Tunneling conductance in strongly correlated materials

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with Jongbae Hong

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1. Introduction and motivation

2. Theory for localized tunneling site

3. Extension to extended interfaces: Application to graphene
Introduction and motivation
Non-equilibrium Kondo systems

Quantum dot SET:

van der Wiel et al., Science 2000.

Quantum point contact:


Single molecule transistor:


STM:

Picture credit: L. Grill
Non-equilibrium Kondo systems

Quantum point contact:

Quantum dot SET:

van der Wiel et al., Science 2000.


Iqbal et al., Nature 2013.

Single molecule transistor:


STM:


Two sources of difficulty in these problems:
- Strong correlations,
- Non-equilibrium dynamics.

Strong correlations $\Rightarrow$ new collective behavior (e.g. Kondo effect).

Nonequilibrium dynamics $\Rightarrow$ no simple intuition.

Need new conceptual and theoretical tools!

We introduce a theory which deals with some of this complexity for a wide range of systems.
- Includes entanglement between source and drain!
- Captures side peaks!
Theoretical technique
Consider single localized level between two "leads".

- e.g. Quantum point contact,
- e.g. STM.

Can use the two reservoir Anderson model to study this:

\[
H = \sum_{\alpha \in \{L,R\}} \left( \epsilon_{k}^{\alpha} - \mu^{\alpha} \right) c_{k\sigma}^{\alpha \dagger} c_{k\sigma}^{\alpha} + \sum_{\sigma} \varepsilon_{d} d_{\sigma}^{\dagger} d_{\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\alpha \in \{L,R\}} \tilde{V} \left( d_{\sigma}^{\dagger} c_{k\sigma}^{\alpha} + c_{k\sigma}^{\alpha \dagger} d_{\sigma} \right)
\]

We want to calculate the Green's function

\[
G_{dd\uparrow}^{\dagger}(t) = -i \theta(t) \langle \{ d_{\uparrow}(t), d_{\uparrow}^{\dagger}(0) \} \rangle.
\]
Calculation of $dI/dV$

- Laplace transform of the Green’s function is:

$$iG_{dd\uparrow}^+(z) = \langle d\uparrow| (z\mathbf{I} + i\mathbf{L})^{-1} |d\uparrow\rangle$$

with $z = -i\omega + \eta$.

- Local DOS at mediating site:

$$\rho_{d\uparrow}(\omega) = -\frac{1}{\pi} \text{Im} G_{dd\uparrow}^+(\omega).$$

- Tunneling conductance:

$$\frac{dI}{dV} = \frac{e}{\hbar} \frac{\Gamma^L \Gamma^R}{\Gamma^L + \Gamma^R} \rho_{d\uparrow}(\omega) \bigg|_{\hbar\omega = eV}$$
Outline of method

Expand the operator

\[ d_{\uparrow}(t) = \sum_{i=1}^{\infty} A_i(t) \hat{e}_i \]

where the set \( \{ \hat{e}_j | j = 1, 2, \ldots, \infty \} \) is a complete basis for the Liouville space.

We specify \( \hat{e}_1 = d_{\uparrow}(0) \).

Find a representation for the basis vectors.

Apply matrix reduction techniques.

Find a 5 × 5 matrix representation of the Liouville operator \( \mathbf{L} \).

• $H_I$ represents isolated part,
  $H_C$ represents connected (i.e. hybridization) part.

