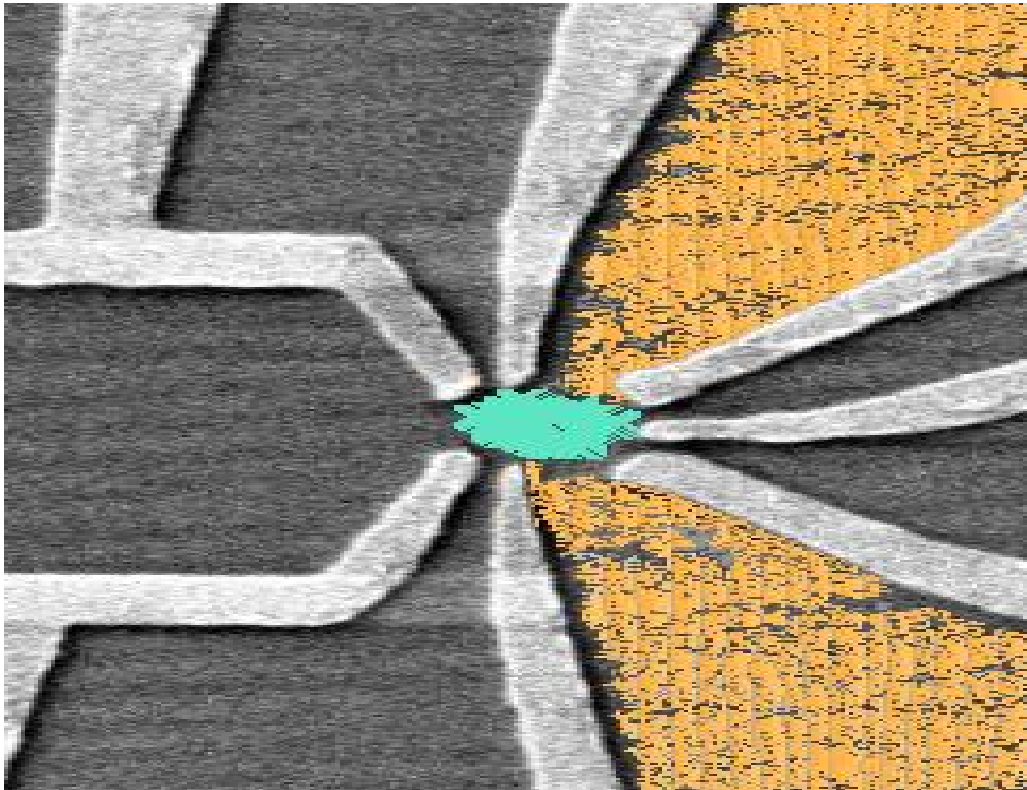


Quantum Impurities Out of Equilibrium



Natan Andrei



With collaborators:

P. Mehta - Princeton

C. Bolech - Rice

A. Jerez - NJIT

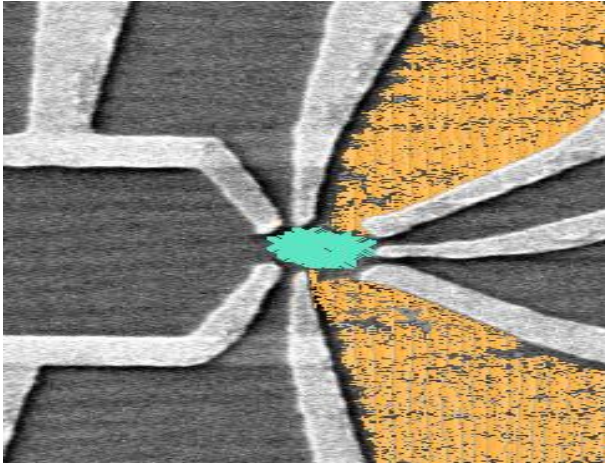
S.-P Chao - Rutgers

G. Palacios - Rutgers

Evora, November 2008

Quantum Impurities out-of-Equilibrium

- **The quantum impurity - experimentally:** Goldhaber-Gordon *et al*, Conenwett *et al*, Schmid *et al*

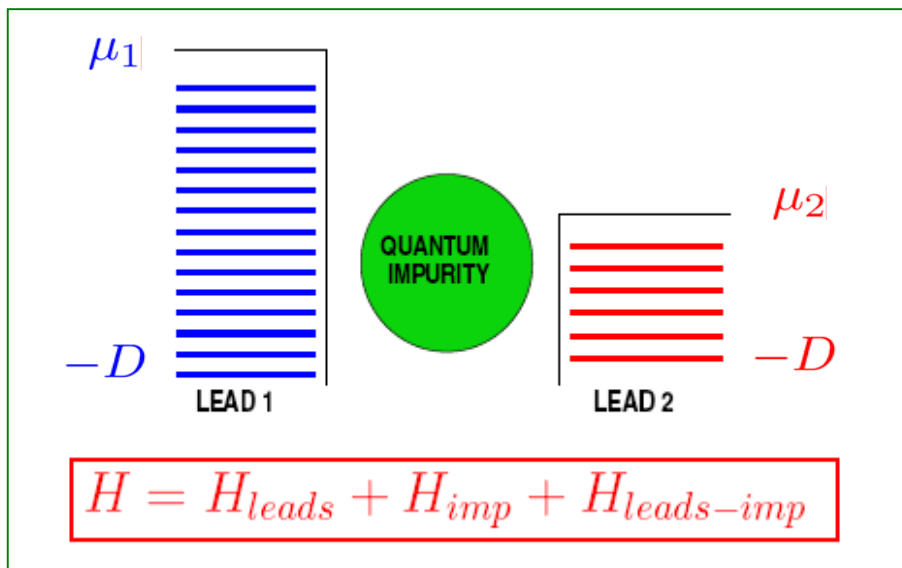


- Couple impurity to leads with $\mu_1 \neq \mu_2$
- Non-equil steady state (NESS) is established:
 - current's flow is time independent (after transients)
- Measure non-equil current in steady state

$$I = I(V, T), \quad V = \mu_1 - \mu_2$$

- **The quantum impurity - theoretically:**

- How to compute $I = I(V, T)$?



Leads = Fermi seas, $i=1,2$

$$H_{leads} = \sum_{i,k} \epsilon_k c_{i\vec{k}}^\dagger c_{i\vec{k}}$$

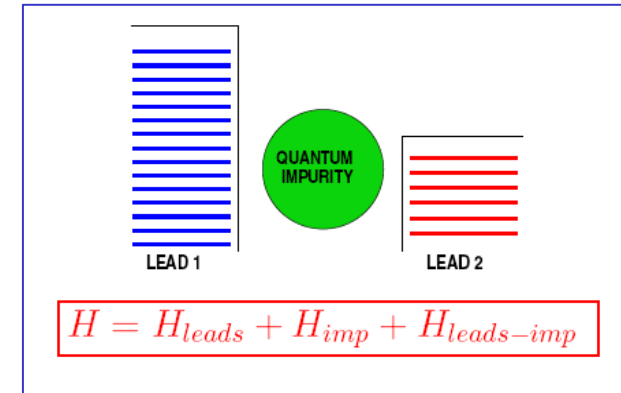
Non-equilibrium

$$V = \mu_1 - \mu_2 \neq 0$$

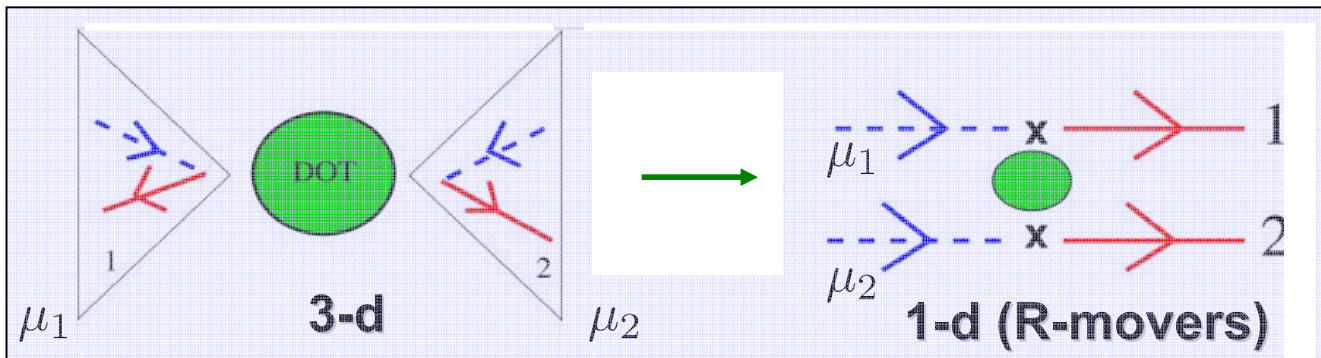
Quantum Impurity Hamiltonian (3d → 1d)

