Superconducting quantum dot in magnetic field: crossing of gap states

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Outline

1. Basic concepts
   - Model description
   - Nambu spinor formalism
   - Magnetic & spin-polarized states
   - Analytic continuation & spectral representation
2. Exact solutions in magnetic field
   - 0 & π phases in the non-interacting dot
   - $0-\pi$ transition in the atomic limit
3. Beyond solvable limits
   - Failure of the mean-field solution
   - Two-particle functions - parquet equations
   - Nambu formalism for 2P functions
4. Conclusions

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

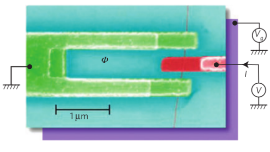
Theoretical description

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

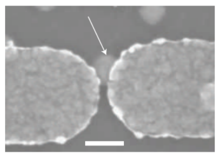
Superconducting Quantum Dot

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

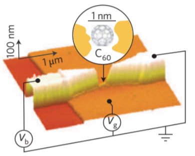
- Various experimental realizations, e.g.:



CNT
Nat. Phys. 6, 965 (2010)



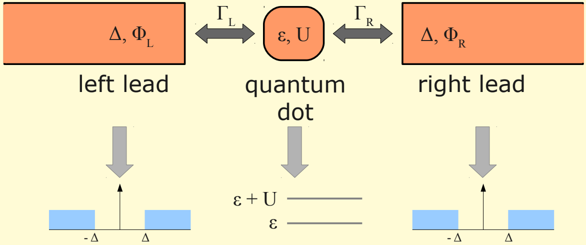
SiGe
Nat. Nano. 5, 458 (2010)



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)

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):

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

- BCS (s-wave) leads:

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

- coupling to the bath:

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

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Spin-dependent Nambu Green's function I

- Imaginary time – the only dynamical variable
- Nambu spinor:

$$\Psi_\sigma(\tau) = \begin{pmatrix} d_\sigma(\tau) \\ d^\dagger_{-\sigma}(\tau) \end{pmatrix}$$

Nambu Green's function:

$$\mathbb{G}_\sigma(\tau) = -\left\langle \mathbb{T}_\tau [\Psi_\sigma(\tau)\Psi^\dagger_\sigma(0)] \right\rangle$$

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

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

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

Spin-dependent Nambu Green's function II

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

$$\widehat{G}_\sigma(z) = \frac{1}{D_\sigma(z)} \begin{pmatrix} -X_{-\sigma}(-z), & -\Delta_\Phi Y_{-\sigma}(-z) \\ -\Delta_\Phi Y_\sigma(z), & X_\sigma(z) \end{pmatrix}$$

$$X_\sigma(z) = z[1 + s(z)] + \sigma h_U - \epsilon_U - \Sigma_\sigma(z)$$
$$Y_\sigma(z) = s(z) - U\nu - \mathcal{S}_\sigma(z)$$

$\epsilon_U = \varepsilon + Un/2,\ h_U = h + Um/2,$

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

- Determinant – zeros determine bound states

$$D_\sigma(z) = -X_\sigma(z)X_{-\sigma}(-z) - \Delta_\Phi^2 Y_\sigma(z)Y_{-\sigma}(-z)$$

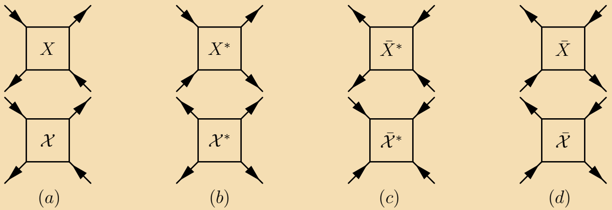
- Determinant is real within the gap $z \in [-\Delta, \Delta]$ (independent of U)
- Symmetries: $G^*_\sigma(z) = -G_{-\sigma}(-z), \qquad \mathcal{G}^*_\sigma(z) = \mathcal{G}_{-\sigma}(-z)$
- Four gap states (ABS): $\omega^\pm_\sigma$ with symmetry $\omega^\pm_\sigma = -\omega^\mp_{-\sigma}$

Elements of diagrammatic representation

- Particle & hole propagators:

