Quantum Impurities Out of Equilibrium



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Non-equilibrium and Strong Correlations

Nonequilibrium - poorly understood



- No unifying theory such as Boltzmann's statistical mechanics
- Many of our standard physical ideas and concepts are not applicable (Scaling? RG? Universality?)
- Non-equilibrium systems are all different- it is unclear what if anything they all have in common.

Strongly correlated -in general- poorly understood.

- Perturbative approaches fail
- New degrees of freedom emerge
- New collective Behavior

Quantum Impurities - Theory and Experiment *Interplay : non-equilibrium and strong correlations*

Outline

Non-equilibrium and Steady State (Quantum impurities)

- Time dependent description (Keldysh)
- The steady State open systems
- Time independent description

Scattering theory, Lippmann-Schwinger equation

- Scattering eigenstates and Non-equilibrium Steady State
- Constructing Scattering States

-Traditional Bethe-Ansatz : closed systems - inadequate

- Equilibrium, Thermodynamics
- Scattering Bethe-Ansatz : open systems new approach (SBA)
 - Non-equilibrium Steady States
 - Scattering states of electrons off magnetic impurities
- Non-equilibrium currents
- Dissipation and Entropy Production

Quantum Impurities out-of-Equilibrium

The quantum impurity (as seen by a theorist)



In the Coulomb blockade regime:

$$H_{qdot} = \sum_{i=1,2} \sum_{\vec{k}a} \epsilon_k c^{\dagger}_{i\vec{k}a} c_{i\vec{k}a} + J \sum_{i\vec{k}a} c^{\dagger}_{i\vec{k}a} (\vec{\sigma})_{aa'} \sum_{i\vec{k'}a'} c_{i\vec{k'}a'} \cdot \vec{S}$$

Quantum Impurities out-of-Equilibrium (1d)

Rewrite exactly as **1-d field theory** (Affleck, Ludwig, Jones)

$$\psi_{i\epsilon a} \equiv \int d^{3}k \, \delta(\epsilon_{\vec{k}} - \epsilon) \, c_{i\vec{k}a}$$

$$\psi_{ia}(x) = \int_{-D}^{D} \frac{d\epsilon}{\nu(\epsilon)^{1/2}} \, e^{i\epsilon x} \, \psi_{i\epsilon a}$$



- Iow-energy physics, universality
 linearize spectrum, take cut-off to infinity
 1-d field theory

 $H_{qdot} = -i \int \sum_{i=1,2} \psi_i^{\dagger}(x) \partial \psi_i(x) \, dx + J(\psi_1^{\dagger}(0) + \psi_2^{\dagger}(0)) \, \vec{\sigma} \, (\psi_1(0) + \psi_2(0)) \cdot \vec{S}$

Non-equilibrium: Time-dependent Description

- Keldysh• $t \leq t_o$, system described by: ρ_o $t = t_o$, couple leads to impurity• $t \geq t_o$, evolve with $H(t) = H_o + e^{\eta t} H_1$

<u>For T > 0:</u>

1. initial condition : ρ_0 **2.** evolution : $U(t, t_o) = T\{e^{-i \int_{t_o}^t dt' H(t')}\}$ **3**. density matrix : $\rho(t) = U^{\dagger}(t, t_o)\rho_o U(t, t_o)$ 4. non-equil value : $\langle \hat{O}(t) \rangle = Tr\{\rho(t)\hat{O}\}$

In equilibrium: $\lim_{t_0 \to -\infty} U^{\dagger}(t, t_o) \rho_o U(t, t_0) = e^{-\beta H}$ (B. Doyon, N. A. 2005)

Non-equilibrium: Time-dependent Description

For T=0 :

1. initial condition: $|\phi_o\rangle$ 2. evolution: $U(t, t_o) = T\{e^{-i\int_{t_o}^t dt' H(t')}\}$ 3. evolved state: $|\psi(t)\rangle = U(t, t_o)|\phi_o\rangle$ 4. non-equil value: $\langle \hat{O}(t) \rangle = \langle \psi(t)|\hat{O}|\psi(t) \rangle$