Impurity Hamiltonian (3d):

$$H^{3d} = \sum_{j=1,2} \sum_{\vec{k}} \epsilon_k c_{j\vec{k}a}^\dagger c_{j\vec{k}a} + t \sum_{j=1,2} \sum_{\vec{k}} (c_{j\vec{k}a}^\dagger d_a + h.c.) + H_{imp}$$



Unfold 3d Hamiltonian → 1d field theory:



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

$$\{\psi_{iea}, \psi_{je'b}^\dagger\} = \delta_{ab} \delta_{ij} \delta(\epsilon - \epsilon') \nu(\epsilon)$$

$$\psi_{ia}(x) = \int_{-D}^D \frac{d\epsilon}{\sqrt{\nu}} e^{i\epsilon x} \psi_{iea}$$

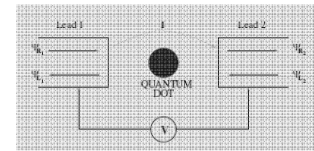
Affleck Ludwig 95'

Field Theory of chiral electrons (R-movers): ($\nu = 1/2\pi$, $v_F = 1$, $D \rightarrow \infty$)

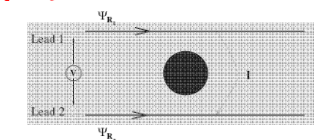
Impurity Hamiltonian (1d): Low-energy universality

$$H^{1d} = -i \sum_{j=1,2} \int \psi_{ja}^\dagger \partial \psi_{ja} dx + t \sum_{j=1,2} (\psi_{ja}^\dagger(0) d_a + h.c.) + H_{imp}$$

The Quantum Impurity:



The Quantum Impurity unfolded:



Non-equilibrium: Time-dependent Description

Given H - how to set up the non-equilibrium problem?

- Keldysh** {
- $t \leq t_0$, leads decoupled, system described by: ρ_0
 - $t = t_0$, couple leads to impurity
 - $t \geq t_0$, evolve with $H(t) = H_0 + e^{\eta t} H_1$

Description of Nonequilibrium requires two elements: H, ρ_0 or H, H_0 ; Equilibrium requires only H .

For $T > 0$:

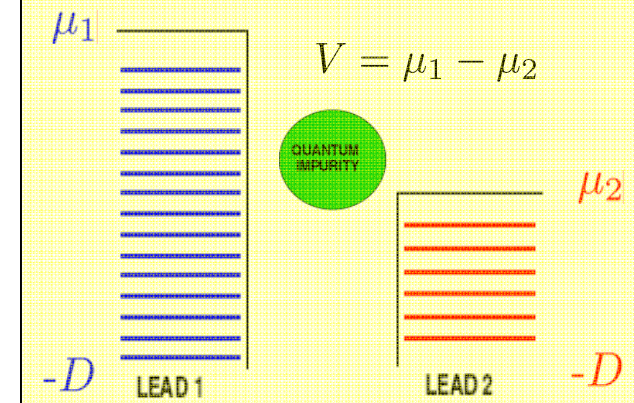
1. initial condition: ρ_0
2. evolution: $U(t, t_0) = T\{e^{-i \int_{t_0}^t dt' H(t')}\}$
3. density matrix: $\rho(t) = U(t, t_0) \rho_0 U^\dagger(t, t_0)$
4. non equil value: $\langle \hat{O}(t) \rangle = Tr\{\rho(t) \hat{O}\}$

For $T = 0$:

1. initial condition: $|\phi_0, V\rangle$
2. evolution: $U(t, t_0) = T\{e^{-i \int_{t_0}^t dt' H(t')}\}$
3. evolved state: $|\psi(t)\rangle_V = U(t, t_0) |\phi_0, V\rangle$
4. non-equil value: $\langle \hat{O}(t) \rangle_V = \langle \psi(t) | \hat{O} | \psi(t) \rangle_V$

The initial condition at $T=0$:

$$|\phi_0\rangle = |\phi_0, V\rangle = |bath1\rangle \otimes |bath2\rangle \otimes |\alpha\rangle$$



The Steady State (open system limit)

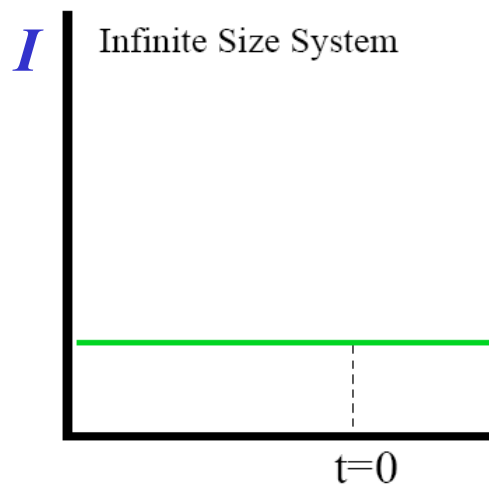
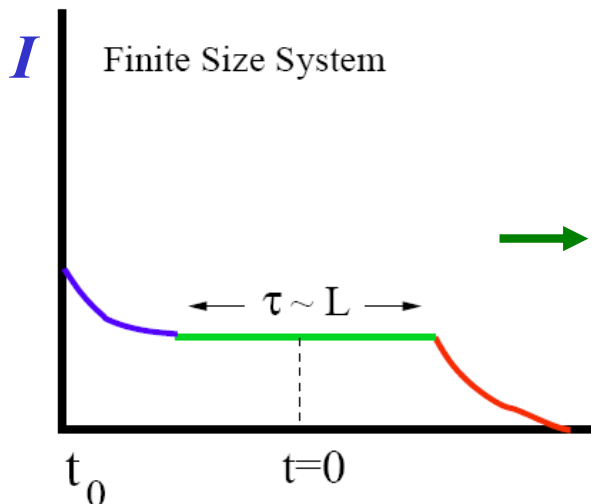
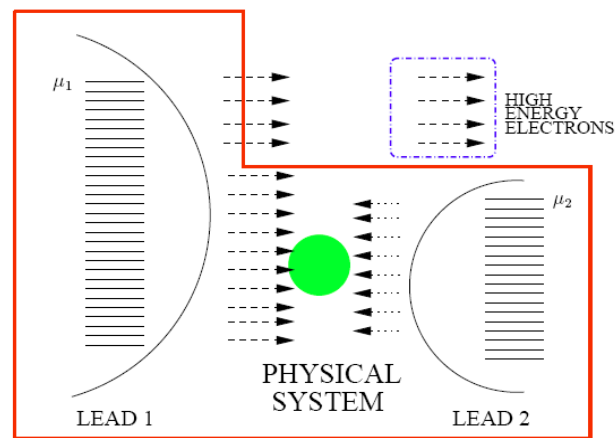
Non-equilibrium steady states (NESS): when do they occur?

- Leads good thermal baths, infinite volume limit - open system

$\Rightarrow \exists \lim_{t_0 \rightarrow -\infty}$, no IR divergences, $\frac{1}{L} \ll \frac{1}{|t_0|} \ll \eta \rightarrow 0$ (B Doyon, NA, PRB '05)
(order by order in P.T.)

Open system limit :

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



A steady state ensues

$$\langle \hat{O}(t) \rangle = \langle \hat{O} \rangle$$

The Steady State – time independent description

The open system limit $\frac{1}{L} \ll \frac{1}{|t_o|} \ll \eta \rightarrow 0$:

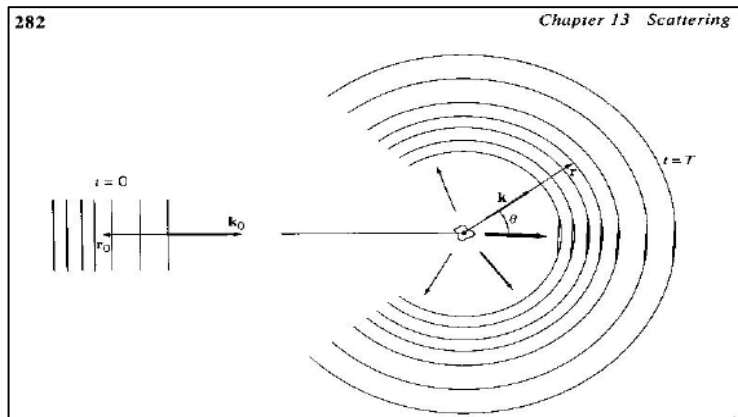
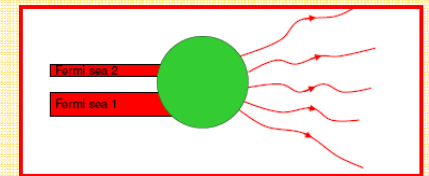
→ $|\psi, V\rangle_s = U(0, -\infty)|\phi_o, V\rangle$ a well defined state.

