigma \\
S
\end{array} = \begin{array}{c}
\Sigma \quad - \quad \Sigma \\
S \quad - \quad S
\end{array}
\]

- interacting Green function: matrix Dyson equation
  \[
  \hat{G}^{-1}(i\omega_n) = \hat{G}_{U=0}^{-1}(i\omega_n) - \hat{\Sigma}(i\omega_n)
  \]

- static self-consistency between input and output Green functions:
  \[
  \Sigma_{HF}^{1} = \frac{U}{\beta} \sum_n G_n[i\omega_n; \Sigma(i\omega_n), S(i\omega_n)] \quad S_{HF}^{1} = \frac{U}{\beta} \sum_n G_a[i\omega_n; \Sigma(i\omega_n), S(i\omega_n)]
  \]

- Josephson current:
  \[
  J = \frac{4}{\beta} \sum_n \text{Im} \left[ G_a(i\omega_n)S^{(0)}(i\omega_n) \right]
  \]

- Spectral functions:
  \[
  \rho_{n/a}(\omega) = -\frac{1}{\pi} \text{Im} \left[ G_{n/a}(\omega + i0) \right]
  \]
two-terminal setup: $\Gamma_N = 0$

ABS frequencies:

\[ \omega / \Delta \]

\[ \Phi / \pi \]

NRG data calculated using NRG Lubliana code (nrgljubljana.ijs.si)

- good agreement with NRG in the 0-phase
- we can extract the position of the $0 - \pi$ transition QCP from ABS frequencies or Josephson current (both experimentally measurable)
- fails completely to describe the $\pi$-phase
- breakdown of the perturbation technique: double-degenerate ground state, violation of the Gell-Mann - Low theorem
Results

two-terminal setup: 2nd order PT vs. NRG

- NRG: $\sim$ hours on a cluster node
- 2nd order PT: $\sim$ minutes on a laptop
- Fundamental theorem of scientific computing: *Nobody cares how fast you can calculate a wrong answer.*
- need to set limits of applicability of 2nd order PT

Phase diagram in $U - \Delta$ plane ($\Phi = 0$)

Andreev bound states

Induced gap $\mu = U\langle d^{\dagger}d^{\dagger} \rangle$
Results  two-terminal setup: 2nd order PT vs. experiment

R. Delagrange et al, PRB 91, 241401(R) (2015).

**two-terminal setup**: quantum dot with sc leads embedded in asymmetric squid setup:

- doped Si substrate + SiO$_2$ layer
- quantum dot: carbon nanotube
- Al electrodes ($T_C = 1.2$K) with Pd/Nb coating
- $T = 50$ mK

**parameters:**

- $\Delta = 0.17$ meV
- $U = 3.2$ meV $\pm 10$
- $\Gamma_L + \Gamma_R = 0.44$ meV, $\Gamma_L / \Gamma_R = 4$
- $\Phi = (2e/\hbar)BS$

Good fit of exp. data obtained by varying $U$ within the error bars.
three-terminal heterostructure (two superconducting and one normal lead):

- NRG is ineffective in this setup, except $\Phi = 0$ case (three-channel problem)
- normal coupling $\Gamma_N$ smears out the phase boundary and mixes 0 and $\pi$ phases: 2nd order PT becomes unreliable (cannot describe the $\pi$-phase)
- normal coupling also populates the gap with non-zero density of states, leading to the onset of the Kondo effect

Test: NRG vs 2nd order PT at $\Phi = 0$:

$(\Gamma_S = \Gamma_L + \Gamma_R)$

- We need a robust method to solve the modified SIAM, capable to describe
  - superconducting pairing
  - both 0 and $\pi$ phase
  - Kondo behavior
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**test: NRG vs 2nd order PT at $\Phi = 0$:**

![Graph showing comparison between NRG and 2nd order PT](image)

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Three-terminal setup: CT-HYB

Continuous-time quantum Monte Carlo [1]:

- In experiment, $U > \Gamma$, so we chose the strong-coupling, hybridization-expansion CT-QMC solver implemented in the triqs package (ipht.cea.fr/triqs) [2,3]

- Include superconducting pairing:
  Particle-hole transformation in the $\sigma = \downarrow$ segment [4]:

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    d_{\uparrow}^\dagger & \rightarrow d_{\uparrow}^\dagger, \\
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- It maps the sc SIAM model on normal SIAM with attractive interaction:

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    \varepsilon_{\sigma} & \rightarrow \sigma \varepsilon_{\sigma}, \\
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- As $\varepsilon_{\sigma} = \varepsilon + \sigma B$, it maps the magnetic field $B$ on the local energy $\varepsilon$ and vice versa

- Gauge invariance under $\Phi_{L,R} \rightarrow \Phi_{L,R} + \Phi_{sh}$ used to keep the hybridizations real

- No fermionic sign problem

- Finite temperatures only

- Green function is calculated in imaginary time, no direct access to spectral functions/ABS frequencies, only the Josephson current, filling and the induced gap can be obtained directly

(1) E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Rev. Mod. Phys. 83, 349 (2011).
(2) O. Parcollet, M. Ferrero, T. Ayral, H. Hafermann, I. Krivenko, L. Messio, and P. Seth, Comput. Phys. Commun. 196, 398 (2015).
(3) P. Seth, I. Krivenko, M. Ferrero, and O. Parcollet, Comput. Phys. Commun. 200, 74 (2016).
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three-terminal setup: CT-HYB

**Induced gap** $\mu = U \langle d^\dagger d \rangle$: test against NRG for $\Phi = 0$

| $\Gamma_N / \Gamma_S$ | NRG | CT-HYB |
|-----------------------|-----|--------|
| 0                     | ![NRG](image1) | ![CT-HYB](image2) |
| 0.01                  | ![NRG](image3) | ![CT-HYB](image4) |
| 0.1                   | ![NRG](image5) | ![CT-HYB](image6) |
| 1                     | ![NRG](image7) | ![CT-HYB](image8) |

$\Delta = \Gamma_S$, $\Phi = 0$

$T = 0$

$\mu U / \Gamma_S$

$\Gamma_N / \Gamma_S = \frac{0.2}{0.25}$

$\Delta = \Gamma_S$, $\Phi = 0$

$T = 0.025\Gamma_S$

$\mu U / \Gamma_S$

CT-HYB, $\Gamma_N / \Gamma_S = \frac{0.01}{1}$

$\Delta = \Gamma_S$, $\Phi = 0$

$T = 0.025\Gamma_S$

$\mu U / \Gamma_S$

Normal coupling $\Gamma_N$ and temperature have qualitatively similar effect on the system: vanishing of the $\pi$-phase (spin-doublet)
**Results**

**three-terminal setup: CT-HYB**

**Induced gap** $\mu = U\langle d^\dagger d \rangle$: test against NRG for $\Phi = 0$

- Normal coupling $\Gamma_N$ and temperature have qualitatively similar effect on the system: vanishing of the $\pi$-phase (spin-doublet)

**Josephson current**: finite $\Gamma_N$ vs. finite temperature
Results

CT-HYB: spectral functions

- in CT-HYB, Green function is calculated in imaginary time, no direct access to spectral functions/ABs frequencies
- analytic continuation $-i\tau \rightarrow t$ of noisy data is a well-known ill-defined problem

\[
G(\tau) = \int d\omega K(\tau, \omega) \rho(\omega)
\]

\[
K(\tau, \omega) = \frac{e^{-\tau \omega}}{1 + e^{-\beta \omega}}
\]

- solvers:
  - Pade approximants (very unstable) [1]
  - maximum-entropy method (cannot resolve sharp features, needs covariance data) [2]
  - stochastic sampling - Mishchenko method (computationally very demanding) [3]