• Definition of Liouville operator:
  \[
iL O = \frac{d}{dt} O = i [H, O]
  \]

• Remember:
  \[
  G_{dd\uparrow}^+(z) = \langle d\uparrow | (zI + iL_I + iL_C)^{-1} |d\uparrow \rangle.
  \]

• Apply identity
  \[
  (\hat{p} + \hat{q})^{-1} = \hat{p}^{-1} - \hat{p}^{-1} \hat{q} (\hat{p} + \hat{q})^{-1}
  \]
  with
  \[
p = zI + iL_I, \quad \text{and} \quad q = iL_C
  \]
  to $G_{dd\uparrow}^+(z)$ to get basis states
  \[
  |\Phi_d\rangle = |iL_C \hat{G}_I d\uparrow \rangle \quad \text{and} \quad |\tilde{d}\uparrow \rangle = |d\uparrow \rangle + |L_C^{-1} (-izI + L) \Phi_d \rangle
  \]
Hopping operators:

\[ j_{d\downarrow}^- = i \sum_k \left( V_{kd\downarrow} d_k^\dagger c_{k\downarrow} - V_{kd\downarrow}^* c_{k\downarrow}^\dagger d_{k\downarrow} \right), \quad j_{d\downarrow}^+ = \sum_k \left( V_{kd\downarrow} d_k^\dagger c_{k\downarrow} + V_{kd\downarrow}^* c_{k\downarrow}^\dagger d_{k\downarrow} \right). \]

where \( k = 1, 2, \ldots, \infty \) are the states in the metallic leads.

The linearly independent components of \( |\Phi_d\rangle \) are:

\[ c_{k\uparrow}, \quad n_{d\downarrow} c_{k\uparrow}, \quad \text{and} \quad j_{d\downarrow}^- d_{\uparrow}. \]

The linearly independent components of \( |\tilde{d}_{\uparrow}\rangle \) break into two sets:

\[ d_{\uparrow}, \quad n_{d\downarrow} d_{\uparrow}, \quad j_{d\downarrow}^- d_{\uparrow}, \quad j_{d\downarrow}^+ d_{\uparrow}, \quad (L_C^n j_{d\downarrow}^\mp) d_{\uparrow}, \quad (L_C^n j_{d\downarrow}^- n_{d\downarrow}) d_{\uparrow}, \]

and

\[ c_{k\uparrow}, \quad n_{d\downarrow} c_{k\uparrow}, \quad j_{d\downarrow}^- c_{k\uparrow}, \quad j_{d\downarrow}^+ c_{k\uparrow}, \quad (L_C^n j_{d\downarrow}^\mp) c_{k\uparrow}. \]

These operators give all ways of annihilating an up-spin in level \( d \) at time \( t \), so span the Liouville space of \( d_{\uparrow}(t) \).

Infinitely many vectors: Need to distinguish physically important ones.
Up until this point, mathematics are exact.

**Full basis:**

\[
d_{\uparrow}, \ n_{d\downarrow}d_{\uparrow}, \ j_{d\downarrow}d_{\uparrow}, \ j_{d\downarrow}^{\uparrow}d_{\uparrow}, \ (L_{C}^{n}j_{d\downarrow}^{\mp})d_{\uparrow}, \ (L_{C}^{n}j_{d\downarrow}^{\mp}n_{d\downarrow})d_{\uparrow}, \\
\ c_{k\uparrow}, \ n_{d\downarrow}c_{k\uparrow}, \ j_{d\downarrow}^{\mp}c_{k\uparrow}, \ j_{d\downarrow}^{\mp}c_{k\uparrow}, \ (L_{C}^{n}j_{d\downarrow}^{\mp})c_{k\uparrow}.
\]

Processes with \(n_{d\downarrow}^{r}d_{\uparrow} = n_{d\downarrow}d_{\uparrow}\) are higher order of \(U\), so are excluded on energetic grounds.

\((L_{C}^{n}j_{d\downarrow}^{\mp})\) is \(n\) trips of a down-spin between MS and reservoir without contact with an up-spin at the MS. Rare process, so ignored.

Contribution from \(j_{d\downarrow}^{\mp}c_{k\uparrow} \ll n_{d\downarrow}c_{k\uparrow}\) so ignored.