Properties:

P. Mehta, N.A. PRL 96, '06

- $|\psi, V\rangle_s$ eigenstate of $H = H_0 + H_1$ (Gellman-Low thm)
- Lippmann-Schwinger equation, $|\phi_o, V\rangle$ -boundary condition

$$|\psi, V\rangle_s = z|\phi_o, V\rangle + \frac{1}{E - H_0 + i\eta} H_1 |\psi, V\rangle_s$$
- $|\phi_o, V\rangle$: Initial condition → boundary condition
- $|\psi, V\rangle_s$ scattering state - eigenstate on the infinite line



from Merzbacher: $\psi(x)$ eigenstate of

$$H = \frac{1}{2m} p^2 + V(x)$$

with incoming boundary condition

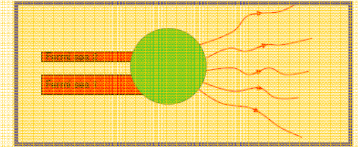
$$\psi(x) \rightarrow \phi_o(x) = e^{i\vec{p}\cdot\vec{x}}$$

(Both H, H_0 enter description)

The Non-equilibrium Steady State

- Non-equilibrium $T=0$ steady state is described by:

$$|\psi, V\rangle_s =$$



- Non-equilibrium value:

$$\langle O \rangle_s = \langle \psi, V | O | \psi, V \rangle_s$$

- For $T=0$, $|\phi_0, V\rangle \xrightarrow{\text{L-S}} |\psi, V\rangle_s$ $|\phi_0, V\rangle$ g.s. of $H_0 - \sum_i \mu_i N_i$
- Generally, $|\phi_n, V\rangle \xrightarrow{\text{L-S}} |\psi_n, V\rangle_s$ where $|\phi_n\rangle \in \mathcal{H}_0^{\perp, V}$
- For $T>0$, "free leads" boundary conditions: $p_n^o = e^{-\beta E_n^o} / Z_o$

$$\rho_o = \sum_n p_n^o |\phi_n\rangle \langle \phi_n| \longrightarrow \rho_s = \sum_n p_n^o |\psi_n\rangle \langle \psi_n|_s$$

and:
$$\langle \hat{O} \rangle_s = \text{Tr} \rho_s \hat{O}$$

In steady state - \exists "non-thermal" density operator!

cf. Hershfield '93

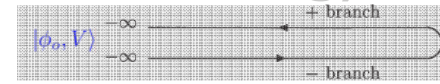
- In equilibrium: $\rho_o \rightarrow \rho_s = \frac{1}{Z} e^{-\beta H}$ (Keldysh \rightarrow Boltzmann)

Doyon, N.A. '05

Steady-states & Scattering States

- Time-dependent (Keldysh) vs. time-independent approach (Scattering)

$$I(V) = \langle \phi_o, V | U^\dagger(0, -\infty) \hat{I} U(0, -\infty) | \phi_o, V \rangle \equiv \langle T_c e^{-i \int_{-\infty}^0 H(t') dt'} \hat{I}(0) \rangle$$



-Keldysh approach

$$= \langle \psi, V | \hat{I} | \psi, V \rangle_s$$



-Scattering approach

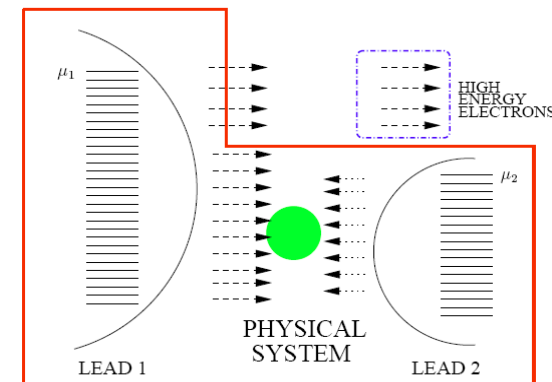
- Scattering approach: $|\psi, V\rangle_s \longleftrightarrow$ non-perturbative Keldysh

- The scattering eigenstate $|\psi, V\rangle_s$ describes all aspects of non-equilibrium steady-state physics (NESS):

- non-equilibrium currents,
- energy dissipation,
- entropy production

Q: How can an eigenstate describe dissipation, entropy production?

A: Scattering eigenstate describes both system and environment (open system)



Entropy production and Dissipation

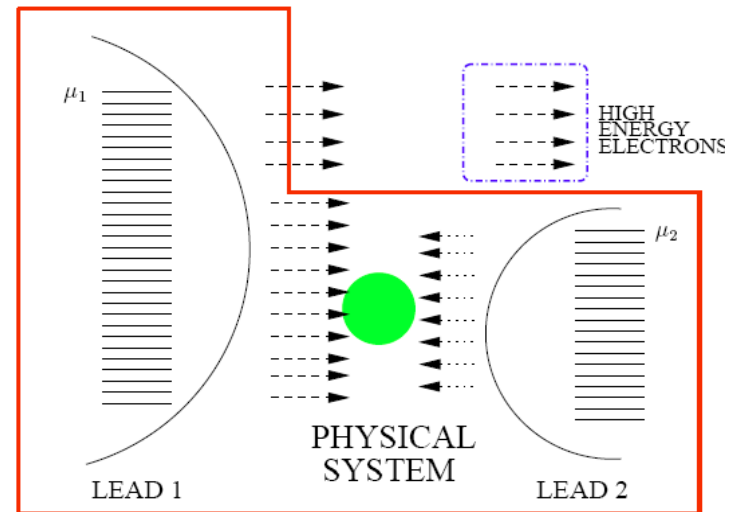
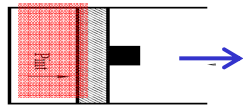
Non-equilibrium currents dissipate heat into environment:

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

$$\delta Q_i = dE_i - \mu_i dN_i$$

Entropy is produced quasi-statically:

- currents ~ 1
- leads $\sim L \rightarrow \text{infy}$



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

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

Entropy production and Dissipation

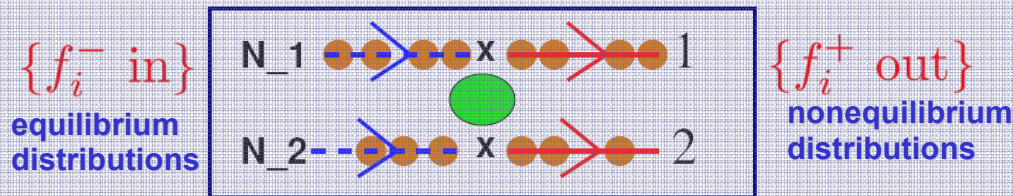
- **“Thermodynamic” approach:** (discontinuous system - defined w.r.t. quasi-equil, $L \sim \infty$)

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

No accumulation
in dot: $I_1 + I_2 = 0$

- **“Boltzmannian” approach – (distributions)**

scattering \rightarrow change of distribution:



$$\sigma = \sum_i \int dp v_F (f_i^+(p) - f_i^-(p)) \frac{p - \mu_i}{T_i}$$

$$f_i^+(p) = f_i^-(p) |R(p)|^2 + f_i^-(p) |T(p)|^2$$

- **“Information Theory” approach – (in the infinite volume limit) :**

$$\sigma = \lim_{L \rightarrow \infty} \frac{1}{L} \sum_{i=1,2} v_F [(S_i^+ - S_i^-) + v_F D_{KL}(f_i^+ || f_i^-)]$$

mixing *relaxation*

P. Mehta, N. A. PRL100, '08

Mixing + Relaxation

$$\begin{cases} \text{mixing} & = \Delta S \\ \text{relaxation} & = D_{KL}(f^+ || f^-) \end{cases}$$

$$S_i^\pm = - \sum_\alpha f_i^\pm(p_\alpha) \ln f_i^\pm(p_\alpha) - \sum_\alpha [1 - f_i^\pm(p_\alpha)] \ln [1 - f_i^\pm(p_\alpha)]$$

$$D_{KL}(f^+ || f^-) = \sum_\alpha f^+(p_\alpha) \ln \frac{f^+(p_\alpha)}{f^-(p_\alpha)}$$