$G_\sigma(z)$ $\quad -G^*_\sigma(-z)$ $\quad \mathcal{G}_\uparrow(z)$ $\quad \mathcal{G}^*_\downarrow(-z)$

- Normal & anomalous elementary 2P vertices

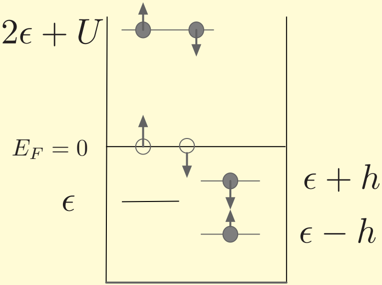


$\overline{X}$ – electron-hole transformation (upper line)

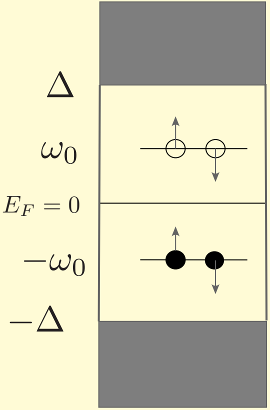
X^* – electron-hole transformation (lower line)

Magnetic field vs. superconductivity

Single atom in magnetic field



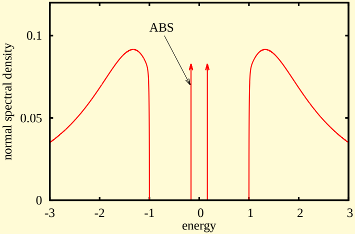
Superconducting atom spin symmetric

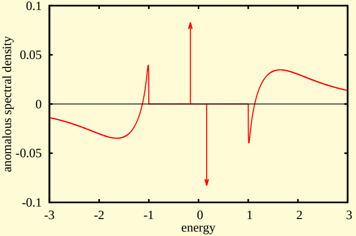


Spin symmetric superconducting dot

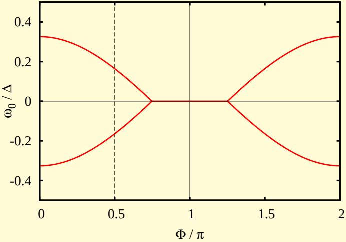
$U = 2\Delta$, $\Gamma = \Delta$, $\Phi/\pi = 0.5$, $\varepsilon = -\Delta$

(height of ABS represents the residue)

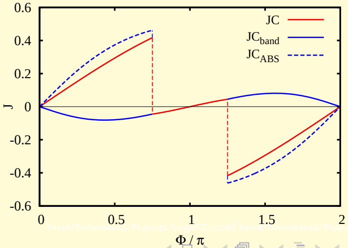




ABS

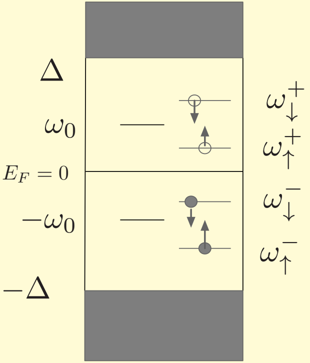


current-phase relation $J(\Phi)$

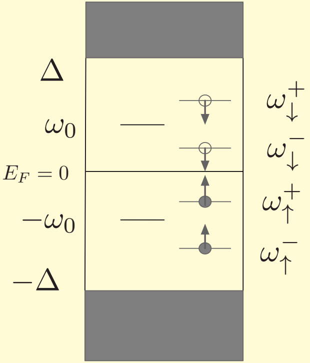


Suoerconducting dot in magnetic field

Superconducting atom in magnetic field - 0-phase



Superconducting atom in magnetic field - π-phase



No singlet Cooper pairs on impurity in π-phase in the atomic limit (no charge fluctuations)

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

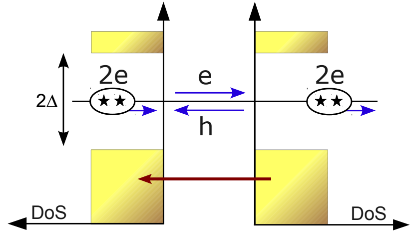
- Decomposition of the (fermionic) Matsubara sum to band & isolated gap states