Operators in black have to be orthogonalised and normalised, but are essentially the basis operators we keep.
### Mathematical details

<table>
<thead>
<tr>
<th>$c_{kT}^L$</th>
<th>$\delta n_{dL} c_{kT}^L$</th>
<th>$\delta j_{dL}^L d_t$</th>
<th>$\delta j_{dL}^L d_\uparrow$</th>
<th>$d_\uparrow$</th>
<th>$\delta j_{dL}^R d_\uparrow$</th>
<th>$\delta j_{dL}^R d_t$</th>
<th>$\delta n_{dL} c_{kT}^R$</th>
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| $\begin{pmatrix} -\xi_d V_{1d} & -\xi_d V_{1d} \\ -\xi_d V_{1d} & -\xi_d V_{1d} \end{pmatrix}$ | $\begin{pmatrix} U_{jL}^L & U_{jL}^L \\ U_{jL}^L & U_{jL}^L \end{pmatrix}$ | $\begin{pmatrix} U_{jL}^L & U_{jL}^L \\ U_{jL}^L & U_{jL}^L \end{pmatrix}$ | $0$ | $0$ | $0$ | $0$ | $0$ | $0$ |
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$(3 \times 3)$

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| $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ | $-\xi_d V_{1d}$ |

$(3 \times 3)$

| $\begin{pmatrix} -\xi_d V_{1d} & -\xi_d V_{1d} \\ -\xi_d V_{1d} & -\xi_d V_{1d} \end{pmatrix}$ | $\begin{pmatrix} U_{jR}^L & U_{jR}^L \\ U_{jR}^L & U_{jR}^L \end{pmatrix}$ | $\begin{pmatrix} U_{jR}^L & U_{jR}^L \\ U_{jR}^L & U_{jR}^L \end{pmatrix}$ | $0$ | $0$ | $0$ | $0$ | $0$ | $0$ |
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$(5 \times 5)$

| $\begin{pmatrix} z + i\epsilon_1 & 0 \\ 0 & \ddots \\ 0 & 0 & z + i\epsilon_\infty \end{pmatrix}$ | $0$ | $0$ | $0$ | $0$ | $0$ | $0$ | $0$ | $0$ |

$(3 \times 3)$
Mathematical details

- **Matrix reduction**: Reservoir degrees of freedom are transformed into self-energy.
- **Matrix equation**:

\[
\begin{pmatrix}
M_{LL} & M_{dL} & 0 \\
M_{Ld} & M_{dd} & M_{Rd} \\
0 & M_{dR} & M_{RR}
\end{pmatrix}
\begin{pmatrix}
C^L_k \\
C^d_d \\
C^R_k
\end{pmatrix} = 0
\]  

(1)

- **Reduction**:

\[
(M_{dd} - M_{Ld}M^{-1}_{LL}M_{dL} - M_{Rd}M^{-1}_{RR}M_{dR}) \equiv M_r C_m
\]

- Where \(M_r\) is a 5 × 5 matrix.
- Green’s function for MS then

\[
iG_{dd\uparrow}^+(z) = (M_r^{-1})_{33}
\]
Liouville operator

- Liouville operator contains the coherent dynamics.
- Third order in hybridization.
- It is:

\[
i L = \begin{pmatrix}
0 & \gamma_{LL} & -U_{j-}^L & \gamma_{SR}^L & \gamma_{AR}^L \\
-\gamma_{LL} & 0 & -U_{j+}^L & \gamma_{AR}^L & \gamma_{SR}^L \\
U_{j-}^L & U_{j+}^L & 0 & U_{j-}^R & U_{j+}^R \\
-\gamma_{SR}^L & -\gamma_{AR}^L & -U_{j+}^R & 0 & -\gamma_{RR}^L \\
-\gamma_{AR}^L & -\gamma_{SR}^L & -U_{j-}^R & \gamma_{RR}^L & 0 \\
\end{pmatrix} + i \Sigma
\]

- $\Sigma$ is a self-energy which doesn’t affect the dynamics.
Liouville operator contains the coherent dynamics.

