Entanglement Effect in a Two-channel Kondo System under Bias

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Two-reservoir Mesoscopic Kondo Systems

& extensions (From Quantum Dot to Cuprate)



A-B ring

Tunneling Current near V≈0



Both entangled singlets perform coherent co-tunneling

Two-reservoir Mesoscopic Kondo Systems

& extensions (From Quantum Dot to Cuprate)



dl/dV formula for a meso. Kondo system 🤿 🖡

Replace one flat dos by sample dos

Task: Understanding Tunneling Conductances



Two-reservoir Mesoscopic Kondo Systems

& extensions (From Quantum Dot to Cuprate)



dl/dV vs. V for a correlated system has in principle three coherent peaks



Revived zero-bias peak in BSCCO



Pan, Nature (2000)

Revived zero-bias peak in BSCCO



Pan, Nature (2000)







Tunneling Current near V≈0



Q2 is related to the experiments applying B field



Weakly & strongly coupled Kondo systems

$$T_{\rm K} = \frac{\sqrt{\Gamma U}}{2} e^{\pi \varepsilon_0 (\varepsilon_0 + U)/\Gamma U}$$

Dimensionless form: $2T_{K}/\Gamma = (U/\Gamma)^{1/2} e^{\pi \varepsilon_{0}(\varepsilon_{0} + U)/\Gamma U}$ Parameter of

coupling strength

QD Singleelectron Transistor Singlemolecule Transistor



Γ/U ~ 0.15 Kogan, PRL (2004)



Γ/U ~ 0.03 Liang, Nature (2002)

Weakly coupled QD Kondo systems



Strongly coupled QD Kondo system





Identifying two side peaks (\checkmark) is another big issue.





van der Wiel, Science (2000)

Identifying two side humps (\checkmark) is another big issue.

New Type: Different-phase Kondo Clouds



Two-channel Kondo system under bias





Keldysh + NCA

Keldysh Perturbation

Real Time RG

Q. Monte Carlo

Scattering-state NRG

They studied independent Kondo clouds sharing an impurity!!



R. Leturcq et al., Phys. Rev. Lett. 95, 126603 (2005)

Realistic mesoscopic Kondo systems:

Phase Coherence Region, Device Dimension, & Kondo Screening Length



In this circumstance, two Kondo clouds are no longer independent. They are coherently supposed: Entangled singlet

Dynamical Descriptions of L-R coherent superpositions

Kondo coupling strength of L-side:



2 and 3 deote exchange



L-R coherent superposition

Transport:



Singlet hopping L-R coherent

superposition

exchange L-R coherent superposition

Dynamical

Descriptions of L-R coherent superpositions

* L-R symmetric superposition



→ Kondo peak at equilibrium

* L-R antisymmetric superposition



At equilibrium, it vanishes. But under bias?

Dynamical

Descriptions of L-R coherent superpositions

* L-R symmetric superposition



* L-R antisymmetric superposition



Under bias, the second parts vanish due to unidirectional motion of the entangled singlet

→ Sym. and antisym. parts become same!!

Dynamical

Descriptions of L-R coherent superpositions

* L-R symmetric superposition







This is the effect of entanglement: The KEY for understanding non-equilibrium Kondo transport

Under bias, the second parts vanish due to unidirectional motion of the entangled singlet Strong E field

→ Sym. and antisym. parts become same!!

In summary,

Spectral function at equilibrium



(1 coherent peak + 2 Coul.-peaks)

Under bias, nonvanishing antisymm. superposition produces two coherent side peaks

Spectral function under bias



(3 coherent peaks + 2 Coul.-peaks)

Tunneling Conductance

Tunneling Current at T=0K:

$$I(V) = \frac{e}{\hbar} \sum_{\sigma} \int_{0}^{eV} d\omega \frac{\Gamma^{L}(\omega) \Gamma^{R}(\omega)}{\Gamma^{L}(\omega) + \Gamma^{R}(\omega)} \rho_{m\sigma}^{ss}(\omega) /_{\omega = eV}$$
Meir & Wingreen;
This formula is valid for $\Gamma^{L}(\omega) \propto \Gamma^{R}(\omega)$
Hershfield et al. (1992)