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

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

Josephson current – 0 & π phases

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



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

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

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

$0-\pi$ transition in magnetic field $(U=0)$

- Spin-dependent propagators $\left(s(\omega)=\Gamma_0/\sqrt{\Delta^2-\omega^2}\right)$

$$G_\sigma(\omega)=\frac{\omega(1+s(\omega))+\epsilon+\sigma h}{D_\sigma(\omega)}$$

$$\mathcal{G}_\sigma(\omega)=-\Delta_\Phi\,\frac{s(\omega)}{D_\sigma(\omega)}$$

- Denominator

$$D_\sigma(\omega)=[\omega(1+s(\omega))+\sigma h]^2-\epsilon^2-\Delta_\Phi^2 s(\omega)^2$$

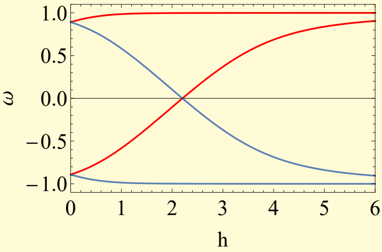
- Reflection symmetry (complex energy): $D_{-\sigma}(z)=D_\sigma(-z)$
- Four spin-dependent gap states

$$\omega_\sigma^\pm\left[1+s\left(\omega_\sigma^\pm\right)\right]=-\sigma h\pm\sqrt{\epsilon^2+\Delta_\Phi^2 s\left(\omega_\sigma^\pm\right)^2}$$

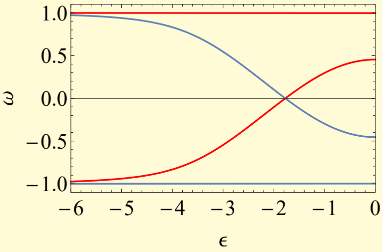
- Crossing of gap states: $\omega_\uparrow^+=-\omega_\downarrow^-=0$
- Critical magnetic field: $h_c=\sqrt{\epsilon^2+\Gamma_0^2\cos^2(\Phi/2)}$

Gap states in magnetic field

Function of magnetic field
($\Delta = \Gamma_0 = 1, \epsilon = -2, \Phi = \pi/4$)



Function of impurity energy
($\Delta = \Gamma_0 = 1, h = 2, \Phi = \pi/4$)



Thermodynamic of the superconducting dot I

- Grand potential

$$\Omega(\Phi_L,\Phi_R) = -\frac{1}{2\beta}\sum_{\sigma}\sum_{\omega_n} e^{\{i\omega_n 0^+\}}\log\left\{\left[i\omega_n\left(1+\frac{\Gamma_0}{\sqrt{\Delta^2-(i\omega_n)^2}}\right) + \sigma h\right]^2 - \epsilon^2 - \Delta^2\frac{\Gamma_0^2\cos\Phi_L\cos\Phi_R}{\Delta^2-(i\omega_n)^2}\right\}$$

- Symmetric leads: $\Phi_R = -\Phi_L = \Phi/2$
- Abbreviations

$$\omega_\sigma = \omega_\sigma^+ = -\omega_{-\sigma}^- \in (-\Delta,\Delta)\,,\quad \mathcal{D}_\sigma = \epsilon^2 + \Delta_\Phi^2 s_\sigma^2$$

$$\Delta_\Phi = \Delta\cos\Phi/2\,,\quad s_\sigma = s(\omega_\sigma) = \Gamma_0/\sqrt{\Delta^2-\omega_\sigma^2}\,,\quad K_\sigma = K_\sigma(\omega_\sigma)\,,$$

$\Delta f_\sigma = f(-\omega_\sigma) - f(\omega_\sigma)$ - responsible for discontinuities at ABS crossing at zero temperature

Thermodynamic of the superconducting dot II

- Derivative of the determinant

$$K_\sigma(\omega) = \frac{dD_\sigma(\omega)}{d\omega} = 2\omega\left\{1 + s(\omega)\left[1 + \frac{\Delta^2 - s(\omega)\left(\Delta_\Phi^2 - \omega^2\right)}{\Delta^2 - \omega^2}\right]\right\} + 2\sigma h\left[1 + s(\omega)\frac{\Delta^2}{\Delta^2 - \omega^2}\right]$$