Third order in hybridization.

It is:

\[
iL = \begin{pmatrix}
0 & \gamma_{LL} & -U_{j-}^L & \gamma_{S}^L & \gamma_{A}^L \\
-\gamma_{LL} & 0 & -U_{j+}^L & \gamma_{A}^L & \gamma_{S}^L \\
U_{j-}^L & U_{j+}^L & 0 & U_{j+}^R & U_{j-}^R \\
-\gamma_{LR} & -\gamma_{A}^L & -U_{j-}^R & 0 & -\gamma_{RR} \\
-\gamma_{LR} & -\gamma_{S}^L & -U_{j-}^R & \gamma_{RR} & 0
\end{pmatrix} + i\Sigma
\]

\(\Sigma\) is a self-energy which doesn’t affect the dynamics.

The \(U\) elements are hybridization of the leads with the MS.
Liouville operator contains the coherent dynamics.

Third order in hybridization.

It is:

\[
iL = \begin{pmatrix}
0 & \gamma_{LL} & -U_{j-}^L & \gamma_{LR} & \gamma_{LR} \\
-\gamma_{LL} & 0 & -U_{j+}^L & \gamma_{LR} & \gamma_{LR} \\
U_{j-}^L & U_{j+}^L & 0 & U_{j+}^R & U_{j+}^R \\
-\gamma_{LR} & -\gamma_{LR} & -U_{j+}^R & 0 & -\gamma_{RR} \\
-\gamma_{LR} & -\gamma_{LR} & -U_{j+}^R & \gamma_{RR} & 0
\end{pmatrix} + i\Sigma
\]

\(\Sigma\) is a self-energy which doesn’t affect the dynamics.

The \(U\) elements are hybridization of the leads with the MS.

The \(\gamma_{LL}\) and \(\gamma_{RR}\) give the Kondo coupling.
Kondo coupling

- Kondo-like elements are $\gamma^{LL}$ and $\gamma^{RR}$ are sum of these exchange and singlet hopping processes.

Exchange process:

Left lead Right lead
Kondo coupling

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**Exchange process:**

![Diagram showing exchange process](image)
Kondo-like elements are $\gamma_{LL}$ and $\gamma_{RR}$ are sum of these exchange and singlet hopping processes.

**Exchange process:**

**Singlet hop process:**
Kondo-like elements are $\gamma^{LL}$ and $\gamma^{RR}$ are sum of these exchange and singlet hopping processes.
Kondo-like elements are $\gamma_{LL}^L$ and $\gamma_{RR}^R$ are sum of these exchange and singlet hopping processes.

**Exchange process:**

- **Left lead**
- **Right lead**

**Singlet hop process:**

- **Left lead**
- **Right lead**
Kondo-like elements are $\gamma^{LL}$ and $\gamma^{RR}$ are sum of these exchange and singlet hopping processes.

- These processes do not carry current.
Liouville operator contains the coherent dynamics.

**Third order** in hybridization.

It is:

\[
i_L = \begin{pmatrix}
0 & \gamma_{LL} & -U_{j-}^L & \gamma_{LR}^S & \gamma_{LR}^A \\
-\gamma_{LL}^L & 0 & -U_{j+}^L & \gamma_{LR}^S & \gamma_{LR}^A \\
U_{j-}^L & U_{j+}^L & 0 & \gamma_A^L & \gamma_{LR}^S \\
-\gamma_{LR}^S & -\gamma_{LR}^S & -U_{j+}^R & 0 & \gamma_{LR}^S \\
-\gamma_{LR}^A & -\gamma_{LR}^A & -U_{j-}^R & \gamma_{LR}^S & 0 \\
\end{pmatrix} + i\Sigma
\]

**\(\Sigma\)** is a self-energy which doesn’t affect the dynamics.

The **U** elements are hybridization of the leads with the MS.

The \(\gamma_{LL}^L\) and \(\gamma_{RR}^R\) give the Kondo coupling.