The initial condition:

 $\begin{aligned} |\phi_o\rangle &= |\phi_o, V\rangle \\ &= |bath1\rangle \otimes |bath2\rangle \otimes |\alpha\rangle \end{aligned}$



The Steady State (open system)

When will a steady state occur? $\frac{1}{L} \ll \frac{1}{|t_0|} \ll \eta \to 0$



- Leads good thermal baths, infinite volume limit open system
 - $\Rightarrow \exists \lim_{t_{\circ} \to -\infty}$, no *IR* divergences (Doyon, NA 2005)



- Dissipation mechanism
- Time-reversal sym. breaking
 Steady-state non- eq. currents







The Steady State – time independent description

The limit $\frac{1}{L} \ll \frac{1}{|t_o|} \ll \eta \to 0$ implies: $\exists |\psi, V\rangle_s = U(0, -\infty) |\phi_o, V\rangle$

fully describes steady-state non-equilibrium

- $|\psi\rangle_s$ eigenstate of $H = H_0 + H_1$ (Gellman-Low thm)
- Lippmann-Schwinger equation, $|\phi_o\rangle$ -boundary condition $|\psi\rangle_s = |\phi_o\rangle + \frac{1}{E - H_0 + i\eta} H_1 |\psi\rangle_s$
- $|\phi_o\rangle$: Initial condition \rightarrow boundary condition
 - $|\psi\rangle_s$ scattering state eigenstate on the infinite line



from Merzbacher: eigenstate of $H = \frac{1}{2m} p^2 + V(x)$ with incoming boundary condition $\psi(x) \to \phi_o(x) = e^{i\vec{p}\cdot\vec{x}}$

The scattering state (many body)

Scattering eigenstate determined by *incoming asymptotics*: *the baths*



For example:

$$\begin{split} I(V) &= \langle \phi_o, V | U^{\dagger}(0, -\infty) \hat{I} U(0, -\infty) | \phi_o, V \rangle \equiv \langle T_c e^{-i \int_{-\infty}^0 H(t') dt'} \hat{I}(0) \rangle \text{ (Keldysh)} \\ &= \langle \psi, V | \hat{I} | \psi, V \rangle_s \end{split}$$
 (Scattering)

Non-equilibrium Steady-states & Scattering States

- A scattering eigenstate describes all aspects of steady-state non-equilibrium physics:
 - non-equilibrium currents, energy dissipation, entropy production
- A scattering eigenstate describes the system <u>and</u> its environment

- At T=0 need a single scattering state
- At T>0 need many scattering states



Steady State at T>0

• For T=0
$$|\phi_0\rangle \rightarrow |\psi\rangle_s$$
 $|\phi_0\rangle$ g.s. of $H_0 - \sum_i \mu_i N_i$

• Generally,
$$|\phi_n\rangle \xrightarrow{L-S} |\psi_n\rangle_s$$
 where $|\phi_n\rangle \in \mathcal{H}_o^{\perp}$

• For T>0 "free leads" boundary conditions: $p_n^o = e^{-\beta E_n^o}/Z_o$ $\rho_o = \sum_n p_n^o |\phi_n\rangle \langle \phi_n| \longrightarrow \begin{cases} \rho_s = \sum_n p_n^o |\psi_n\rangle \langle \psi_n|_s \\ \langle \hat{O} \rangle = Tr \rho_s \hat{O} \end{cases}$

The Scattering Bethe-Ansatz

HOW TO CONSTRUCT $|\psi\rangle_s$, (for T = 0)? **OR** ρ_s , (for T > 0)?