Kullback-Leibler divergence:
- amount of work obtained
when f^+ relaxes to f^-

- **Entropy production rate strictly positive, $\sigma > 0$**

The Scattering Bethe-Ansatz

Nonequilibrium described by open-system eigenstates

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

- Keldysh perturbation theory - fails in general (IR div)
- RG ? - $|\phi_o, V\rangle$ highly excited

Recent developments: Freq dep-RG
TD-DMNRG, TD-DMRG, FRG, Flow-eq

Develop a Bethe Ansatz approach to non-equilibrium:

- **Traditional Bethe-Ansatz - inapplicable** $H|\psi\rangle = E|\psi\rangle$ (+PBC)
- Periodic boundary conditions
- **Closed System:** Equilibrium, Thermodynamics
- **New technology → Scattering States**
- Asymptotic Boundary conditions on the infinite line
- **Open System:** Non-equilibrium, scattering problems

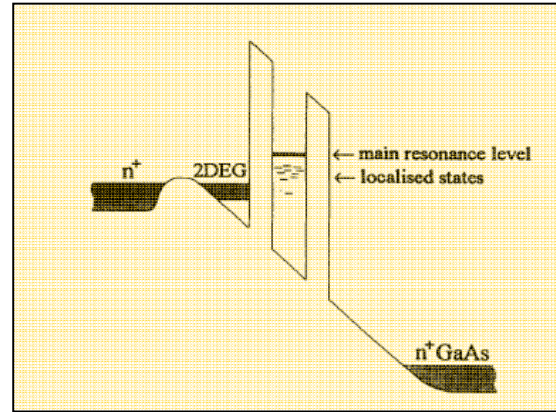
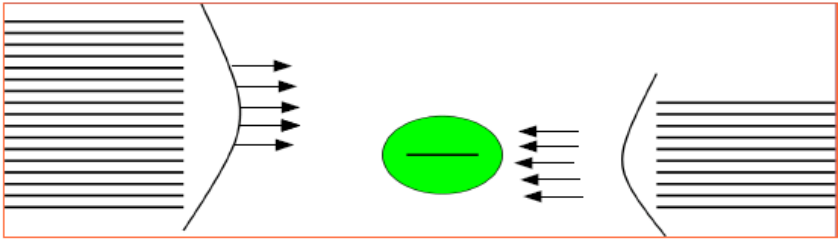
Scattering (Open) Bethe-Ansatz:

$H|\psi\rangle_s = E|\psi\rangle_s$
scattering BC on ∞ -line

1. *Non-equil Interacting Resonance Level model (Non-equil FES)*
2. *Non-equil Anderson model (Quantum Dot – Non-equil Kondo effect)*

The Interacting Resonance Level model out-of-equilibrium

• Non-equil IRL Model:



Non-equil FES

Geim et al 93'

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

• The 1-d Field Theory

Thermodynamic BA Filyov, Wiegman 80'

$$H_{IRL} = -i \sum_j \int \psi_j^\dagger(x) \partial \psi_j(x) + \epsilon_d d^\dagger d + t \sum_j (\psi_j^\dagger(0) d + h.c.) + U \sum_j \psi_j^\dagger(0) \psi_j(0) d^\dagger d$$

Diagonalize H via the Open Bethe-Ansatz:

- directly on the infinite line (open system)

- construct 1-particle eigenstates (with boundary conditions)
- construct N-particle eigenstates out of 1-particle states

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

IRL: The Scattering State

Single-particle scattering eigenstates -

Level width:

$$\Delta = \frac{1}{2}t^2$$

Phase shift:

$$e^{i\delta_p} = \frac{p - \epsilon_d - \Delta}{p - \epsilon_d + i\Delta}$$

$|1p\rangle$

$$\begin{aligned} |1p\rangle &= \int dx e^{ipx} \{ [\theta(-x) + R_p \theta(x) + s(x)] \psi_1^\dagger(x) \\ &\quad + [T_p \theta(x) - s(x)] \psi_2^\dagger(x) + e_p d^\dagger \delta(x) \} |0\rangle \\ &= \int dx e^{ipx} \alpha_{1p}^\dagger(x) |0\rangle \end{aligned}$$

$|2p\rangle$

$$\begin{aligned} |2p\rangle &= \int dx e^{ipx} \{ [\theta(-x) + R_p \theta(x) - s(x)] \psi_2^\dagger(x) \\ &\quad + [T_p \theta(x) + s(x)] \psi_1^\dagger(x) + e_p d^\dagger \delta(x) \} |0\rangle \\ &= \int dx e^{ipx} \alpha_{2p}^\dagger(x) |0\rangle \end{aligned}$$

Impurity amp.

$$e_p = \frac{t}{p - \epsilon_d + i\Delta}$$

Reflec. amp.

$$R_p = \frac{1}{2} [e^{i\delta_p} + 1]$$

Trans. amp.

$$T_p = \frac{1}{2} [e^{i\delta_p} - 1]$$

Trans. coeff.

$$|T_p|^2 = \frac{\Delta^2}{(p - \epsilon_d)^2 + \Delta^2}$$

Renormalization prescription

$$\theta(x)\delta(x) = \frac{1}{2}\delta(x)$$

Local discontinuity

$$s(x) = \begin{cases} 0 & x \neq 0 \\ \frac{e^{i\delta_p} - 1}{2} & x = 0 \end{cases} \text{ constant - consistent with prescription}$$

Boundary condition

$$\alpha_{ip}^\dagger(x) \xrightarrow{x \rightarrow -\infty} \psi_{ip}^\dagger(x)$$

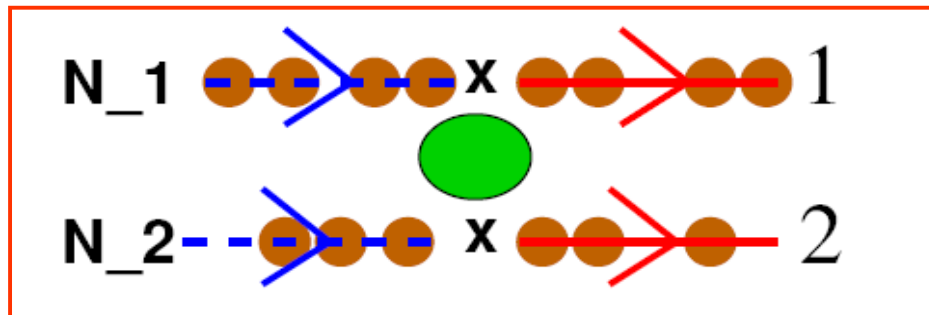
IRL: The Scattering State

Multi-particle scattering state - N_1 lead-1, N_2 lead-2, $N_i \sim \mu_i$

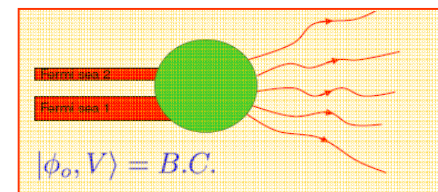
$$|\{p\}, N_1, N_2\rangle_s = \int dx e^{i \sum_j^N p_j x_j} e^{i \sum_{j<l}^N \Phi(p_j, p_l) \text{sgn}(x_j - x_l)} \prod_u^{N_1} \alpha_{1p}^\dagger(x_u) \prod_v^{N_2} \alpha_{2p}^\dagger(x_v) |0\rangle$$

with

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



- $|\{p\}, N_1, N_2\rangle_s$ eigenstate of H for any choice of Bethe momenta $\{p\}$.
- **Choose distributions $\rho_i(p)$ to impose non-eq BC:**
- incoming particles arrive from free leads at μ_i
- **Distributions $\rho_i(p)$ must satisfy SBA equation.**



(Free baths Fermi-Dirac $\rho_i = f_i$ in Fock basis. Here – free baths in Bethe basis)