The \(\gamma_{LR}^A\) and \(\gamma_{LR}^S\) give the coherent current-generating terms.
Singlet hop: $\gamma_1$

Left lead  

\[ \begin{array}{c}
\downarrow \\
\downarrow \\
\downarrow \\
\downarrow \\
\end{array} \quad \begin{array}{c}
\downarrow \\
\downarrow \\
\downarrow \\
\downarrow \\
\end{array} \]

Right lead  

\[ \begin{array}{c}
\uparrow \\
\uparrow \\
\uparrow \\
\uparrow \\
\end{array} \quad \begin{array}{c}
\downarrow \\
\downarrow \\
\downarrow \\
\downarrow \\
\end{array} \]

Current-generating elements are:

\[ \gamma_{LR} \rightarrow = \gamma_1 + \gamma_2 \]

\[ \gamma_{LR} \uparrow = \gamma_1 - \gamma_2 \]

With no bias, $\gamma_1 = \gamma_2$ so $\gamma_{LR} \uparrow = 0$.

Only $\gamma_{LR} \rightarrow$ finite, which gives zero bias peak.

With left-to-right bias, $\gamma_2$ suppressed.

Implies $\gamma_{LR} \rightarrow \approx \gamma_{LR} \uparrow \neq 0$.

It is $\gamma_{LR} \uparrow$ which generates side peaks.
Singlet hop: $\gamma_1$

Current-generating elements are:

$$\gamma_{LR}^S = \gamma_1 + \gamma_2$$

$$\gamma_{LR}^A = \gamma_1 - \gamma_2$$

With no bias, $\gamma_1 = \gamma_2$ so $\gamma_{LR}^A = 0$.

Only $\gamma_{LR}^S$ finite, which gives zero bias peak.

With left-to-right bias, $\gamma_2$ suppressed.

Implies $\gamma_{LR}^S \approx \gamma_{LR}^A \neq 0$.

It is $\gamma_{LR}^A$ which generates side peaks.
Singlet hop: $\gamma_1$

Left lead

Right lead

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Singlet hop: $\gamma_1$

Left lead

Right lead

Current-generating elements are:

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Singlet hop: $\gamma_1$

Left lead

Right lead

Singlet hop: $\gamma_2$

Left lead

Right lead

Current-generating elements are:

$$\gamma_{LR} = \gamma_1 + \gamma_2$$

$$\gamma_{LR}^A = \gamma_1 - \gamma_2$$

With no bias, $\gamma_1 = \gamma_2$ so $\gamma_{LR}^A = 0$.

Only $\gamma_{LR}^S$ finite, which gives zero bias peak.

With left-to-right bias, $\gamma_2$ suppressed.

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It is $\gamma_{LR}^A$ which generates side peaks.

D.S.L. Abergel
Singlet hop: $\gamma_1$

- **Current-generating elements are:**
  \[
  \gamma_{LR}^S = \gamma_1 + \gamma_2 \\
  \gamma_{LR}^A = \gamma_1 - \gamma_2
  \]

- **With no bias, $\gamma_1 = \gamma_2$ so $\gamma_{LR}^A = 0$. Only $\gamma_{LR}^S$ finite, which gives zero bias peak.**

Singlet hop: $\gamma_2$
Singlet hop: $\gamma_1$

Left lead

Right lead

- Current-generating elements are:
  \[
  \gamma_{LR}^S = \gamma_1 + \gamma_2 \\
  \gamma_{LR}^A = \gamma_1 - \gamma_2
  \]

- With no bias, $\gamma_1 = \gamma_2$ so $\gamma_{LR}^A = 0$.
  Only $\gamma_{LR}^S$ finite, which gives zero bias peak.