- Keldysh perturbation theory fails in general (IR div)
- RG is inapplicable, $|\Phi_o\rangle$ highly excited
- Can the Bethe-Ansatz be used?
 - Traditional Bethe-Ansatz inapplicable
 - Periodic boundary conditions
 - Closed System: Equilibrium, Thermodynamics
 - New technology → Scattering States
 - Asymptotic Boundary conditions on the infinite line
 - **Open System**: Non-equilibrium, scattering problems

Scattering Bethe-Ansatz

the new technology

- consistency of non-eq BC and integrability (YBE)
- integrability out-of-equilibrium

IRL: The Scattering State I

• The Interacting Resonance Level Model:



$$H_{IRL} = \sum_{i=1,2\vec{k}} \epsilon_k c_{i\vec{k}}^{\dagger} c_{i\vec{k}} + \epsilon_d d^{\dagger} d + t \sum_{i=1,2\vec{k}} (c_{i\vec{k}}^{\dagger} d + h.c) + 2U \sum_{i=1,2\vec{k}} c_{i\vec{k}}^{\dagger} c_{i\vec{k}} d^{\dagger} d$$

The hamiltonian :

$$\begin{cases} \cdot \text{ low-energy physics, c.o. independence} \\ \cdot \text{ field theory, universality, renormalizability} \end{cases}$$

$$H_{IRL} = -i\sum_{i=1,2} \int dx \,\psi_i^{\dagger}(x) \partial \psi_i(x) + \epsilon_d d^{\dagger} d + t \sum_i \left(\psi_i^{\dagger}(0)d + h.c.\right) + 2U\sum_i \psi_i^{\dagger}(0)\psi_i(0)d^{\dagger} d$$

Diagonalize H via Scattering Bethe-Ansatz: diagonalize directly on the infinite line (open system)

1. construct 1-particle eigenstates (with boundary conditions)

2. construct 2-paricle eigenstates ..

$$H|F_N\rangle = E_N|F_N\rangle$$
 $N = 1, 2...$

IRL: The Scattering State II

Single-particle scattering states: $\delta_p = 2tan^{-1} \left[\frac{t^2}{2(p-\epsilon_d)} \right]$, phase shift

$$\begin{aligned} |1p\rangle &= \int dx e^{ipx} \left[\left(\left[\theta(-x) + \frac{e^{i\delta_p} + 1}{2} \theta(x) \right] \psi_1^{\dagger}(x) + \left[\frac{e^{i\delta_p} - 1}{2} \theta(x) \right] \psi_2^{\dagger}(x) \right) + e_p d^{\dagger} \delta(x) \right] |0\rangle \\ &\equiv \int dx e^{ipx} \alpha_{1p}^{\dagger}(x) |0\rangle \end{aligned}$$

$$\begin{aligned} |2p\rangle &= \int dx e^{ipx} \left[\left(\left[\theta(-x) + \frac{e^{i\delta_p} + 1}{2} \theta(x) \right] \psi_2^{\dagger}(x) + \left[\frac{e^{i\delta_p} - 1}{2} \theta(x) \right] \psi_1^{\dagger}(x) \right) + e_p d^{\dagger} \delta(x) \right] |0\rangle \\ &\equiv \int dx e^{ipx} \alpha_{2p}^{\dagger}(x) |0\rangle \end{aligned}$$



The scattering states satisfy incoming bc: $\alpha_i(x) = \psi_i(x)$ for x < 0

IRL: The Scattering State III

Multi-particle scattering state: N₁ lead-1, N₂ lead-2

 $|\{p\}\rangle_{s} = \int dx \, e^{i\sum_{j=1}^{N} p_{j}x_{j}} e^{i\sum_{j=1}^{N} \Phi(p_{j},p_{l})sgn(x_{j}-x_{l})} \Pi_{u}^{N_{1}} \alpha_{1}^{\dagger}(x_{u}) \Pi_{v}^{N_{2}} \alpha_{2}^{\dagger}(x_{v})|0\rangle$

with

$$e^{2i\Phi(p_i,p_j)} \equiv S(p_i,p_j) = \frac{i - \frac{U}{2} \frac{p_i - p_j}{p_i + p_j - 2\epsilon_d}}{i + \frac{U}{2} \frac{p_i - p_j}{p_i + p_j - 2\epsilon_d}}$$



|{p}⟩_s scattering eigenstate for any choice of {p}
impose non-eq boundary conditions to determine {p} *Why not choose* {p} *Fermi-Dirac distribution?*