Tunneling Conductance at T=0K:

$$\frac{dI}{dV} = \frac{e^2}{\hbar} \left[\frac{\Gamma^{\rm L}(\omega) \Gamma^{\rm R}(\omega)}{\Gamma^{\rm L}(\omega) + \Gamma^{\rm R}(\omega)} \rho_m^{ss}(\omega) \right]_{\omega = eV} \qquad \rho_m^{ss}(\omega) \neq \rho_m^{eq}(\omega)$$

$$\rho_m^{ss}(\omega) : bias - independent$$

$$\rho_{m\sigma}^{ss}(\omega) = (-1/\pi) \operatorname{Im} G_{mm\sigma}^{+ss}(\omega)$$
 The quantity we obtain

Theoretical Procedure for

getting $G^{+}_{mm\sigma}(\omega)$

Resolvent Green's function

(1)
$$G^{\pm}_{mm\sigma}(\omega) = \langle u_{m\sigma} | (\omega \pm i\eta - \hat{H})^{-1} | u_{m\sigma} \rangle$$
 Schrödinger
(2) $G^{\pm}_{mm\sigma}(\omega) = \langle c_{m\sigma} | (\omega \pm i\eta - L)^{-1} | c_{m\sigma} \rangle$ Heisenberg $Lc_{m\sigma} = [H, c_{m\sigma}]$

 (1) → Construct Hamiltonian matrix in terms of a complete set of basis state vectors

(2) → Construct Liouvillian matrix in terms of a complete set of basis operators

Hamiltonian approach vs. Liouvillian approach

Nontrivial Toy Model

Two-site Hubbard Model:

$$\begin{array}{c} \bullet \\ \bullet \\ \mathbf{2} \\ H = -t \, \Sigma_{i \neq j,\sigma} c_{i\sigma}^{+} c_{j\sigma} + I \, \Sigma_{i} \, n_{i\uparrow} n_{i\downarrow} \end{array}$$

Hamiltonian Formulation:

Harris & Lange, PR 157, 295 (1967)

$$\begin{split} \rho_{1\sigma}(\omega) &= \sum_{n} \delta(\omega - E_{n}^{N+1} + E_{0}^{N}) \left| \left\langle \Psi_{0}^{N} \mid c_{1\sigma} \mid \Psi_{n}^{N+1} \right\rangle \right|^{2} - \sum_{n} \delta(\omega + E_{n}^{N-1} - E_{0}^{N}) \left| \left\langle \Psi_{0}^{N} \mid c_{1\sigma}^{+} \mid \Psi_{n}^{N-1} \right\rangle \right|^{2} \\ \mathfrak{o}^{\dagger}_{\{\uparrow\downarrow\}}(E) &= \frac{(1 - \lambda_{-})^{2}}{4(1 + \lambda_{-}^{2})} \,\delta(E - I + t + E_{-}) + \frac{(1 + \lambda_{-})^{2}}{4(1 + \lambda_{-}^{2})} \,\delta(E - I - t + E_{-}) \\ &+ \frac{(1 + \lambda_{-})^{2}}{4(1 + \lambda_{-}^{2})} \,\delta(E - E_{-} + t) + \frac{(1 - \lambda_{-})^{2}}{4(1 + \lambda_{-}^{2})} \,\delta(E - E_{-} - t) \qquad \lambda_{-} = \frac{1}{4t} \left(I - \sqrt{16t^{2} + I^{2}} \right) \end{split}$$



Two-reservoir Anderson impurity model

VS.

Hamiltonian formulation

Obtaining **basis state vectors** is hopeless

Liouvillian formulation

Obtaining **basis operators** is possible

(1) JH, J. Phys.: Condens, Matter vol. 23, 225601 (2011)

(2) JH, J. Phys.: Condens, Matter vol. 23, 275602 (2011)

Determining basis vectors:

$$\mathbf{i}\mathbf{G}_{\mathrm{mm}\uparrow}^{+} = \langle c_{m\uparrow} / (\mathbf{z}\mathbf{I} + \mathbf{i}\mathbf{L}_{I} + \mathbf{i}\mathbf{L}_{C})^{-1} / c_{m\uparrow} \rangle = \langle c_{m\uparrow} / (\hat{A} + \hat{B})^{-1} / c_{m\uparrow} \rangle$$
$$\hat{A} = (z\mathbf{I} + i\mathbf{L}_{I}), \quad \hat{B} = i\mathbf{L}_{C},$$