Singlet hop: $\gamma_2$

Left lead

Right lead

- With left-to-right bias, $\gamma_2$ suppressed.
- Implies $\gamma_{LR}^S \approx \gamma_{LR}^A \neq 0$.
- It is $\gamma_{LR}^A$ which generates side peaks.
Spectral function $\text{Im}G_{dd}^{+}(\omega)$.

Finite-bias tunneling via resonant levels

Quantum point contact:


STM:


- Red line: Experimental data.
- Blue line: Theoretical prediction.
Application to graphene
“Strongly correlated” $\equiv$ non-Fermi liquid ground state.

In the case of multilayer graphene, probably an antiferromagnetic order.

- Monolayer: No.

We apply this new theory for tunneling conductance to bilayer and trilayer graphene.
Is graphene a strongly correlated material?

“Strongly correlated” ≡ non-Fermi liquid ground state.

In the case of multilayer graphene, probably an antiferromagnetic order.

- Monolayer: No.
- Bilayer: Big debate.
Is graphene a strongly correlated material?

“Strongly correlated” ≡ non-Fermi liquid ground state.

In the case of multilayer graphene, probably an antiferromagnetic order.

- Monolayer: No.
- Bilayer: Big debate.
- ABC-stacked trilayer: Probably.
- ABA-stacked trilayer: No.
Is graphene a strongly correlated material?

- We apply this new theory for tunneling conductance to bilayer and trilayer graphene.

  “Strongly correlated” \equiv non-Fermi liquid ground state.

In the case of multilayer graphene, probably an antiferromagnetic order.

- Monolayer: No.

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- ABC-stacked trilayer: Probably.

- ABA-stacked trilayer: No.
Two-terminal conductance $dI/dV$ usually interpreted as effective single particle DOS.

Number of mediating sites $N_c$. 

In steady state, electron in $\Rightarrow$ electron out. $\Rightarrow$ i.e. only tunneling into graphene affects conductance.

Frequency-dependent DOS $\Gamma_R(\omega)$ in "right lead".

Tunneling conductance becomes:

$$
\frac{dI}{dV} = N_c e \hbar \Gamma_L \Gamma_R(\omega) \Gamma_L + \Gamma_R(\omega) \rho d \uparrow(\omega) \bigg|\bigg| \hbar \omega = eV
$$
Systems with extended interfaces

- Two-terminal conductance $dI/dV$ usually interpreted as effective single particle DOS.
- Number of mediating sites $N_c$.

In steady state, electron in $\Rightarrow$ electron out.

- I.e. only tunneling into graphene affects conductance.
- Frequency-dependent DOS $\Gamma^R(\omega)$ in “right lead”.
- Tunneling conductance becomes:

$$\frac{dI}{dV} = N_c \frac{e}{\hbar} \frac{\Gamma^L \Gamma^R(\omega)}{\Gamma^L + \Gamma^R(\omega)} \rho_{d\uparrow}(\omega) \bigg|_{\hbar\omega = eV}$$
- ABC-stacked trilayer graphene.

\[ \text{Gap size } \approx 20 \text{ meV} \]

\[ \Delta_0 = 40 \text{ meV} \]

\[ \phi_0 = 0.012 \Delta_0 \]

ABC-stacked trilayer graphene.

\[ \Delta_0 = 40 \text{ meV} \]

\[ \phi_0 = 0.012 \Delta_0 \]

Gap size \( \approx 20 \text{ meV} \).

Results

- ABC-stacked trilayer graphene.
  
  \[ \Delta_0 = 40 \text{ meV} \]
  \[ \phi_0 = 0.012 \Delta_0 \]

- Bilayer graphene

\[ \Delta_0 \approx 1 \text{ meV} \]


- Gap size \( \approx 20 \text{ meV} \).
- Gap size \( \approx 1 \text{ meV} \).
Summary

- Tunneling current in strongly correlated systems qualitatively explained through analysis of most important physical processes.

- Side peaks understood by inter-lead coherence.

- Extension of theory to extended systems allows for reinterpretation of tunneling conductance in graphene systems.