The Boundary Conditions I (The Bethe Basis)



The Boundary Conditions II

Turn the BA equations into integral equations for : ρ_1, ρ_2

•Non-eq BC \rightarrow momentum distributions $\rho_1(p), \ \rho_2(p)$:

- TBA eqns with upper cut-offs $k_o^j = k_o(\mu^j)$, lower cut-off, D:

$$\rho_{1}(p) = \frac{1}{2\pi} \theta(k_{o}^{1} - p) - \sum_{j=1,2} \int_{-D}^{k_{o}^{j}} \mathcal{K}(p,k) \rho_{j}(k) \, dk$$
$$\rho_{2}(p) = \frac{1}{2\pi} \theta(k_{o}^{2} - p) - \sum_{j=1,2} \int_{-D}^{k_{o}^{j}} \mathcal{K}(p,k) \rho_{j}(k) \, dk$$
with:
$$\mathcal{K}(k,p) = \frac{U}{\pi} \frac{\epsilon_{d} - k}{(k+p-2\epsilon_{d})^{2} + \frac{U^{2}}{4} + (k-p)^{2}}$$

TBA eqns describe the free leads on a ring (in the Bethe basis)
For U=0 distributions reduce to Fermi-Dirac distributions

Comment:

These TBA eqns valid for: $\epsilon_d \geq 0$ otherwise, eqns more complicated

IRL: Current & Dot Occupation

• Current and dot-occupation:

$$\hat{I} = \frac{i}{\sqrt{2}} t \sum_{j=1,2} (-1)^j (\psi_j^{\dagger}(0)d - h.c)$$
$$\hat{n}_d = d^{\dagger}d$$

• Expectation values: \hat{I}, \hat{n}_d in Scattering State: $|\{p\}\rangle_{L\to\infty}^{\mu_1,\mu_2}$

$$\Delta = t^2/2 \qquad \begin{aligned} \langle I \rangle_s^{\mu_1,\mu_2} &= \int dp \left[\rho_1(p) - \rho_2(p) \right] \frac{\Delta^2}{(p - \epsilon_d)^2 + \Delta^2} \\ \langle n_d \rangle_s^{\mu_1,\mu_2} &= \int dp \left[\rho_1(p) + \rho_2(p) \right] \frac{\Delta}{(p - \epsilon_d)^2 + \Delta^2} \end{aligned}$$

- For U=0, Landauer expressions (from the scattering eigenstate!)
- For U>0, in the Bethe-Anzatz basis, expressions look "simple":
 - Excitations undergo phase shifts only
 - Choice of momenta incorporates interactions and boundary conditions

IRL: Current vs. Voltage

• Compute Exactly current and dot occupation as a function of Voltage:

Can easily generalize to finite temperature case

 Universality out of equilibrium: change in D can be compensated by change in U and∆

Traditional vs Scattering BA

The construction of $|\psi\rangle_s$ is an example of the SBA approach:

	SBA	TBA
System	Infinite	Finite
Boundary condition	asymptotic (open)	periodic
Wavefunctions	used explicitly	not used
Thermodynamics	difficult	easy
Scattering Properties	possible	not possible
Nonequilibrium Generalization	Yes	No

More applications:

- Scattering S-matrix of electrons off magnetic impurities
 - elastic and inelastic cross sections
- Calculation single particle Green's functions, spectral functions
 - finite temperature resistivity (resistance minimum)

The Kondo Impurity Out of Equilibrium

Inoshita:Science 24 July 1998: Vol. 281. no. 5376, pp. 526 - 527

- Can control the number of electrons on the dot using gate voltage
- For odd number of electrons- quantum dot acts like a quantum impurity (Kondo, Interacting Resonant Level Model)
 - •Quantum impurity models exhibit new collective behaviors such as the Kondo effect

The Kondo Impurity out-of- Equilibrium

 $N_{1} = N_{0} + \Delta N/2 \qquad Nu$ $N_{2} = N_{0} - \Delta N/2 \qquad Nu$ $N_{e} = N_{1} + N_{2} = 2N_{0} \qquad To$ $\Delta N = VL/2\pi$