- Crossing odd symmetry: $K_{-\sigma}(0) = -K_\sigma(0)$
- Charge density

$$n = \frac{1}{\beta}\sum_{\omega_n}\sum_\sigma G_\sigma(i\omega_n) = \sum_\sigma \frac{\sqrt{\mathcal{D}_\sigma}\left(1 + s_\sigma\right) - \sigma h s_\sigma + \epsilon\Delta f_\sigma}{K_\sigma}$$

$$- \sum_\sigma\left[\int_{-\infty}^{-\Delta} + \int_\Delta^\infty\right]\frac{d\omega f(\omega)}{\pi}\Im\left[\frac{\omega + \epsilon + \sigma h + \omega s(\omega + i0^+)}{D_\sigma(\omega + i0^+)}\right]$$

Thermodynamic of the superconducting dot III

- Spin density

$$m = \frac{1}{\beta}\sum_{\omega_n}\sum_{\sigma}\sigma G_\sigma(i\omega_n) = -\sum_{\sigma}\frac{[\sqrt{\mathcal{D}_\sigma}\,(1+s_\sigma))]\Delta f_\sigma - \sigma\epsilon}{K_\sigma}$$

$$-\sum_{\sigma}\sigma\left[\int_{-\infty}^{-\Delta}+\int_{\Delta}^{\infty}\right]\frac{d\omega f(\omega)}{\pi}\Im\left[\frac{\omega+\epsilon+\sigma h+\omega s(\omega+i0^+)}{D_\sigma(\omega+i0^+)}\right]$$

- Anomalous charge density

$$\nu = \frac{1}{\beta}\sum_{\omega_n}\sum_{\sigma}\frac{\mathcal{G}_\sigma(i\omega_n)}{\Delta_\Phi} = \sum_{\sigma}\frac{s_\sigma\Delta f_\sigma}{K_\sigma}$$

$$+\sum_{\sigma}\left[\int_{-\infty}^{-\Delta}+\int_{\Delta}^{\infty}\right]\frac{d\omega f(\omega)}{\pi}\Im\left[\frac{s(\omega+i0^+)}{D_\sigma(\omega+i0^+)}\right]$$

Thermodynamic of the superconducting dot IV

- Josephson current with band-states contribution (symmetric leads)

$$J_{super} = \frac{\partial \Omega}{\partial \Phi_R} = -\frac{\Gamma_0^2 \Delta^2 \sin\Phi}{2} \sum_{\sigma,\alpha=\pm 1} \frac{f(\sigma\alpha\omega_\alpha)}{(\Delta^2 - \omega_\alpha^2)\, K_\sigma(\sigma\alpha\omega_\alpha)}$$

$$+ \Gamma_0^2 \Delta^2 \sin\Phi \left[\int_{-\infty}^{-\Delta} + \int_{\Delta}^{\infty}\right] \frac{d\omega\, f(\omega)}{4\pi\,(\omega^2 - \Delta^2)} \sum_\sigma \frac{\Im D_\sigma(\omega + i0^+)}{|D_\sigma(\omega)|^2}$$

Discontinuities at the transition (zero temperature)

- Jump of the Josephson current at the transition

$$\delta J_{super} = \frac{\Gamma_0^2 \sin\Phi}{K_\uparrow(0)} = \frac{\Gamma_0^2 \Delta \sin\Phi}{2\sqrt{\epsilon^2 + \Delta^2\cos^2(\Phi/2)}\,[\Delta + \Gamma_0]}$$

- Jump in density of Cooper pairs

$$\delta\nu = \frac{\Gamma_0}{\Delta K_\uparrow(0)} = \frac{\Gamma_0}{\sqrt{\epsilon^2 + \Delta^2\cos^2(\Phi/2)}\,[\Delta + \Gamma_0]}$$

- Jump in particle density

$$\delta n = -\frac{2\epsilon}{K_\uparrow(0)} = -\frac{\epsilon\Delta}{\sqrt{\epsilon^2 + \Delta^2\cos^2(\Phi/2)}\,[\Delta + \Gamma_0]}$$

