Quantum dot attached to two superconducting leads: Andreev bound states

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Outline

Nano-structures attached to leads

Experimental realization

- Carbon nanotubes with well separated energy levels and strong electron repulsion
- Nanotube attached to metallic leads – formation of local magnetic moment
- Nanotube attached to superconducting leads – tunneling of Cooper pairs

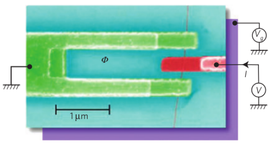
Theoretical description

- Singe-impurity Anderson model
- Metallic leads – no spontaneous magnetization (Kondo)
- BCS superconducting leads – induce superconducting gap on impurity (Josephson junction)

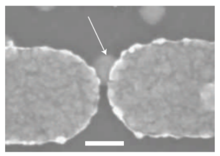
Superconducting Quantum Dot

A single-level quantum dot connected to superconducting BCS leads:

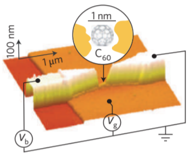
- Various experimental realizations, e.g.:



CNT
Nat. Phys. 6, 965 (2010)



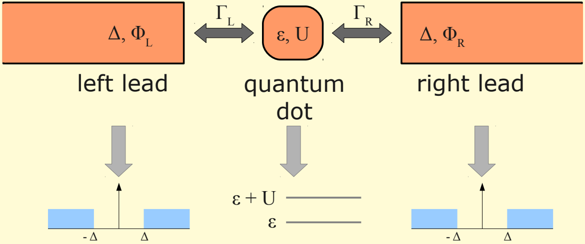
SiGe
Nat. Nano. 5, 458 (2010)



C_{60}
Nat. 453, 633 (2008)

- These devices are generalized Josephson junctions!
- They allow to explore a wide range of phenomena, including electron transport, Kondo physics, quantum entanglement, different quasiparticles or $0 - \pi$ phase transition

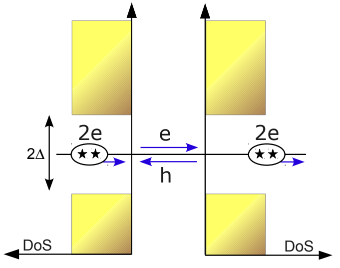
Model system

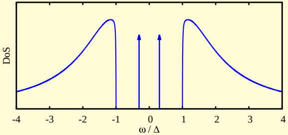


- U - on-site Coulomb interaction
- ε - on-site energy level
- Δ - superconducting gap
- Φ_α - superconducting order parameter phase
- $\Phi = \Phi_R - \Phi_L$ - phase difference
- Γ_α - tunneling rate (dot-lead coupling)

Andreev reflections and gap states

- Electron at the right QD-S interface: creation of a Cooper pair, hole reflected to the left
- Hole at the left QD-S interface: annihilation of a Cooper pair, electron reflected to the left
- Multiple Andreev reflections form resonant standing waves
  - Andreev bound states at $\pm\omega_0$ ($\omega_0 < \Delta$ - lie within the sc gap)





- ABS carry supercurrent

$$J_{ABS} = \frac{2e}{\hbar}\frac{\partial\omega_0}{\partial\Phi}$$

- Classical analog - Fabry - Perot interferometer

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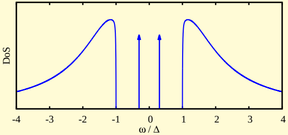

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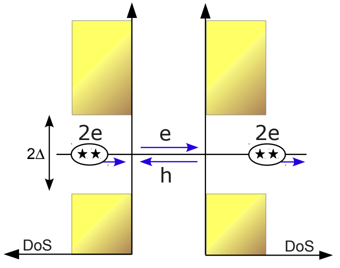

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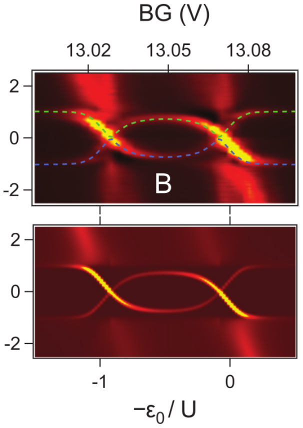
Behavior of gap states with electron repulsion



ε_0 – impurity energy level (chemcal potential)