I: isolated part *c*: connecting part

Using operator identity
$$\frac{1}{\hat{A}+\hat{B}} = \frac{1}{\hat{A}} - \frac{1}{\hat{A}}\hat{B}\frac{1}{\hat{A}} + \frac{1}{\hat{A}}\hat{B}\frac{1}{\hat{A}}\hat{B}\frac{1}{\hat{A}}\hat{B}\frac{1}{\hat{A}} - \cdots,$$

$$iG_{mm\uparrow}^{+}(\omega) = \left\langle c_{m\uparrow} \middle| \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})+i\mathbf{L}_{C}} \middle| c_{m\uparrow} \right\rangle$$

$$= \left\langle c_{m\uparrow} \middle| \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})} \middle| c_{m\uparrow} \right\rangle \quad \left\langle \Leftarrow \frac{1}{\hat{A}} \right\rangle$$

$$- \left\langle c_{m\uparrow} \middle| \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})} i\mathbf{L}_{C} \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})} c_{m\uparrow} \right\rangle \quad \left\langle \Leftarrow -\frac{1}{\hat{A}} \hat{B} \frac{1}{\hat{A}} \right\rangle$$

$$+ \left\langle c_{m\uparrow} \middle| \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})} i\mathbf{L}_{C} \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})} i\mathbf{L}_{C} \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})} i\mathbf{L}_{C} \frac{1}{(z\mathbf{I}+i\mathbf{L}_{1})} \right\rangle$$

$$iG_{mm\uparrow}^{+}(\omega) = \left\langle c_{m\uparrow} \left| \hat{G}_{\mathrm{I}} \right| c_{m\uparrow} \right\rangle - \left\langle c_{m\uparrow} \left| \hat{G}_{\mathrm{I}} \right| \Phi_{m} \right\rangle + \left\langle \Phi_{m} \left| \hat{G} \right| \Phi_{m} \right\rangle \quad \text{where} \quad \begin{array}{c} \hat{G}_{\mathrm{I}} = (z\mathbf{I} + i\mathbf{L}_{\mathrm{I}})^{-1} \\ \Phi_{m} = i\mathbf{L}_{C}(z\mathbf{I} + i\mathbf{L}_{\mathrm{I}})^{-1} c_{m\uparrow} \end{array}$$

Expressing this in a matrix form yields

$$\mathbf{i}\mathbf{G}_{\mathbf{m}\mathbf{m}\uparrow}^{+}(\boldsymbol{\omega}) = (\langle \mathbf{c}_{\mathbf{m}\uparrow} \mid \langle \Phi_{\mathbf{m}} \mid) \begin{pmatrix} \hat{\mathbf{G}}_{\mathbf{I}} & -\hat{\mathbf{G}}_{\mathbf{I}} \\ \mathbf{0} & \hat{\mathbf{G}} \end{pmatrix} \begin{pmatrix} |\mathbf{c}_{\mathbf{m}\uparrow}\rangle \\ |\Phi_{\mathbf{m}}\rangle \end{pmatrix}$$

Similarity transformation using $U = \begin{pmatrix} 1 & -\frac{\widehat{G}_I}{\widehat{G} - \widehat{G}_I} \\ 0 & 1 \end{pmatrix}$

diagonalizes
$$\hat{G}$$
: $\hat{G}_d = \bigcup \hat{G} \bigcup^{-1} = \begin{pmatrix} \hat{G}_I & 0 \\ 0 & \hat{G} \end{pmatrix}$

Then, we obtain

$$iG_{mm\uparrow}^{\pm}(\omega) = (\langle \widetilde{c}_{m\uparrow} \mid \langle \Phi_m \mid) \begin{pmatrix} \hat{G}_I & 0 \\ 0 & \hat{G} \end{pmatrix} \begin{pmatrix} | \widetilde{c}_{m\uparrow} \rangle \\ | \Phi_m \rangle \end{pmatrix}$$

where

$$\widetilde{c}_{m\uparrow} = c_{m\uparrow} + \frac{z\mathbf{I} + i\mathbf{L}}{i\mathbf{L}_{C}}\Phi_{m}, \quad \Phi_{m} = i\mathbf{L}_{C}(z\mathbf{I} + i\mathbf{L}_{I})^{-1}c_{m\uparrow}$$

A complete set of linearly independent basis vectors is given by collecting the linearly independent components of the vector/ $\tilde{c}_{m\uparrow}$ >.