- Jump in magnetization

$$\delta m = -\frac{2h_c}{K_\uparrow(0)} = -\frac{\Delta}{\Delta + \Gamma_0}$$

HF grand potential - exact in the atomic limit

- Static solution exact in the atomic limit $\Delta \to \infty$
- Static parameters: particle (n_σ), hole $(1 - n_\sigma)$ densities & density of Cooper pairs (ν)
- Grand potential particle & holes mixed

$$2\Omega(n_\sigma, n^*_\sigma; \nu) = -\frac{1}{\beta} \sum_{\omega_n} \sum_{\sigma} e^{\{i\omega_n 0^+\}} \log \Big[(i\omega_n(1 + s(i\omega^*_n)) + \sigma h - \epsilon - U n_{-\sigma}) \times (i\omega_n(1 + s(i\omega_n)) + \sigma h + \epsilon + U n^*_\sigma) - \Delta^2_\Phi \left(s(i\omega_n) - \frac{U\nu}{\Delta} \right)^2 \Big] - U n_\uparrow n_\downarrow - U(1 - n^*_\uparrow)(1 - n^*_\downarrow) - 2U \cos^2(\Phi/2)\nu^2$$

$$s(i\omega_n) = \Gamma_0 / \sqrt{\omega^2_n + \Delta^2}, \ \Delta_\Phi = \Delta \cos \Phi/2$$

- Equilibrium symmetry (stationary point): $n_\sigma = n^*_\sigma$
- Atomic limit: $\lim_{\Delta \to \infty} \Delta s(\omega) = \Gamma_0$

0 and π phases – atomic limit at zero temperature I

- Only discrete gap (Andreev) states
  – no band states and no Kondo asymptotics
- Hartree-Fock solution - exact for integer fillings
- Spin-dependent propagators

$$G_\sigma(\omega) = \frac{\omega + \epsilon_U + \sigma h_U}{D_\sigma(\omega)}, \quad \mathcal{G}_\sigma(\omega) = -\frac{\Gamma_U \cos(\Phi/2)}{D_\sigma(\omega)}$$

$$\epsilon_U = \epsilon + \frac{U}{2}n,\ h_U = h + \frac{U}{2}m,\ \Gamma_U = \Gamma_0 - U\nu$$

- Reflection symmetry: $G_{-\sigma}(-\omega) = -G_\sigma(\omega)$, $\mathcal{G}_{-\sigma}(-\omega) = \mathcal{G}_\sigma(\omega)$
- Denominator ($n = n_\uparrow + n_\downarrow$, $m = n_\uparrow - n_\downarrow$)

$$D_\sigma(\omega) = (\omega + \sigma h_U)^2 - \epsilon_U^2 - \cos^2(\Phi/2)\,\Gamma_U^2$$

- Reflection symmetry (complex energy): $D_{-\sigma}(z) = D_\sigma(-z)$

0 and π phases – atomic limit at zero temperature II

- Four spin-dependent gap states

$$\omega_\sigma^\pm = -\sigma h_U \pm \sqrt{\epsilon_U^2 + \cos^2(\Phi/2)\,\Gamma_U^2}$$

- Symmetry: $\omega_\sigma^\pm = -\omega_{-\sigma}^\mp$
- 0-phase: low-magnetic (singlet) state ($\omega_\uparrow^- < 0,\ \ \omega_\uparrow^+ > 0$)
- Particle occupation (zero temperature)

$$n_\uparrow = n_\downarrow = \frac{\sqrt{\epsilon_U^2 + \cos^2(\Phi/2)\,\Gamma_U^2} - \epsilon_U}{2\sqrt{\epsilon_U^2 + \cos^2(\Phi/2)\,\Gamma_U^2}}$$

- Density of Cooper pairs (zero temperature)

$$\nu = \frac{\Gamma_U}{2\sqrt{\epsilon_U^2 + \cos^2(\Phi/2)\,\Gamma_U^2}}$$

0 and π phases – atomic limit at zero temperature III

- π-phase: high-magnetic (doublet) state ($\omega_\uparrow^- < 0, \ \omega_\uparrow^+ < 0$)
- Particle occupation (zero temperature)

$$n_\uparrow = m = \frac{\omega_\uparrow^- + \epsilon_U + h_U}{\omega_\uparrow^- - \omega_\uparrow^+} + \frac{\omega_\uparrow^+ + \epsilon_U + h_U}{\omega_\uparrow^+ - \omega_\uparrow^-} = 1$$