The Boundary Conditions II

The boundary conditions become OBA equations for: ρ_1, ρ_2

$$2\rho(p) = \frac{1}{2\pi} - \int_{-D}^{B_2} 2\rho(k)\mathcal{K}(k,p)dk - \int_{B_2}^{B_1} \rho(k)\mathcal{K}(k,p)dk$$

$$\rho_2(p) = \rho(p) \quad p \leq B_2$$

$$\rho_1(p) = \rho(p) \quad p \leq B_1$$

$$\mathcal{K}(p,k) = \frac{U}{\pi} \frac{k - \epsilon_d}{(p+k-2\epsilon_d)^2 + \frac{U^2}{4}(p-k)^2}$$

Bethe chemical potentials B_1, B_2
determined from μ_1, μ_2 minimizing:

$$F = \int_{-D}^{B_1} dp (p - \mu_1)\rho_1(p) + \int_{-D}^{B_2} dp (p - \mu_2)\rho_2(p)$$

- For $U=0$ distributions reduce to Fermi-Dirac distributions

These are **OBA** eqns for: $\epsilon_d \geq B_j$ (in **co-tunneling regime**)

- otherwise, eqns more complicated – include complex solutions (Non-equil FES)

Current and Dot Occupation

The scattering state $|\{p\}\rangle_s^{\mu_1\mu_2}$ is determined in terms of ρ_1, ρ_2

- **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: $|\{p\}\rangle_{L \rightarrow \infty}^{\mu_1, \mu_2}$**

$$\Delta = t^2/2$$

Hybridization
width

$$\langle I \rangle_s^{\mu_1, \mu_2} = \int dp [\rho_1(p) - \rho_2(p)] \frac{\Delta^2}{(p - \epsilon_d)^2 + \Delta^2}$$

$$\langle n_d \rangle_s^{\mu_1, \mu_2} = \int dp [\rho_1(p) + \rho_2(p)] \frac{\Delta}{(p - \epsilon_d)^2 + \Delta^2}$$

- For $U=0$, Landauer-Buttiker formulas $\rho_i(p) \rightarrow f_i(p)$
- For $U>0$, in the Bethe-basis, expressions look “simple”:
 - excitations undergo phase shifts only
 - $\rho_i(p)$ incorporate interactions and boundary conditions

Current vs. Voltage IRL

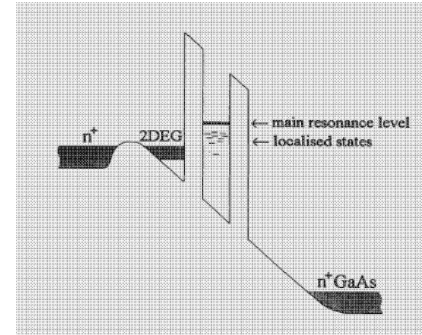
• Compute exactly current as a function of Voltage:

Non-monotonicity in U

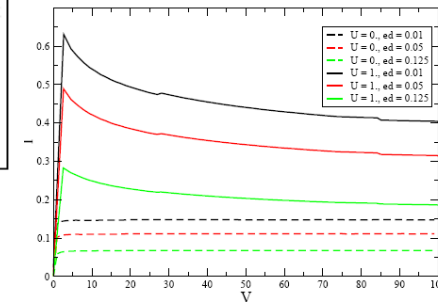
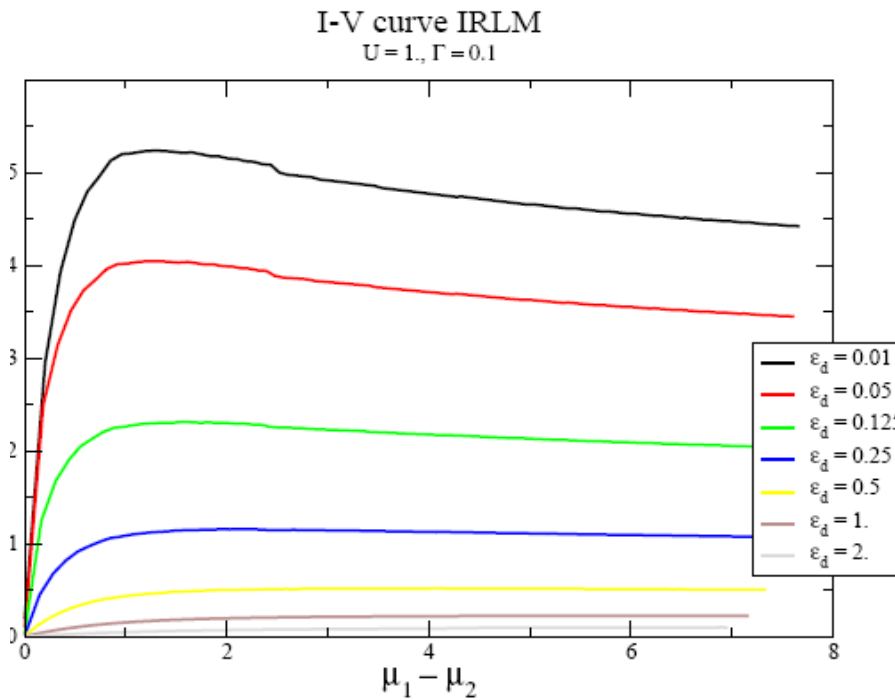
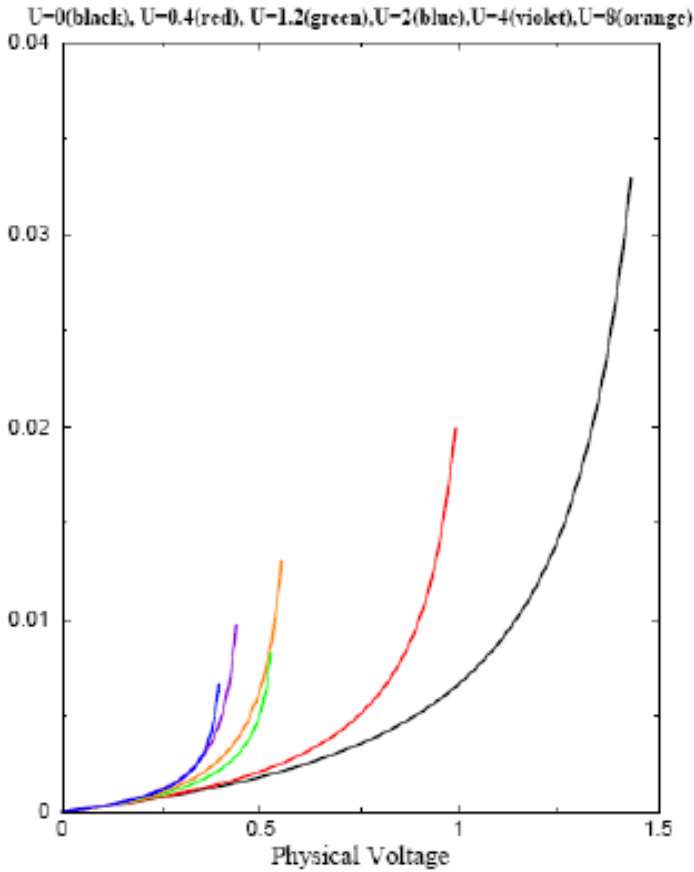
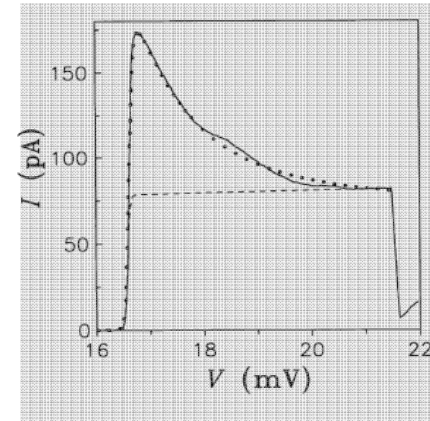
- FES : repulsion vs IR Catastrophe (Borda et al)
- Duality : $U/2 \rightarrow 1/(U/2)$ (Schiller NA)

Fermi Edge Singularity
out of equilibrium

(Matveev & Larkin, Levitov, Abanin..)