Crossing of gap states

- Experiment: continuous crossing of Andreev states at the Fermi level
- Crossing of gap staes coincides with $0 - \pi$ transition in Josephson current
- Numerical RG results in good agreement with experimental data
- Missing reliable analytic approach to explain the phenomenon

Single-impurity Anderson model with SC leads

$$\mathcal{H} = \mathcal{H}_{dot} + \sum_{\alpha=R,L} \left(\mathcal{H}^{\alpha}_{lead} + \mathcal{H}^{\alpha}_{c}\right)$$

- quantum dot (single - level):

$$\mathcal{H}_{dot} = \varepsilon \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow}$$

- BCS (s-wave) leads:

$$\mathcal{H}^{\alpha}_{lead} = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) c^{\dagger}_{\alpha,\mathbf{k}\sigma} c_{\alpha,\mathbf{k}\sigma} - \Delta \sum_{\mathbf{k}} \left(e^{i\Phi_{\alpha}} c^{\dagger}_{\alpha,\mathbf{k}\uparrow} c^{\dagger}_{\alpha,-\mathbf{k}\downarrow} + \mathrm{H.c.}\right) \qquad \alpha = R, L$$

- coupling to the bath:

$$\mathcal{H}^{\alpha}_{c} = -t_{\alpha} \sum_{\mathbf{k}\sigma} \left(c^{\dagger}_{\alpha,\mathbf{k}\sigma} d_{\sigma} + \mathrm{H.c.}\right) \qquad \Gamma_{\alpha} = 2\pi\rho_{\alpha} |t_{\alpha}|^{2}$$

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Nambu Green's function I

- Imaginary time – the only dynamical variable
- Nambu spinor: Nambu Green's function:

$$\Psi(\tau) = \begin{pmatrix} d_{\uparrow}(\tau) \\ d^{\dagger}_{\downarrow}(\tau) \end{pmatrix} \qquad \mathbb{G}(\tau) = -\left\langle \mathbb{T}_{\tau}[\Psi(\tau)\Psi^{\dagger}(0)] \right\rangle$$

- 2×2 matrix with normal (diagonal) and anomalous (off-diagonal) components

$$\mathbb{G}_{\sigma}(\tau - \tau') = -\begin{pmatrix} \left\langle \mathbb{T}\left[d_{\sigma}(\tau)d^{\dagger}_{\sigma}(\tau')\right]\right\rangle, & \left\langle \mathbb{T}\left[d_{\sigma}(\tau)d_{-\sigma}(\tau')\right]\right\rangle \\ \left\langle \mathbb{T}\left[d^{\dagger}_{-\sigma}(\tau)d^{\dagger}_{\sigma}(\tau')\right]\right\rangle, & \left\langle \mathbb{T}\left[d^{\dagger}_{-\sigma}(\tau)d_{-\sigma}(\tau')\right]\right\rangle \end{pmatrix}$$

$$= \begin{pmatrix} G_{\sigma}(\tau - \tau'), & \mathcal{G}_{-\sigma}(\tau - \tau') \\ \mathcal{G}^{*}_{\sigma}(\tau - \tau'), & G^{*}_{-\sigma}(\tau - \tau') \end{pmatrix}$$

Nambu Green's function II

- One-particle GF & self-energies (normal Σ and anomalous $\mathcal{S}$)

$$\widehat{G}(z) = \frac{1}{D(z)} \begin{pmatrix} z[1+s(z)] + \varepsilon + \Sigma(-z)\,, & -\Delta_\Phi\,[s(z) - \mathcal{S}(z)] \\ -\Delta_\Phi\,[s(z) - \mathcal{S}(-z)]\,, & z[1+s(z)] - \varepsilon - \Sigma(z) \end{pmatrix}$$

$\Delta_\Phi = \Delta\cos(\Phi/2)$, $s(z) = i\Gamma_0 \mathrm{sgn}(\Im z)/\zeta$, $\zeta^2 = z^2 - \Delta^2$