Number of electrons in lead 1 Number of electrons in lead 2 Total number of electrons

Kondo Impurity: The Scattering State I

• The leads-dot interaction:

$$H_I = (\psi_1^{\dagger}(0) + \psi_2^{\dagger}(0)) \,\vec{\sigma} \,(\psi_1(0) + \psi_2(0)) \cdot \vec{S}$$

- Induces the S-matrices: (satisfy YBE out of equilibrium)
 - Electron-electron (same as for the 2-channel Kondo)

$$S^{ij} = P_f^{ij} S_K^{ij} = P_f^{ij} P_s^{ij}$$

- Electron-impurity

$$S^{j0} = \begin{pmatrix} (S_K^{j0} + 1_s^{j0})/2 & (S_K^{j0} - 1_s^{j0})/2 \\ (S_K^{j0} - 1_s^{j0})/2 & (S_K^{j0} + 1_s^{j0})/2 \end{pmatrix}_j \qquad S_K^{j0} = \frac{I_s^{j0} - icP_s^{j0}}{1 - ic}$$

The scattering state is constructed with these S-matrices

Kondo Impurity: The Scattering State II

The scattering state:

$$|\Psi\rangle_{s} = \int dx \sum_{Q} \theta(x_{Q}) e^{i\sum_{j} k_{j} x_{j}} (S_{Q}A)^{\alpha_{1}\dots\alpha_{N}}_{a_{1}\dots a_{N}} \psi^{\dagger}_{a_{1}\alpha_{1}}(x_{1}) \cdots \psi^{\dagger}_{a_{N}\alpha_{N}}(x_{N})|0\rangle$$

The Bethe-momenta {k}:
$$k_{\delta}^{\pm} = k_{\delta} \pm i \wedge c/2, \quad \delta = 1 \cdots N_2$$
 $k_j, \quad j = 1 \cdots \Delta N$

$$e^{i2k_{\delta}L} = \prod_{\gamma=1}^{N_0} \frac{\chi_{\gamma} + ic}{\chi_{\gamma} - ic} \qquad \delta = 1, \dots, N_2 \qquad (2 - strings)$$
$$e^{ik_jL} = \prod_{\gamma=1}^{N_0} \frac{\chi_{\gamma} + i\frac{c}{2}}{\chi_{\gamma} - i\frac{c}{2}} \qquad j = N_2 + 1, \dots, N_1 (1 - strings)$$

ÎI

The spin momenta $\{\chi_{\gamma}\}$ *are determined from:*

$$-\prod_{\beta=1}^{N_0} \frac{\chi_{\gamma} - \chi_{\beta} + ic}{\chi_{\gamma} - \chi_{\beta} - ic} = \left(\frac{\chi_{\gamma} + i\frac{c}{2}}{\chi_{\gamma} - i\frac{c}{2}}\right)^{N_1 - N_2} \left(\frac{\chi_{\gamma} + ic}{\chi_{\gamma} - ic}\right)^{N_2}$$

Kondo: The Scattering State III

The 1-string and 2-string densities $\rho_1(p) \rho_2(p)$ satisfy: (Andres Jerez)

$$\rho_{1}^{-}(p) + \rho_{1}^{+}(p) = \frac{\Delta N e^{ipB_{1}}}{2ch(p/2)} + \rho_{2}^{-}(p) \frac{e^{ik(B_{1}-B_{2})}}{2ch(p/2)}$$
$$\rho_{2}^{-}(p) + \rho_{2}^{+}(p)(1+e^{-|p|}) = \frac{1}{2}N_{2}e^{-|p|/2}e^{ipB_{2}} + \rho_{1}^{-}(p)e^{-|p|/2}e^{i(B_{2}-B_{1})}$$

With:

(mag. field)
$$h \sim e^{\pi B_2}$$

(voltage) $V \sim e^{-\pi (B_1 - B_2)}$

Thus:

$$\rho_i^{\pm}(p) = \rho_i^{\pm}(p; V)$$

Kondo: The Current (in progress)