(1) H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. 29, 179 (1977).
(2) M. Jarrell and J. E. Gubernatis, Phys. Rep. 269, 133 (1996).
(3) A. S. Mishchenko, N. V. Prokof’ev, A. Sakamoto, and B. V. Svistunov, Phys. Rev. B 62, 6317 (2000).
Results  CT-HYB: spectral functions

**Experiment:**
J.-D. Pillet et al., Phys. Rev. B, 88 045101 (2013).

- two-terminal setup, CNT with Al leads
- $\Delta = 150\mu eV$, $T=35mK$
- $U = 13.3\Delta$, $\Gamma = 0.9\Delta$
- spectral function measured via STM
- good agreement between experiment and NRG

Spectral function from CT-HYB:
stochastic sampling method

$T = 44mK$ ($0.025\Delta$)
- good agreement with $T = 0$ NRG results in 0-phase
- good agreement around QCP
- ABS from CT-HYB shifted w.r.t. NRG in $\pi$-phase
Other possible applications

multiple-quantum dot systems:

\[ \Delta_L e^{i\Phi_L} \rightleftharpoons \varepsilon_L, U_L \rightleftharpoons \varepsilon_R, U_R \rightleftharpoons \Delta_R e^{i\Phi_R} \]

\[ \Delta = 0 \quad \Delta = 0 \]

R. Žitko et al, Phys. Rev. Lett. 105, 116803 (2010).
R. Žitko, Phys. Rev. B 91, 165116 (2015).
D. Sherman et al., Nat. Nanotech. 12, 212 (2017).
Z. Su et al., Nat. Commun. 8, 585 (2017).

InSb nanowire with NbTiN leads
\[ \Delta \approx 400 \mu eV, \quad U = 1 - 2 meV \]

▶ singlet, doublet and triplet Andreev molecular states
▶ superexchange effects (tunable by interdot coupling \( t_{LR} \))
▶ fingerprints of Majorana bound states (?)
▶ interesting for applications in topological quantum computing
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\[ \Gamma_L \uparrow \Gamma_{NL} \downarrow \Delta = 0 \]

\[ \Gamma_R \uparrow \Gamma_{NR} \downarrow \Delta = 0 \]

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Conclusions

**second order of perturbation theory:**
- fast, simple, charge conserving (if $\Delta_L = \Delta_R$) and thermodynamically consistent approximation, does not break spin symmetry, direct access to spectral functions/ABS frequencies
- gives reliable results for 0-phase properties (spectral/transport) and phase boundaries in realistic range of parameters (outside the Kondo region)
- present formulation not applicable to the $\pi$-phase - double degenerate ground state - violation of the Gell-Mann - Low theorem
- not reliable in the three-terminal setup due to the mixing of 0 and $\pi$ phases

**hybridization-expansion CT-QMC:**
- based on the TRIQS CT-HYB solver (ipht.cea.fr/triqs)
- works well in both the two-terminal and the three-terminal setups
- able to describe all phases including the $\pi$-phase and the Kondo regime
- works only for finite temperatures
- formulated in imaginary time: no direct access to spectral functions/ABS frequencies without analytic continuation
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reading:
- M. Žonda, V. Pokorný, V. Janiš, and T. Novotný, Sci. Rep. 5, 8821 (2015). (2ndPT)
- M. Žonda, V. Pokorný, V. Janiš, and T. Novotný, PRB 93, 024523 (2016). (2ndPT)
- T. Domański, M. Žonda, V. Pokorný, G. Górski, V. Janiš, and T. Novotný, PRB 95, 045104 (2017). (3-terminal, QMC)
- V. Pokorný, M. Žonda, arXiv:1001.2700 (2017). (2-terminal, QMC)
- www.fzu.cz/~pokornyv/pages/research (more resources, including this presentation)

codes:
- 2nd order PT solver: github.com/pokornyv/SQUAD
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Thank you for your attention.
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