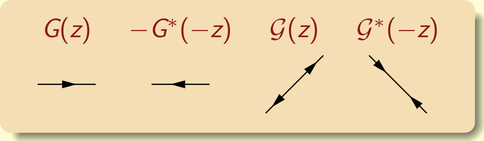
- Determinant – zeros determine bound states

$$D(z) = z\,[1 + s(z)]\,[z\,(1 + s(z)) - \Sigma(z) + \Sigma(-z)] \\ - [\epsilon + \Sigma(z)]\,[\epsilon + \Sigma(-z)] - \Delta_\Phi^2\,[s(z) - \mathcal{S}(z)]\,[s(z) - \mathcal{S}(-z)]$$

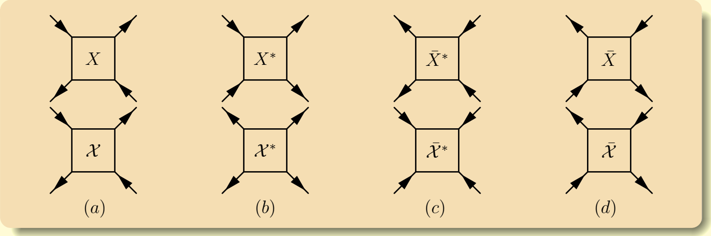
- Determinant is real within the gap $z \in [-\Delta, \Delta]$ (independent of U)
- Symmetries: $G^*(z) = -G(-z)$, $\mathcal{G}^*(z) = \mathcal{G}(-z)$
- Enrgies of Andreev bound states (ABS): $\pm\omega_0$

Elements of diagrammatic representation

- Particle & hole propagators:



- Normal & anomalous elementary 2P vertices

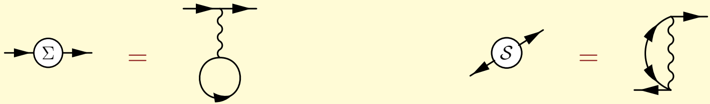


$\overline{X}$ – electron-hole transformation (upper line)

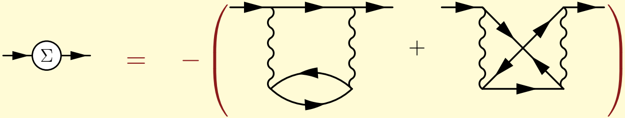
X^* – electron-hole transformation (lower line)

Simple diagrams

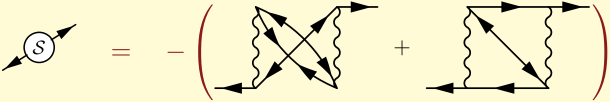
- Hatree-Fock approximation



- Second-order PE: normal SE

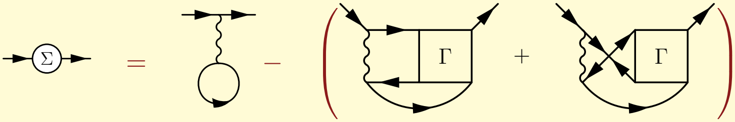


- Second-order PE: anomalous SE

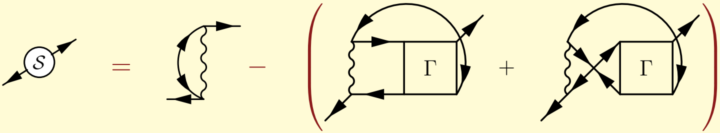


Schwinger-Dyson equations

- Normal self-energy (electron-hole channel)



- Anomalous self-energy (electron-hole channel)



Matsubara frequencies & analytic continuation

- Energy variables in diagrams → Matsubara frequencies
  fermionic: $\omega_n = (2n+1)\pi T$, bosonic: $\nu_m = 2m\pi T$
- Thermodynamic quantities – sums over Matsubara frequencies

> Matsubara formalism carries no information about spectrum of eigenstates & ABS

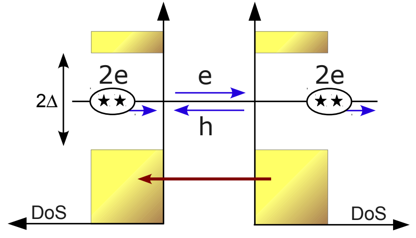
- Decomposition of the (fermionic) Matsubara sum to band & isolated gap states

$$\frac{1}{\beta}\sum_n F(i\omega_n) \to \sum_i f(x_i)\,\mathrm{Res}[F,x_i] - \left[\int_{-\infty}^{-\Delta} + \int_{\Delta}^{\infty}\right]\frac{dx}{\pi} f(x)\Im F(x+i0)$$

where $\pm\Delta$ are gap edges (independent of interaction)