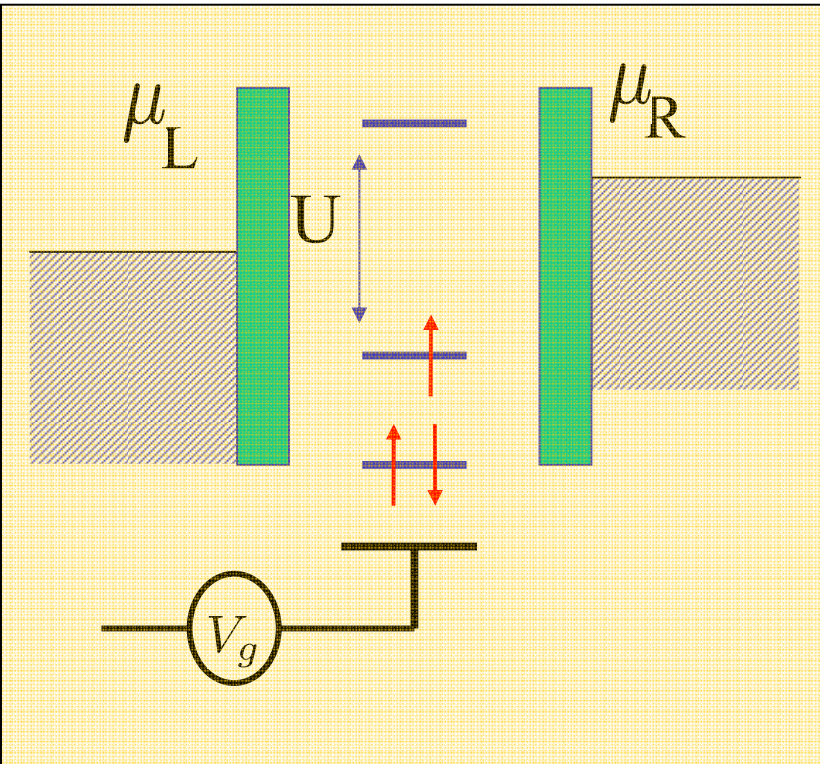
(Geim et al '93)



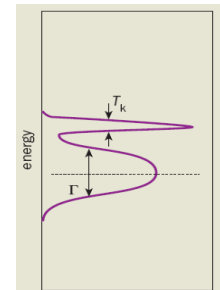
Other approaches:

1. Perturbative RG Borda, Zawadowski 06'
2. Perturbative expansion Doyon 07'
3. DMRG Scmitteckert 07'
4. Model at self-dual point ($U=2$) \rightarrow BSG : BA + dressed Landauer: Boulat, Saleur (08') cf Fendley, Ludwig, Saleur 95'

The Quantum Dot - equilibrium

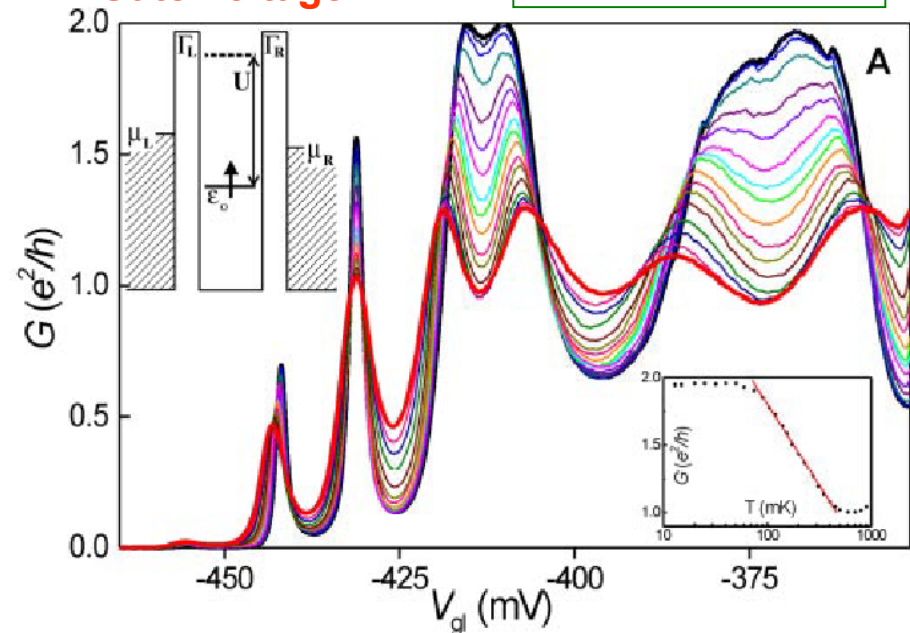


- Can control number of electrons on dot using gate voltage
- For odd number of electrons- quantum dot acts as **quantum impurity**
- New collective behaviours, e.g. **Kondo effect**
 - formation of narrow peak at the Fermi surface as $T \rightarrow 0$

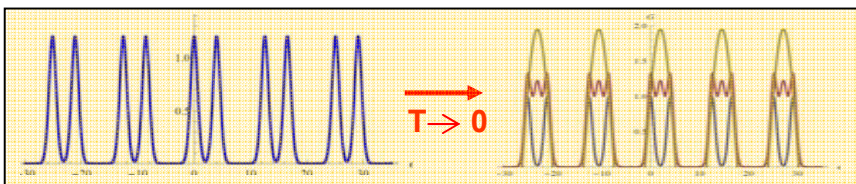


Conductance vs Gate voltage

van der Wiel *et al.*
Science 2000



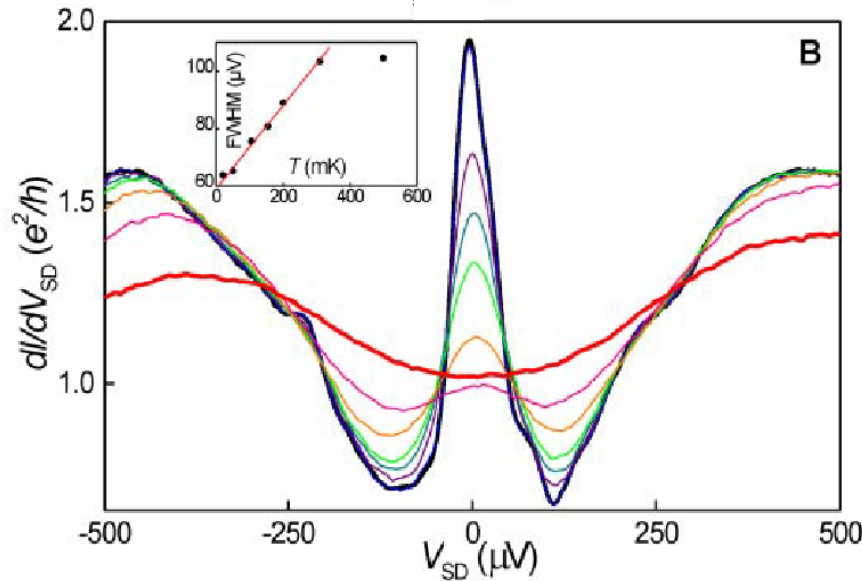
Kondo effect - zero bias (equilibrium):
filling of odd valleys of Coulomb Blockade at low T



The Quantum Dot - nonequilibrium

van der Wiel *et al.*,
Science 2000

Conductance vs. bias voltage



• Questions:

- The nonequilibrium Kondo Effect
- Effects of temperature,
- magnetic field
- DOS in and out of equilibrium
- Decoherence

• Nonequilibrium Anderson model:

small dots:
 $\delta \geq U, V ; T_k = \frac{1}{\pi} \sqrt{2U\Gamma} e^{\pi\epsilon_d(\epsilon_d+U)/(2U\Gamma)} \ll \Theta_D$

$$H = -i \sum_{j=1,2} \int \psi_{ja}^\dagger \partial \psi_{ja} dx + \epsilon_d d_a^\dagger d_a + t \sum_{j=1,2} (\psi_{ja}^\dagger(0) d_a + h.c.) + U n_{d\uparrow} n_{d\downarrow}$$

Equilibrium BA: *Wiegmann & Tselik, Kawakami & Okiji '80-'83*

• Solve:

Previous attempt - *Konik, Ludwig, Saleur '02* - valid only close to equilibrium

Approach: Landauer + *dressed BA*, developed by Fendley Ludwig Saleur '95

- Based on dressed excitations: holon, spinon. But voltage in leads acts on bare electrons
- **Approximation**: electron \sim spinon + holon. (No spinon-antispinons, no holon-antiholons are included.)
- **Approximation invalid** in general - except for $V=0$, (cf *N.A. '82*)

Anderson Model of the single-level Quantum Dot

Anderson model out equilibrium: Open Bethe Ansatz (H=0 T=0)