- Density of Cooper pairs (zero temperature)

$$\nu = \frac{\Gamma_U}{\omega_\uparrow^- - \omega_\uparrow^+} + \frac{\Gamma_U}{\omega_\uparrow^+ - \omega_\uparrow^-} = 0$$

- Critical interaction/field (exact for integer filling):

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

only for $\epsilon < 0$

Non-zero temperature I

- Particle density ($\Delta f_\sigma = f(-\omega_\sigma) - f(\omega_\sigma)$)

$$n = \frac{1}{2\sqrt{\mathcal{D}_U}}\left[2\sqrt{\mathcal{D}_U} - \left(\epsilon + \frac{U}{2}n\right)(\Delta f_\downarrow + \Delta f_\uparrow)\right]$$

- Magnetization

$$m = \frac{1}{2\sqrt{\mathcal{D}_U}}\left[\sqrt{\mathcal{D}_U}(\Delta f_\downarrow - \Delta f_\uparrow)\right] = f\left(\sqrt{\mathcal{D}_U} - \frac{U}{2}m\right) - f\left(\sqrt{\mathcal{D}_U} + \frac{U}{2}m\right)$$

- Magnetic instability (physical) due to gap states ($h = 0$)

$$k_B T_c < Uf(\omega_0)\left[1 - f(\omega_0)\right]$$

$$\omega_0 = \sqrt{\mathcal{D}_U} = \sqrt{\left(\epsilon + \frac{U}{2}n\right)^2 + (\Gamma_0 - U\nu)^2}$$

- Magnetic and non-magnetic states may coexist

Non-zero temperature II

- Cooper pairs

$$\nu = \frac{\Gamma_0 - U\nu}{2\sqrt{\mathcal{D}_U}} \left(\Delta f_\downarrow + \Delta f_\uparrow\right)$$

- Gap states

$$\omega_\sigma = -\sigma\left(h + \frac{U}{2}m\right) + \sqrt{\mathcal{D}_U}$$

- Crossing of gap states (continuous)

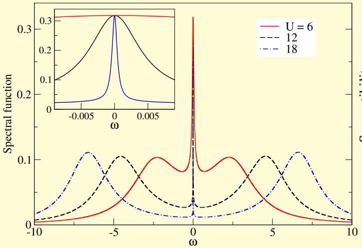
$$\left(h + \frac{U}{2}m\right)^2 = \left(\epsilon + \frac{U}{2}n\right)^2 + (\Gamma_0 - U\nu)^2$$

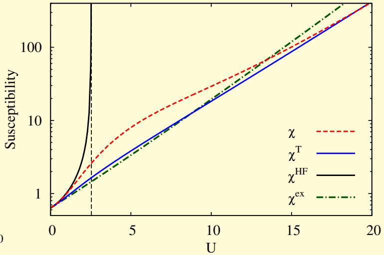
- Magnetic solution matches the non-magnetic one

Crossing of gap states - transition from non-magnetic to magnetic state

Quantum dot – metallic leads

- No gap & no discrete gap states
- Kondo strong-coupling regime
- Exponential Kondo scale in the spectral function & magnetic susceptibility (zero temperature)

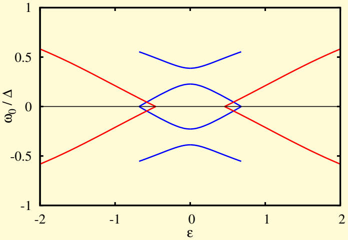




- HF – no Kondo regime, spurious magnetic state (insulator)

Spin-polarized HF solution – superconducting leads

- Transition to a magnetic state before ABS reach Fermi energy
- Discontinuous crossing of gap states

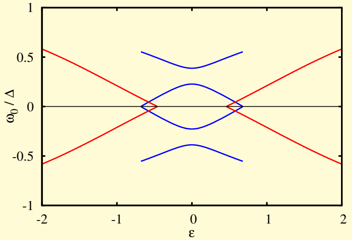


- π phase coincides with the magnetic state
- Magnetic transition spurious and due to continuous band states
- Magnetic solution does not match the non-magnetic one