Josephson current - 0 & π phases

$$J_{super} = -2\Delta\Gamma_0 \left[\frac{\mathrm{Res}[\mathcal{G}^*, -\omega_0]}{\sqrt{\Delta^2 - \omega_0^2}} + \int_{-\infty}^{-\Delta} \frac{d\omega}{\pi} \frac{\Re\mathcal{G}^*(\omega)}{\sqrt{\omega^2 - \Delta^2}} \right] \sin(\Phi/2)$$



$$J_{ABS} \sim \sin(\Phi/2)$$

$$J_{band} \sim \sin(\Phi)$$

- 0 phase – contribution from Andreev bound states dominant: direct current via the impurity level
- π phase – only contribution from band states: reverse tunneling current

0 and π phases – infinite gap (atomic) limit

- Only discrete gap (Andreev) states
  – no band states, no Kondo limit
- Static hybridization self-energy: $\lim_{\Delta\to\infty} \Delta s(\omega) = \Gamma_0$
- 0 phase BCS spin singlet: $|\pm\rangle = \mp u_{\mp}|\uparrow\downarrow\rangle + u_{\pm}|0\rangle$

$$\omega_{\pm} = \pm\sqrt{\left(\varepsilon + \frac{U}{2}n\right)^2 + \cos^2(\Phi/2)\left(\Gamma_0 - U\nu\right)^2}$$

- Degenerate spin doublet: $|\uparrow\rangle, |\downarrow\rangle$ states at energy $E_d = 0$
- 0 phase being the ground state: $\omega_- < E_d = 0$
- $0 - \pi$ transition: $\omega_{\pm} = 0$
- Critical interaction (HFA exact):

$$\frac{U_c}{2} = \sqrt{\left(\varepsilon + \frac{U_c}{2}\right)^2 + \cos^2(\Phi/2)\Gamma_0^2}$$

only for $\varepsilon < 0$

Hartree-Fock solution – spin symmetric state I

- Separation of gap and band contributions

$$n = \frac{x_0(1+s_0) - \epsilon(1+K_0\mathcal{I}_0) + K_0(\mathcal{J}_\sigma + \mathcal{J}_0)}{U + K_0(1+U\mathcal{I}_0)}\,, \quad \nu = \frac{s_0 + K_0\mathcal{I}_\sigma}{U + K_0(1+U\mathcal{I}_0)}$$

with $K_0 = K(x_0), s_0 = s(x_0)$

$$K(x) = \frac{dD(x)}{dx} = 2x\left[1 + \Gamma_0\frac{2\Delta^2 + U\Delta_\Phi^2\nu - x^2}{(\Delta^2 - x^2)^{3/2}} + \Gamma_0^2\frac{\Delta^2 - \Delta_\Phi^2}{(\Delta^2 - x^2)^2}\right]$$

- Band contributions ($|x| > \Delta$)

$$\mathcal{I}_0 = -\int_{-\infty}^{-\Delta}\frac{dx}{\pi}\frac{\Im D(x)}{|D(x)|^2}\,, \quad \mathcal{I}_\sigma = \int_{-\infty}^{-\Delta}\frac{dx}{\pi}\frac{\Gamma_0\Re D(x)}{|D(x)|^2\sqrt{x^2 - \Delta^2}}$$

$$\mathcal{J}_0 = -\int_{-\infty}^{-\Delta}\frac{dx}{\pi}\frac{x\Im D(x)}{|D(x)|^2}\,, \quad \mathcal{J}_\sigma = \int_{-\infty}^{-\Delta}\frac{dx}{\pi}\frac{\Gamma_0 x\Re D(x)}{|D(x)|^2\sqrt{x^2 - \Delta^2}}$$

Hartree-Fock solution – spin symmetric state II

- Determinant (in band)

$$\Re D(x) = x^2 - (\epsilon + Un)^2 - \Delta_\Phi^2 U^2 \nu^2 - \Gamma_0^2 \frac{x^2 - \Delta_\Phi^2}{x^2 - \Delta^2}$$

$$\Im D(x) = 2\Gamma_0 \, \mathrm{sgn}(x) \frac{x^2 + \Delta_\Phi^2 U\nu}{\sqrt{x^2 - \Delta^2}}$$