- Similar construction of scattering eigenstates

- Bethe momenta - complex strings $k_{\pm}(\lambda) = x(\lambda) \pm y(\lambda)$

$$x(\lambda) = \epsilon_d + \frac{U}{2} - \left[\frac{\lambda + (\epsilon_d + \frac{U}{2})^2 + ((\lambda + (\epsilon_d + \frac{U}{2})^2)^2 + U^2\Gamma^2)^{1/2}}{2} \right]^{1/2}$$

$$y(\lambda) = \left[\frac{-(\lambda + (\epsilon_d + \frac{U}{2})^2) + ((\lambda + (\epsilon_d + \frac{U}{2})^2)^2 + U^2\Gamma^2)^{1/2}}{2} \right]^{1/2}$$

- Satisfying

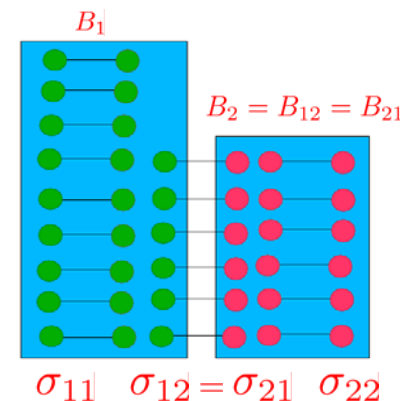
$$e^{2ix(\lambda_{\alpha})L} = \prod_{\beta} \frac{\lambda_{\alpha} - \lambda_{\beta} + i2U\Gamma}{\lambda_{\alpha} - \lambda_{\beta} - i2U\Gamma}$$

- Four types of momentum-strings: 11, 12, 21, 22

described by distributions

$$\sigma_{11}(\lambda), \sigma_{22}(\lambda), \sigma_{12}(\lambda), \sigma_{21}(\lambda)$$

- Distributions determined by SBA-eqn : **free leads in Bethe basis**



$$4\sigma(\lambda) = -\frac{1}{\pi} \frac{dx(\lambda)}{d\lambda} - \frac{1}{\pi} \int_{B_2}^{\infty} d\lambda' 4\sigma(\lambda') \frac{2U\Gamma}{(2U\Gamma)^2 + (\lambda - \lambda')^2} - \frac{1}{\pi} \int_{B_1}^{B_2} d\lambda' \sigma(\lambda') \frac{2U\Gamma}{(2U\Gamma)^2 + (\lambda - \lambda')^2}$$

$$\sigma_{12}(\lambda) = \sigma_{21}(\lambda) = \sigma_{22}(\lambda) = \sigma(\lambda),$$

$$B_2 \leq \lambda \leq \infty$$

$$B_1 \leq B_2 = B_{12} = B_{21} \leq \infty$$

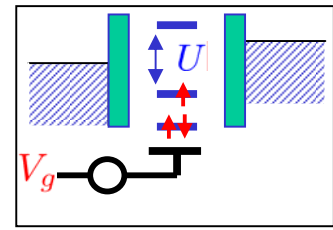
$$\sigma_{11}(\lambda) = \sigma(\lambda),$$

$$B_1 \leq \lambda \leq \infty$$

- Bethe chemical potentials: B_1, B_2 determined by physical potentials μ_1, μ_2 , minimizing

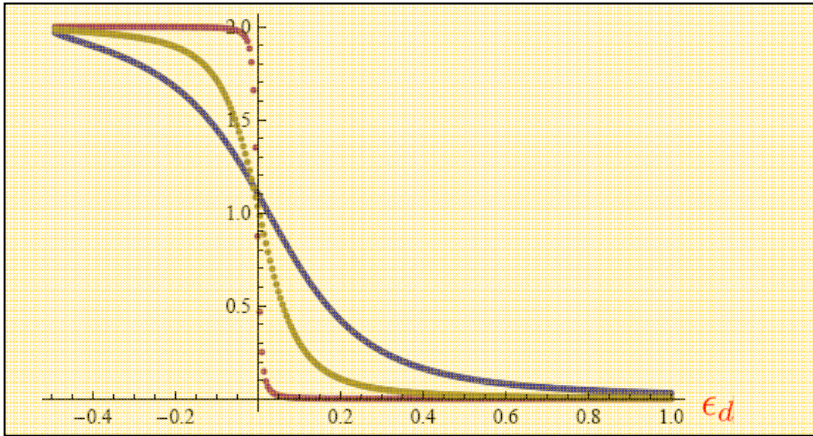
$$F = \int_{B_1}^{\infty} 2(x(\lambda) - \mu_1)\sigma_{11}(\lambda)d\lambda + \int_{B_{12}}^{\infty} (2x(\lambda) - \mu_1 - \mu_2)(\sigma_{12}(\lambda) + \sigma_{21}(\lambda))d\lambda + \int_{B_2}^{\infty} 2(x(\lambda) - \mu_2)\sigma_{22}(\lambda)d\lambda$$

Conductance in and out of equilibrium



Conductance $G(V=0, \epsilon_d)$ vs. gate voltage ϵ_d

$\Gamma = 0.125, 0.05,$ and 0.005 for blue, brown, and purple.

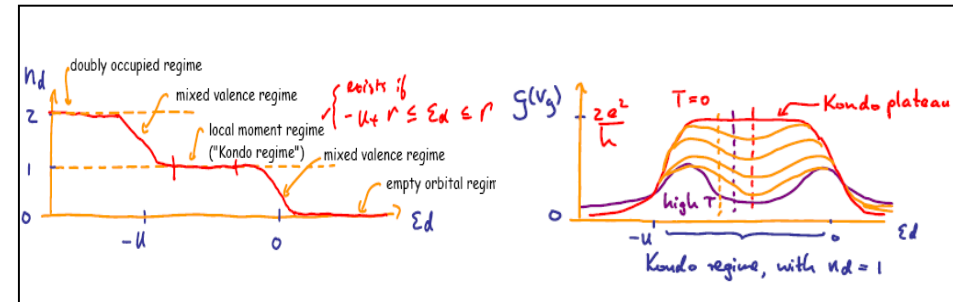


- Direct calculation from current.

- Verifies Friedel SR

- TBA vs SBA

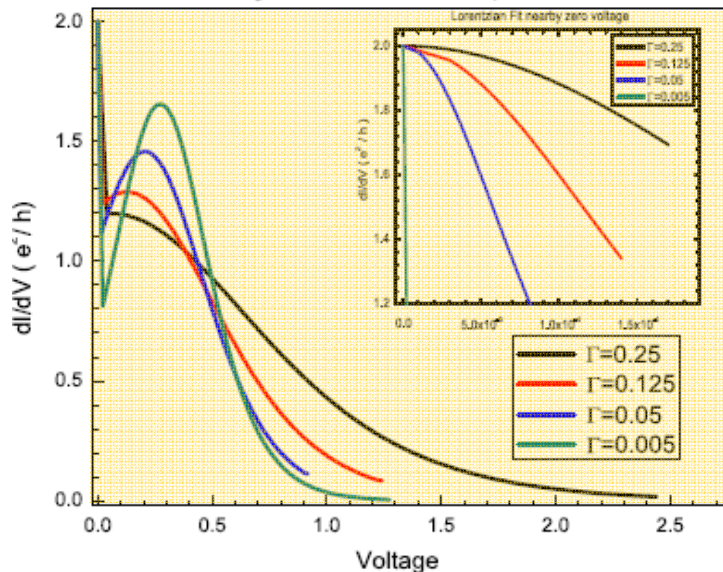
$$G = \frac{e^2}{h} \sum_{\sigma} \sin^2(\pi n_{d,\sigma})$$



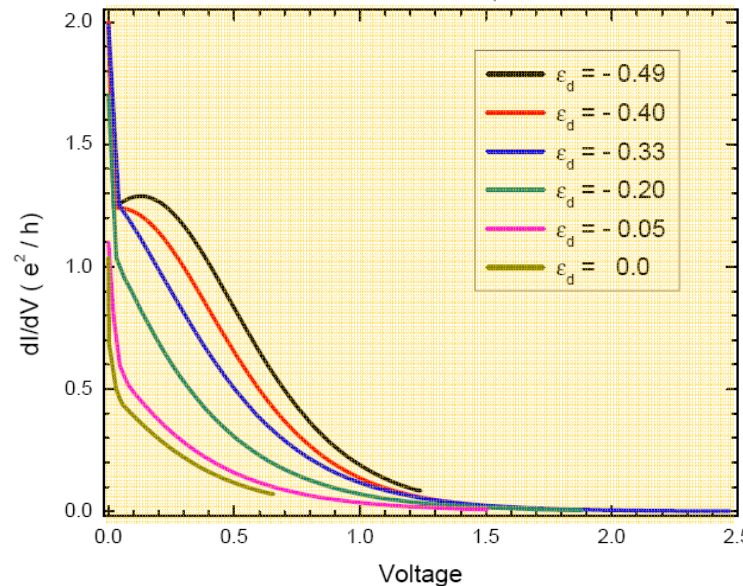
Von Delft, notes

Conductance $G(V, \epsilon_d, \Gamma)$ vs. bias voltage V (preliminary)