Complete Set of basis vectors for $c_{m\uparrow}(t)$:



number of hopping of \downarrow -spin electron

Neglect multiple hoppings: Effect of entanglement under bias

number of hopping of \downarrow -spin electron

APPROXIMATION: Neglect in Kondo regime & self-energy



number of hopping of **-spin electron

Orthonormalized basis vectors:

$$C_{m\uparrow}, \frac{(\delta j_{m\downarrow}^{-L,R})c_{m\uparrow}}{\sqrt{\langle (\delta j_{m\downarrow}^{-L,R})^2 \rangle}}, \frac{(\delta j_{m\downarrow}^{+L,R})c_{m\uparrow}}{\sqrt{\langle (\delta j_{m\downarrow}^{+L,R})^2 \rangle}} \Rightarrow 5 \text{ peaks}$$

$$c_{k\uparrow}^{L,R}, \frac{(\delta n_{m\downarrow})c_{k\uparrow}^{L,R}}{\sqrt{\langle (\delta n_{m\downarrow})^2 \rangle}}, k = 1, 2, \cdots, \infty$$

 peak widening

Constructing Liouvillian matrix: $\mathbf{M} = z \mathbf{I} + i \mathbf{L}$



Constructing Liouvillian matrix: $\mathbf{M} = z \mathbf{I} + i \mathbf{L}$





Constructing Liouvillian matrix: $\mathbf{M} = z \mathbf{I} + i \mathbf{L}$



Matrix Reduction: Löwdin's Partitioning technique

P.O. Löwdin, J. Math. Phys. Vol. 3, 969 (1962)

Matrix equation:

$$\begin{pmatrix} M_{LL} & M_{mL} & 0 \\ M_{Lm} & M_{mm} & M_{Rm} \\ 0 & M_{mR} & M_{RR} \end{pmatrix} \begin{pmatrix} C_k^L \\ C_m \\ C_m^R \\ C_k^R \end{pmatrix} = 0 \qquad k = 0, 1, 2, \dots, \infty \\ C_m = (C_1, C_2, C_3, C_4, C_5)^T$$

$$(M_{mm} - M_{Lm}M_{LL}^{-1}M_{mL} - M_{Rm}M_{RR}^{-1}M_{mR})C_{m} \equiv M_{r}C_{m}$$

$$M_{r} = M_{mm} - M_{Lm}M_{LL}^{-1}M_{mL} - M_{Rm}M_{RR}^{-1}M_{mR}$$

$$iself-energy$$

$$iself-energy$$

$$iself-energy$$

$$iG_{mm}^{+}(\omega) = (\mathbf{M}_{\mathbf{r}}^{-1})_{33} \quad \rho_{m}^{ss}(\omega) = (1/\pi)\operatorname{Re}(\mathbf{M}_{\mathbf{r}}^{-1})_{33}$$

Reservoir degrees of freedom are transformed into **self-energy** by matrix reduction process

 $\rho_{\rm m}^{\rm ss}(\omega) = (1/\pi) \, {\rm Re} \left({\rm M}_{\rm r}^{-1} \right)_{33}$

$$\mathbf{M}_{\mathbf{r}} = \begin{bmatrix} -i\omega & -\gamma_{LL} & U_{j^{-}}^{L} & \gamma_{LR} & \gamma_{j} \\ \gamma_{LL} & -i\omega & U_{j^{+}}^{L} & \gamma_{j} & \gamma_{LR} \\ -U_{j^{-}}^{L^{*}} & -U_{j^{+}}^{L^{*}} & -i\omega & -U_{j^{+}}^{R^{*}} & -U_{j^{-}}^{R^{*}} \\ -\gamma_{LR} & -\gamma_{j} & U_{j^{+}}^{R} & -i\omega & \gamma_{RR} \\ -\gamma_{j} & -\gamma_{LR} & U_{j^{-}}^{R} & -\gamma_{RR} & -i\omega \end{bmatrix}$$