Resolution: Suppression of the spurious magnetic transition

Spin-polarized HF solution – superconducting leads

- Transition to a magnetic state before ABS reach Fermi energy
- Discontinuous crossing of gap states

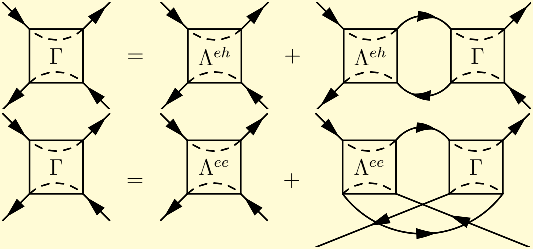


- π phase coincides with the magnetic state
- Magnetic transition spurious and due to continuous band states
- Magnetic solution does not match the non-magnetic one

Resolution: Suppression of the spurious magnetic transition

Suppressing spurious magnetic transition

- Two-particle self-consistency needed to suppress divergence in the magnetic susceptibility
- Simplest solution – parquet approach
  - Bethe-Salpeter equations in the singlet *eh* and *ee* channels



  - Parquet equation: $\Gamma = \Lambda^{eh} + \Lambda^{ee} - U$
- Consistency between 1P and 2P functions – ambiguous
- Schwinger-Dyson equation incompatible with the Ward identity

Reduced parquet equations – metallic leads

- Full parquet equations – do not reproduce the Kondo regime
- Reduction scheme
  - Decomposition of the full vertex: $\Gamma = \Lambda + K$
  - Irreducible vertex: $\Lambda = U - K\,[GG]_{ee}\,\Lambda$
  - Reducible vertex: $K = -\Lambda\,[GG]_{eh}\,(\Lambda + K)$
- One-particle self-energy
  - Thermodynamic self-energy (linearized WI & generalized HF)

$$\Sigma^{T} = \Lambda G^{T}$$

  - Spectral self-energy

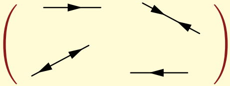
$$\Sigma^{sp} = \Sigma_{HF} - U\left[G^{T}G^{T}\right]_{eh}\Gamma G^{T}$$

  - G^{T} renormalized with thermodynamic self-energy
- Both self-energies share the same critical behavior (qualitatively)
- Simplification of frequency and momentum depedednce