Differential Conductance vs Voltage with different Γ
($\epsilon_d = -0.49, U=1, D=80, \mu_1 \sim 0.0$)

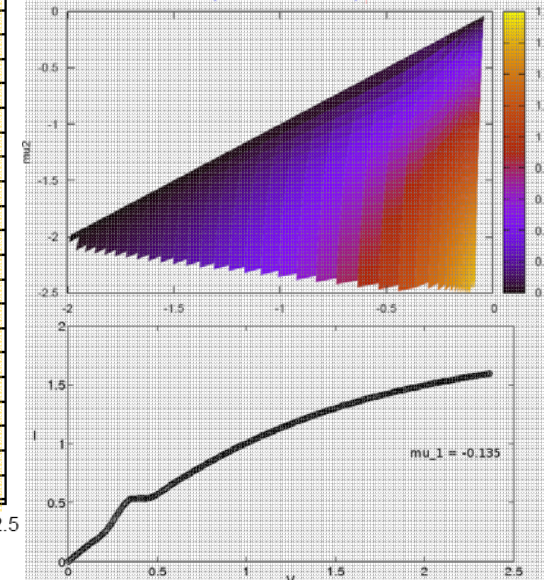


Differential Conductance vs Voltage with different ϵ_d
($\Gamma = 0.125, U=1, D=80, \mu_1 \sim 0.0$)



Full description:

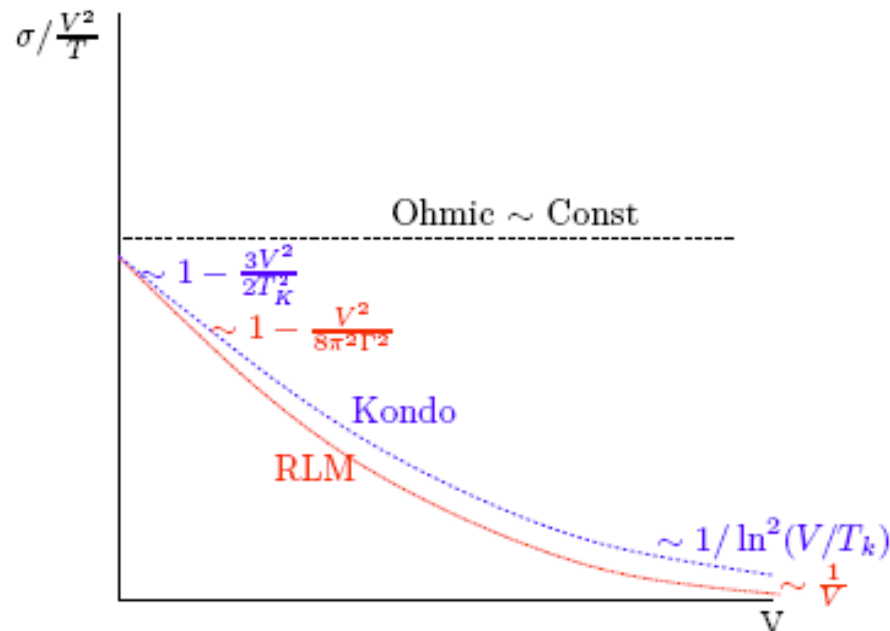
$$I(\mu_1, \mu_2)$$



The Kondo effect forms as ϵ_d is decreased, destroyed as the bias voltage is increased

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

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)*

Conclusions

- **Showed:**
Scattering eigenstates with non-eq BC – Steady States
- **Computed:**
Steady state current, entropy production rate
- **Many Generalizations and applications:**

Non-equilibrium Impurity

- Non-equilibrium in other impurity models
Multichannel versions
- Non-equilibrium at $T > 0, T_1 \neq T_2$, thermal currents
- More leads: non-equilibrium DOS (*Lebanon&Schiller*)

Non-equilibrium Wire

- The Luttinger liquid (*e.g.* nanotubes)
- AB Interferometers (with/without impurities)

Scattering

- Inclusive, exclusive scattering amplitudes
- Elastic, inelastic scattering amplitudes $T > 0$

Quantum full counting statistics, Entropy fluctuations, noise, Onsager relations

Bethe basis vs. Fock basis

- **To the left of the impurity** $|\{p\}\rangle$ **is eigenstate of** $H_0 - \sum_i \mu_i N_i$ **in the Bethe - basis**
- **Choose momenta so incoming state consists of two free Fermi seas in the Bethe - basis**

S-Matrix	$S=1$	$S \neq 1$
Basis	Fock Basis	Bethe Basis
Fermi-sea momenta	Fermi – Dirac distributions $\rho_i^0 = \theta(\mu_i - p)$	Bethe distributions $\rho_i(p)$

- *How to determine $\rho_i(p)$, i.e. what is the ground state of $H_0 - \sum_i \mu_i N_i$ in the Bethe basis?*
- *Not a scattering problem! Solve on the ring \rightarrow Bethe Ansatz equations.*

The Boundary Conditions III

How to choose the momenta $\{p\}$ so as to have the ground state?

Auxiliary problem: in \mathcal{H}_0 find the ground state in Bethe basis on a ring of length L :

$$e^{ip_j L} = \prod_{l=1}^N S(p_j, p_l)$$

Or:

$$p_j = \frac{1}{L} \sum_{l=1}^N \ln S(p_j, p_l) + \frac{2\pi}{L} I_j$$

- ***The BA eqns describe the free leads on a ring (in the Bethe basis)***
- ***For the ground state choose: $I_{j+1} = I_j + 1$***

Quantum Impurities: strong correlations out-of-equilibrium

Experimentally well studied : *Goldhaber-Gordon et al, Cronenwett et al, Schmid et al*

Theoretically - example of interplay of **strong correlation** and **nonequilibrium**

• **Nonequilibrium** - **poorly understood**



- Non-equilibrium systems are all different- it is unclear what if anything they all have in common.
 - **No unifying theory such as Boltzmann's statistical mechanics**
- Many of our standard physical ideas and concepts are not applicable (Scaling? RG? Universality?)
- New inherently non-equilibrium phenomena:
 - e.g. **entropy production, dissipation**

• **Strong correlations** - **poorly understood**

Perturbative approaches fail

- **New degrees of freedom emerge at low energy**
- **New collective behavior e.g. Kondo effect in and out of equilibrium**

Can fully discuss issues – in quantum impurity context

The Boundary Conditions I

Why not choose Fermi-Dirac distribution for the momenta?

- *Fermi-Dirac* distributions describe free leads in the **Fock basis**,
- plane waves $F_{\text{fock}}(x_1, \dots, x_N) = e^{i\sum_j^N p_j x_j}$ eigenstates of leads $H_o = -i \sum_j \partial_j$
- The wave functions on the left of the impurity (using $\alpha_{ip}(x) \rightarrow \psi_i(x)$)
 $F_{\text{bethe}}(x_1, \dots, x_N) = e^{i\sum_j^N p_j x_j} e^{i\sum_{s<t}^N \Phi(p_s, p_t) \text{sgn}(x_s - x_t)}$
- also eigestates of $H_o = -i \sum_j \partial_j$ written in the **Bethe Basis**

Why different bases?

- All fermions are right-movers with same velocity $\Rightarrow E = k_1 + k_2 = (k_1 + q) + (k_2 - q)$.
- Energy levels infinitely degenerate.
- Scattering matrix **S** corresponds to a choice of basis in degenerate space.
- $e^{ik_1 x_1 + ik_2 x_2} [A\theta(x_1 - x_2) + (SA)\theta(x_2 - x_1)]$ is eigenstate of $H_o = -i(\partial_1 + \partial_2)$ for any S
- $S = 1$ corresponds to the **Fock basis**
- $S = e^{2i\Phi}$ corresponds to the **Bethe basis** -the natural basis to turn on the interaction
cf. degenerate perturbation theory