with additional $i\beta_{ij}[\Sigma^{L}_{0}(\omega) + \Sigma^{R}_{0}(\omega)]$ except U-terms





$$\rho_{\rm m}^{\rm ss}(\omega) = (1/\pi) \, {\rm Re} \left({\rm M}_{\rm r}^{-1} \right)_{33}$$

$$\mathbf{M}_{\mathbf{r}} = \begin{bmatrix} -i\omega & -\gamma_{LL} & U_{j^{-}}^{L} & \gamma_{LR} & \gamma_{j} \\ \gamma_{LL} & -i\omega & U_{j^{+}}^{L} & \gamma_{j} & \gamma_{LR} \\ -U_{j^{-}}^{L^{*}} & -U_{j^{+}}^{L^{*}} & -i\omega & -U_{j^{+}}^{R^{*}} & -U_{j^{-}}^{R^{*}} \\ -\gamma_{LR} & -\gamma_{j} & U_{j^{+}}^{R} & -i\omega & \gamma_{RR} \\ -\gamma_{j} & -\gamma_{LR} & U_{j^{-}}^{R} & -\gamma_{RR} & -i\omega \end{bmatrix}$$

with additional $i\beta_{ij}[\Sigma^{L}_{0}(\omega)+\Sigma^{R}_{0}(\omega)]$ except U-terms

* Conventional Kondo System: (Single Reservoir)



Single Reservoir:

$$\mathbf{M}_{r} = \begin{bmatrix} -i\omega & -\gamma_{LL} & U_{j^{-}}^{L} \\ \gamma_{LL} & -i\omega & U_{j^{+}}^{L} \\ -U_{j^{-}}^{L*} & -U_{j^{+}}^{L*} & -i\omega \end{bmatrix}$$

$$U_{j^{\pm}}^{L} = U/2\sqrt{2}$$

with additional self-energy terms $i\beta_{ij}\Sigma^{L}_{0}(\omega)$ except U-elements

$$\gamma_{LL} = \langle \sum_{k} V_{km}^* c_{k\uparrow} c_{m\uparrow}^+ j_{m\downarrow}^{-L} j_{m\downarrow}^{+L} \rangle$$

$$\gamma_{LL} = (U/2) \sqrt{\frac{Z_s}{1 - Z_s}}$$

$$Z_{S} = Z_{S}^{BA} = (4/\pi)\sqrt{U/\Gamma} e^{-\frac{\pi U}{4\Gamma}}$$

Our APPROXIMATION is reasonable!!



Information from Liouvillian Matrix: *i*L



Information from Liouvillian Matrix: *i*L



Reproducing dl/dV line shapes (some of my results)



Adsorbed magnetized atom on an insulating layer covering metallic substrate



γ_{LL}	γ_{RR}	$\gamma_{j,LR}$	$\mathrm{Re}U_{j}^{L,R}$	${ m Re}U_{j^+}^L$	${\rm Re}U^R_{j^+}$	$\mathrm{Im}U^{L,R}_{j^{\pm}}$
0.8	0.7	0.43	2.8	7.0	1.62	0

Otte, N. Phys. 2008







0.4

0.6

 $G(2e^2/h)$

0.8

0.0

1.0

0.04

0.0

0.2

Sarkozy, PRB (2009)



Conclusions

- (1) We study mesoscopic Kondo systems and find that the entanglement effect (coherent superposition between two Kondo clouds) is critical to explain the experimental line shapes of tunneling conductance.
- (2) We show that antisymmetric superposition does not vanish under bias and gives two coherent side peaks.
- (3) We recover the bias-dependent Kondo peak splitting by treating a system having independent Kondo clouds.
- (4) We reproduce the experimental dl/dV line shapes obtained for various mesoscopic Kondo systems.



(5) More things are left to fully appreciate the entangled singlet dynamics imbedded in mesoscopic Kondo systems and strongly correlated samples.