- Gap-states contribution ($|x| < \Delta$)

$$\mathrm{Res}[G, x] = \frac{1}{K(x)} \left[x \left(1 + \frac{\Gamma_0}{\sqrt{\Delta^2 - x^2}} \right) + \epsilon + Un \right]$$

$$\mathrm{Res}[\mathcal{G}, x] = -\frac{\Delta_\Phi}{K(x)} \left(\frac{\Gamma_0}{\sqrt{\Delta^2 - x^2}} - U\nu \right)$$

Hartree-Fock solution – spin symmetric state III

- Energies of the gap states ($\pm x_0$)

$$\left[1 + \frac{\Gamma_0}{\sqrt{\Delta^2 - x_0^2}}\right]^2 x_0^2 = (\epsilon + Un)^2 + \Delta_\Phi^2 \left[U\nu - \frac{\Gamma_0}{\sqrt{\Delta^2 - x_0^2}}\right]^2$$

- Saturation: gap states reach the Fermi energy ($x_0 \to 0$, $K_0 \to 0$), second-order pole
- Critical interaction for vanishing of 0-phase

$$U_c^2 = \left\{U_c + 2\left(1 + \frac{\Gamma_0}{\Delta}\right)\left[\epsilon + U_c(\mathcal{J}_\sigma + \mathcal{J}_0)\right]\right\}^2 + 4\Delta_\Phi^2 \left(1 + \frac{\Gamma_0}{\Delta}\right)^2 \left[\sigma_0(1 + U_c\mathcal{I}_0) - U_c\mathcal{I}_\sigma\right]^2$$

- Saturated solution ($U > U_c$): $x_0 = 0$, $n = -\epsilon/U$, $\nu = \Gamma_0/U\Delta$ – ABS freeze at the Fermi energy no ABS crossing

Analytic methods – diagrammatic expansion

Dynamical solutions – spin symmetric

- Dynamical corrections (DC) with only static self-consistence
- Fully dynamically self-consistent corrections (FDC)
- High numerical precision of 2^{nd} order (up to intermediate coupling)

Mean field – spin polarized (to be overcome)

- 0-π first order transition (no gap-state crossing)
- 0 (nonmagnetic) and π (magnetic) phases overlap
- π phase – spurious magnetic state due to band states

Dynamical approximations by now applicable only in 0 phase and zero temperature

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Numerical simulations & solutions

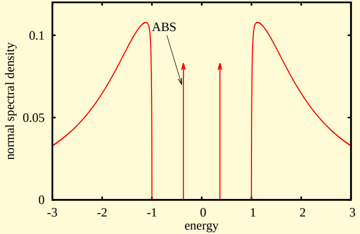
- Numerical Renormalization Group (NRG) - reference
  - Accurate results at zero temperature
    $0 - \pi$ transition & crossing of ABS
  - Suitable for both 0 (spin singlet) and π (spin doublet) phases
  - Only ground state
  - Only spin-symmetric situation (no magnetic field)

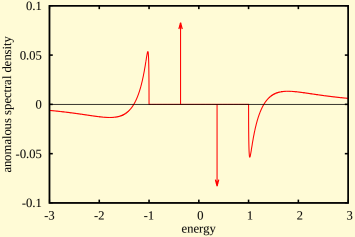
- CT Quantum Monte Carlo (CTQMC)
  - Only non-zero temperatures
  - Ground and excited states mixed up
  - Only spin-symmetric situation (no magnetic field)

Non-interacting case

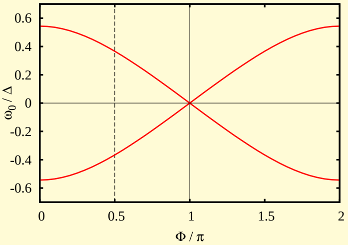
$U = 0$, $\Gamma = \Delta$, $\Phi/\pi = 0.5$, $\epsilon = 0$

(height of ABS represents the residue)