Application to SC QD – Nambu spinors I

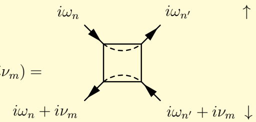
- 1P propagator

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

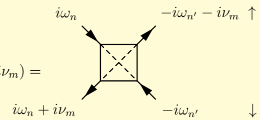


- Normal and anomalous vertices

$X(i\omega_n, i\omega_{n'}; i\nu_m) =$

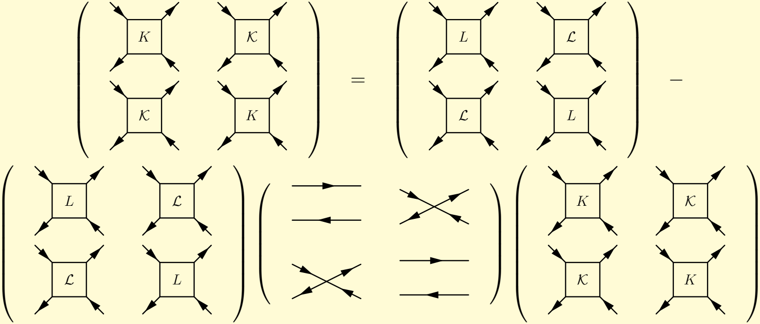


$\mathcal{K}(i\omega_n, i\omega_{n'}; i\nu_m) =$



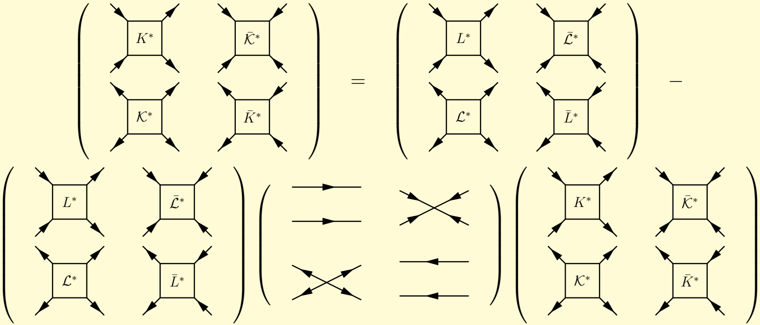
Application to SC QD – Nambu spinors II

- Bethe-Salpeter equation: *eh* channel



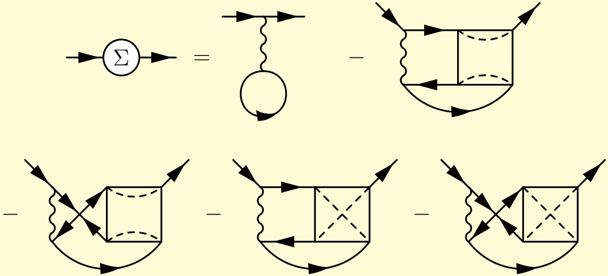
Application to SC QD – Nambu spinors III

- Bethe-Salpeter equation: ee channel



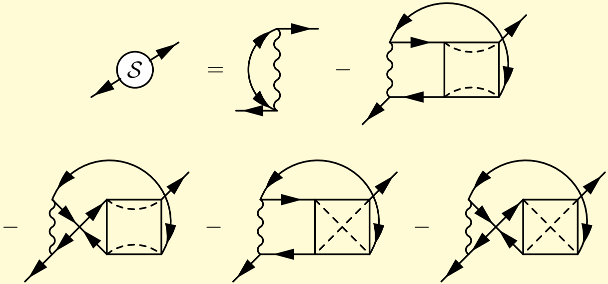
Application to SC QD – Nambu spinors IV

- Spectral self-energy (normal)



Application to SC QD – Nambu spinors V

- Spectral self-energy (anomalous)



Matrix reduced parquet equations

- Simplified frequency dependence: $\widehat{\Lambda}_{\uparrow\downarrow}(\omega), \widehat{K}_{\uparrow\downarrow}(\omega,\Omega)$
- Factorization of the reducible vertex: $\widehat{K}_{\uparrow\downarrow}(\omega,\Omega) = \widehat{\Lambda}_{\uparrow\downarrow}(\omega)\widehat{\kappa}_{\uparrow\downarrow}(\Omega)$
- Reduced algebraic matrix equations

$$\widehat{\Lambda}\left\{\widehat{1} + \widehat{\kappa}\left[\widehat{GG}\right]_{ee}\widehat{\Lambda}\right\} = \widehat{U}$$

$$\widehat{\kappa}\left\{\widehat{1} + \left[\widehat{GG}\right]_{eh}\widehat{\Lambda}\right\} = -\left[\widehat{GG}\right]_{eh}\widehat{\Lambda}$$

- Thermodynamic self-energy

$$\widehat{\Sigma}^{T} = \widehat{\Lambda}\widehat{G}$$

- Spectral self-energy (dynamical part)

$$\widehat{\Sigma}^{sp} = -\widehat{U}\widehat{\kappa}\widehat{G}$$

- Spin-polarized solution matches the spin-symmetric one

Conclusions I

Phases in SC quantum dot

1. Spin singlet – non-degenerate non-magnetic (0 phase)
2. Spin doublet – degenerate spin-polarized state (π phase)
3. Beyond $0-\pi$ transition – only in spin polarized theory
4. Magnetic field lifts spin degeneracy
5. Spin-polarized gap states with cross symmetry
6. Two solutions – low and high magnetic states (may coexist)
7. Cooper pairs suppressed in the high-magnetic state

Continuous ABS crossing only if the low-magnetic and high-magnetic solutions match

Conclusions II

Consistent diagrammatic many-body approach

1. Mean field (HFA) breaks down – the magnetic solution does not match the non-magnetic one
2. Spurious transition due to band states responsible
3. Remedy – two-particle self-consistency
4. Reduced parquet equations
   – restore Kondo regime
   – suppress spurious magnetic transition
5. Nambu formalism– spin-polarized matrix parquet equations

Full control of spin-polarized gap states necessary.
Reduction of the impact of band states important.