The Current:

$$\widehat{I} = \psi_1^{\dagger}(\epsilon)\psi_1(\epsilon) - \psi_1^{\dagger}(-\epsilon)\psi_1(-\epsilon) = \vec{J}_x \cdot \vec{S}$$

Evaluated in the scattering state:

$$\langle \hat{I} \rangle_{neq}^{V} = V \int dp \left(\rho_{1}^{+}(p;V)e^{-|p|/2} + \rho_{2}^{+}(p;V)e^{-|p|} \right)$$

$$= V \sum_{n=0}^{\infty} (-1)^{n} \rho_{1}^{-}(i(2n+1)\pi)e^{(2n+1)B_{1}}$$

I-V curves? – please stay tuned.

Entropy production I

Non-equilibrium currents dissipate heat into environment:

 $\delta Q_i = dE_i - \mu_i dN_i$

- Scattering state describes system +environment
- Dissipation mechanism:
 electrons reaching infinity
- Lost high energy electrons generate entropy (entanglement)

Recall: currents ~ 1 leads ~ $L \rightarrow infty$

 $\frac{dE_1}{dt} \equiv \langle \frac{d\hat{E}_1}{dt} \rangle_s = \langle i[\hat{H}, \hat{H}_{01}] \rangle_s = -\langle I_E \rangle_s$

 $\frac{dN_1}{dt} \equiv \langle \frac{d\hat{N}_1}{dt} \rangle_s = \langle i[\hat{H}, \hat{N}_1] \rangle_s = -\langle I_N \rangle_s$

Entropy production II

- The rate of entropy production "thermodynamically" defined:
 - discontinuous system:

$$\sigma \equiv \frac{dS}{dt} = \frac{1}{T_1} \frac{\delta Q_1}{dt} + \frac{1}{T_2} \frac{\delta Q_2}{dt} = \left(\frac{1}{T_1} - \frac{1}{T_2}\right) \langle I_E \rangle_s + \left(\frac{\mu_1}{T_1} - \frac{\mu_2}{T_2}\right) \langle I_N \rangle_s$$

Note: i) entropy and energy are defined w.r.t quasi –equil, (L ~ infty) *ii)* maximal entropy per lead *iii)* no entropy production in dot

- Can compute rate explicitly
- "Microscopic" derivation entanglement (?):

from: $\rho_s \equiv \rho_{12} = \sum_n p_n^0 |\psi_n\rangle \langle \psi_n|$ define: $\rho_1 = Tr_2 \rho_s$, $\rho_2 = Tr_1 \rho_s$ then:

 $\sigma = \frac{1}{T_1} \frac{d}{dt} T r_1 \rho_1 \ln \rho_1 + \frac{1}{T_2} \frac{d}{dt} T r_2 \rho_2 \ln \rho_2$

- Considering: $I_N, I_E = I_N, I_E(\Delta T, \Delta \mu)$
 - Out-of-equilibrium thermo-electric (Onsager) relations
 - Quantum-dot refrigerator

Entropy Production: Effects of Correlations

How does the Kondo effect manifest itself?

• The RLM describes the Kondo model at Strong coupling

- Stronger correlations suppress entropy production
- To measure: perform spectroscopy of emerging electrons

Conclusions

• Showed:

Scattering States with non-eq BC - Steady State

• Computed:

The Steady State Current: IRLM at T = 0

• Exact results:

A strongly correlated impurity system out of equilibrium

• Many generalizations and applications:

Non-equilibrium Impurity Problems:

- Non-equilibrium in other impurity models: Kondo, Anderson, Multichannel versions
- Non-equilibrium at $T > 0, T_1 \neq T_2, B$
- Thermal Currents, spin currents
- More leads: non-equilibrium DOS

Scattering Problems:

- Inclusive, exclusive scattering amplitudes
- Inelastic scattering amplitudes T > 0

More ambitious:

- Non-equilibrium description of *bulk* systems
- Non-equilibrium RG