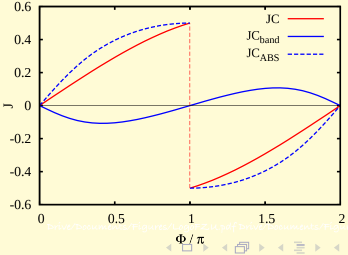




ABS



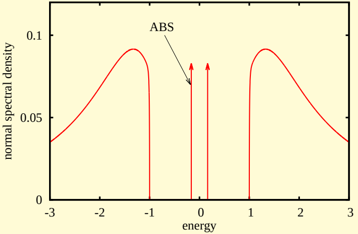
current-phase relation $J(\Phi)$

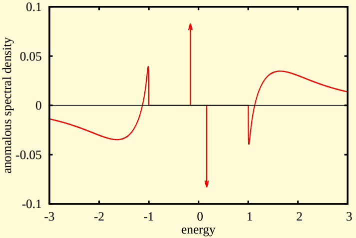


HFA results

$U = 2\Delta$, $\Gamma = \Delta$, $\Phi/\pi = 0.5$, $\varepsilon = 0$

(height of ABS represents the residue)





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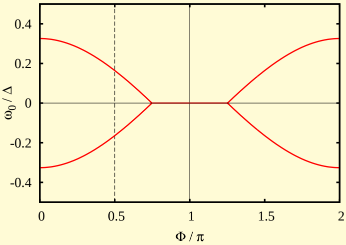

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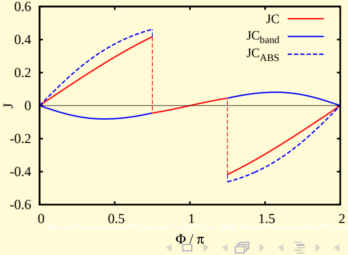
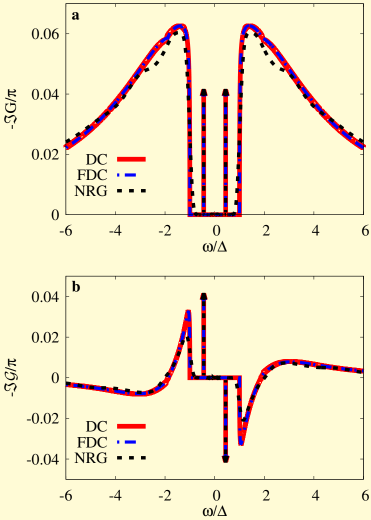
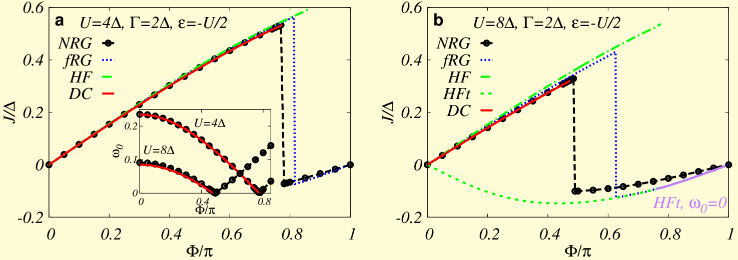


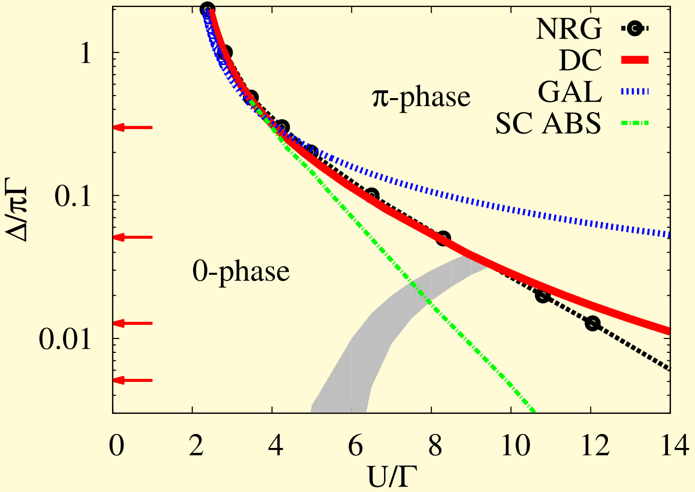
Normal & anomalous GF – dynamical corrections



Josephson current & ABS crossing



$U-\Delta$ Phase diagram



Beyond the crossing of gap states

What the crossing of gap states means?
How to describe π phase beyond MFT?

Suppressing spurious magnetic state due to band states in the spin polarized state.
Dynamical solution in magnetic field.

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Solution in an external magnetic field I

- Spin-dependent propagators $G_\sigma(\omega)$, $\mathcal{G}_\sigma(\omega)$ in magnetic field
- Denominator - spin dependent ($n = n_\uparrow + n_\downarrow$, $m = n_\uparrow - n_\downarrow$)

$$D_\sigma(\omega) = \left[\omega(1 + s(\omega)) + \sigma\left(h + \frac{U}{2}m\right)\right]^2 - \left(\epsilon + \frac{U}{2}n\right)^2 - \Delta_\Phi^2\left(s(\omega) - U\nu\right)^2$$

(Mean-field approximation)

- Reflection symmetry: $D_{-\sigma}(\omega) = D^*_\sigma(-\omega)$
- Four resolved spin-dependent gap states

$$\omega_\sigma^\pm\left(1 + s_\sigma^\pm\right) = -\sigma\left(h + \frac{U}{2}m\right) \pm \sqrt{\left(\epsilon + \frac{U}{2}n\right)^2 + \Delta_\Phi^2\left(s_\sigma^\pm - U\nu\right)^2}$$

- Spin-reflection symmetry: $\omega_\sigma^\pm = -\omega_{-\sigma}^\mp$

Solution in an external magnetic field II

- Crossing of gap states ($h \searrow 0$): $\omega^+_\uparrow = \omega^-_\downarrow = 0$
  - 0 phase: $\omega_\sigma = \omega$

$$n_c = -\frac{2\varepsilon}{U}\,, \qquad \Delta\nu_c = \frac{2\Gamma_0}{U}$$

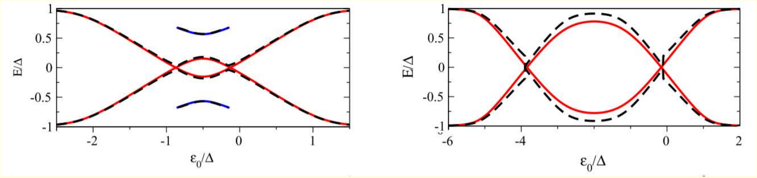
  - π phase: $\omega_\uparrow \neq \omega_\downarrow$

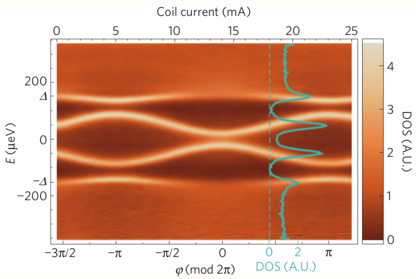
$$\frac{U^2}{4} m^2 = \left(\varepsilon + \frac{U}{2} n\right)^2 + \Gamma_0^2 \cos^2(\Phi/2)$$

  - Atomic limit: $n_\downarrow = 0, m = n = 1, \nu = 0$, & exact critical U_c
- 0 phase: low-magnetic (singlet) state ($\omega^-_\uparrow < 0,\ \omega^+_\uparrow > 0$)
- π phase: high-magnetic (doublet) state ($\omega^-_\uparrow < 0,\ \omega^+_\uparrow < 0$)
- No Andreev bound states in π-phase

Spin polarized Andreev states

$U = \Delta$ $\quad\quad$ $U = 4\Delta$





- Four Gap states in the π phase
- Jump in particle density, magnetization & Josephson current
- Continuous crossing of gap states beyond Hartee-Fock solution (free of spurious magnetic transition due to band states)

SC interacting quantum dot – spectral representation

1. Induced SC gap on impurity - normal & anomalous GF
2. Gap states – remnants of the impurity level
3. MB perturbation theory – convolutions of poles & cuts in GF

Gap states, Josephson current and 0 and π phases

1. Two contributions to JC: Direct (ABS) & tunneling (inverse)
2. $0-\pi$ transition – crossing of ABS to spin-dependent JC
3. Spin symmetric solution (beyond static HF):
   - Two ABS (spin degenerate) symmetric around FE
   - No crossing - saturation due to freezing at FE & vanishing of anomalous GF
4. Spin polarized solution:
   - Four resolved ABS – two for each spin (asymmetric w.r.t. FE)
   - Crossing of ABS – low-spin to high-spin transition
5. Dynamics to suppress spurious magnetic state due to band states

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