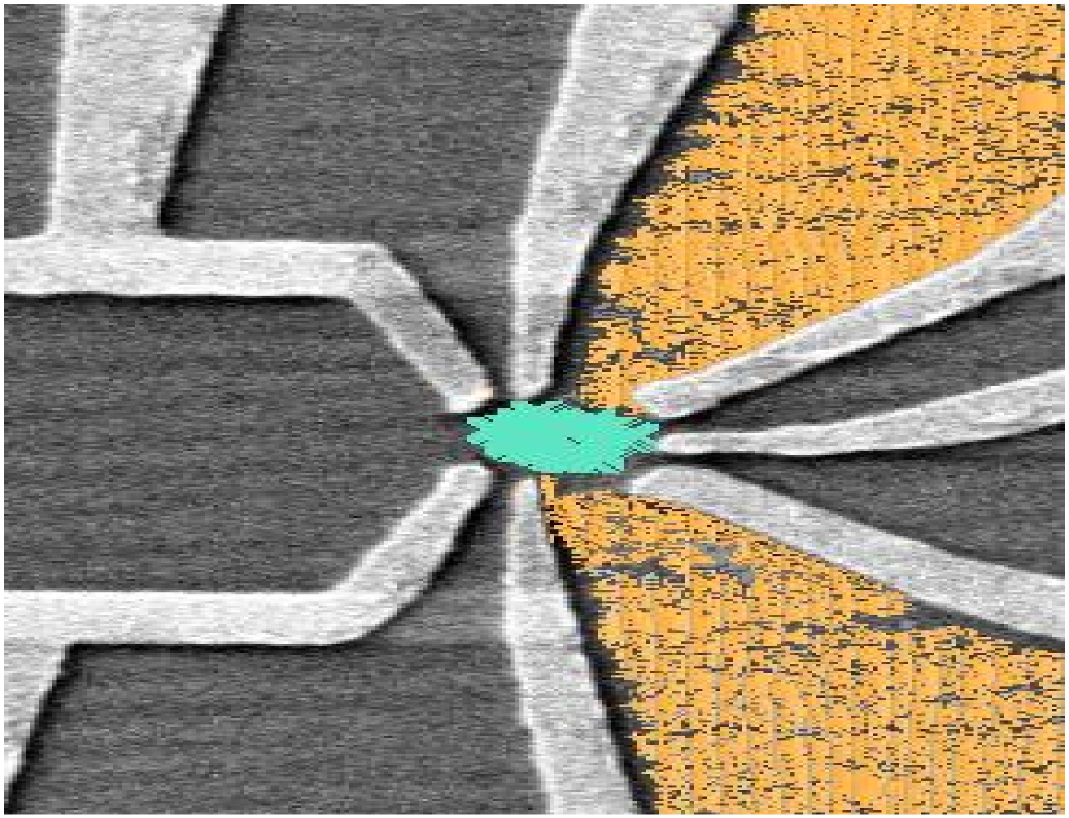
Quantum Impurities Out of Equilibrium



Natan Andrei

Rutgers
Department of
Physics and Astronomy

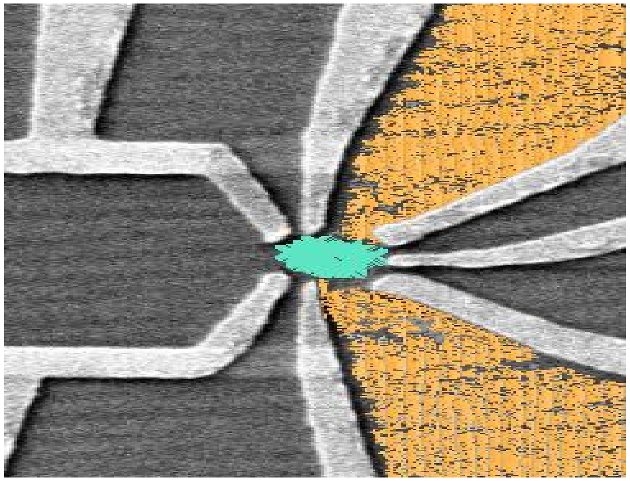
With collaborators:

P. Mehta **- Princeton**
C. Bolech **- Rice**
A. Jerez **- NJIT**
S.-P Chao **- Rutgers**
G. Palacios **- Rutgers**

Florence, September 2008

Quantum Impurities out-of-Equilibrium

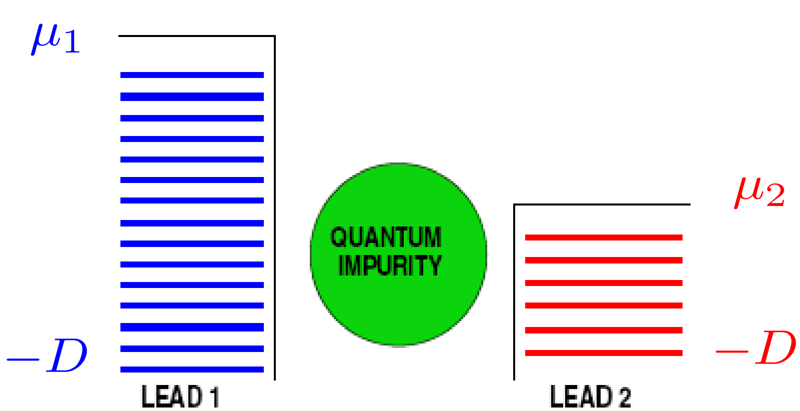
- **The quantum impurity - *experimentally*:** Goldhaber-Gordon *et al*, Conenwett *et al*, Schmid *et al*



- **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** $I = I(V,T)$?



$$\boxed{H = H_{leads} + H_{imp} + H_{leads-imp}}$$

Leads = Fermi seas, i=1,2

$$\boxed{H_{leads} = \sum_{i,k} \epsilon_k c^\dagger_{i\vec{k}} c_{i\vec{k}}}$$

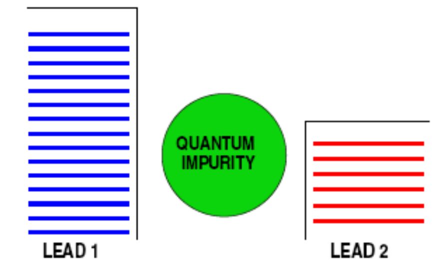
Non-equilibrium

$$\boxed{V = \mu_1 - \mu_2 \neq 0}$$

Quantum Impurity Hamiltonian $(3d \rightarrow 1d)$

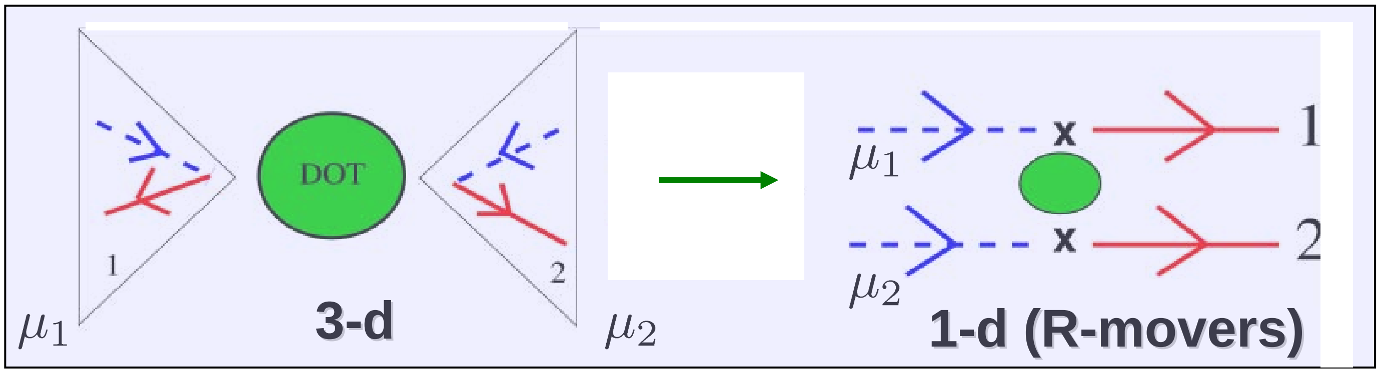
- **Impurity Hamiltonian (3d):**

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



$$H = H_{leads} + H_{imp} + H_{leads-imp}$$

Unfold 3d Hamiltonian $\longrightarrow$ 1d field theory:



$$\begin{aligned} \psi_{i\epsilon a} &\equiv \int d^3k\, \delta(\epsilon_{\vec{k}} - \epsilon)\, c_{i\vec{k}a} \\ \{\psi_{i\epsilon a}, \psi^\dagger_{j\epsilon' b}\} &= \delta_{ab}\,\delta_{ij}\,\delta(\epsilon - \epsilon')\nu(\epsilon) \\ \psi_{ia}(x) &= \int_{-D}^{D} \frac{d\epsilon}{\sqrt{\nu}}\, e^{i\epsilon x}\, \psi_{i\epsilon a} \end{aligned}$$

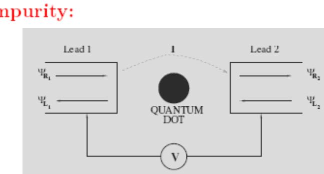
Affleck Ludwig 95'

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

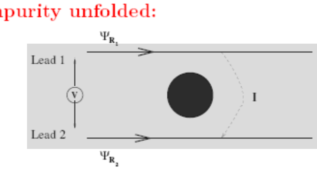
- **Impurity Hamiltonian (1d): Low-energy universality**

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

The Quantum Impurity:



The Quantum Impurity unfolded:



Non-equilibrium: Time-dependent Description

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

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

Description of Nonequilibrium requires two elements: H, ρ_o or H, H_o; Equilibrium requires only H.

For T > 0 :

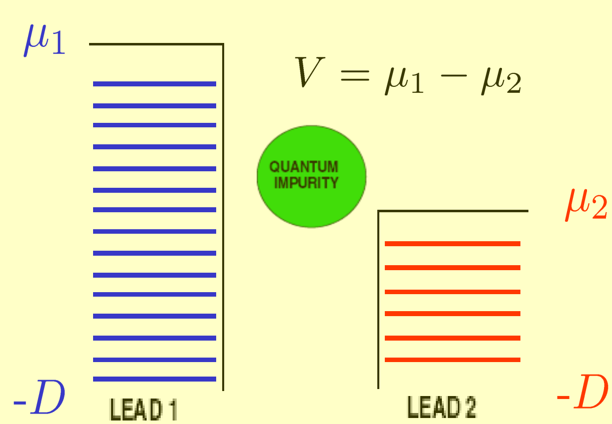
1. initial condition: ρ_o
2. evolution: $U(t,t_o) = T\{e^{-i\int_{t_o}^{t} dt' H(t')}\}$
3. density matrix: $\rho(t) = U(t,t_o)\rho_o U^\dagger(t,to)$
4. non equil value: $\langle\hat{O}(t)\rangle = Tr\{\rho(t)\hat{O}\}$

For T = 0 :

1. initial condition: $|\phi_o, V\rangle$
2. evolution: $U(t,t_o) = T\{e^{-i\int_{t_o}^{t} dt' H(t')}\}$
3. evolved state: $|\psi(t)\rangle_V = U(t,t_o)|\phi_o, V\rangle$
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:

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



The Steady State (open system limit)

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

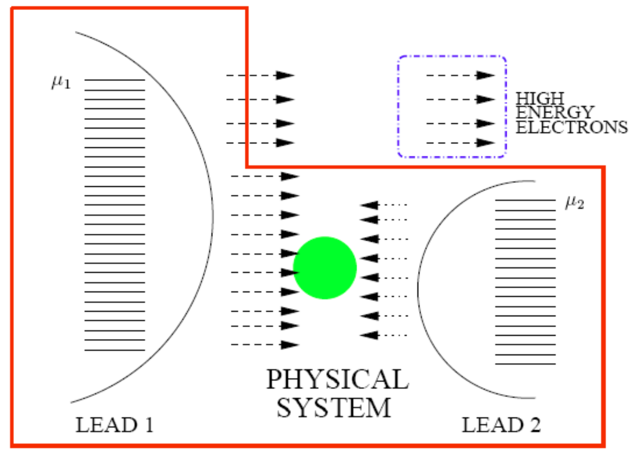
- **Leads good thermal baths, infinite volume limit - open system**

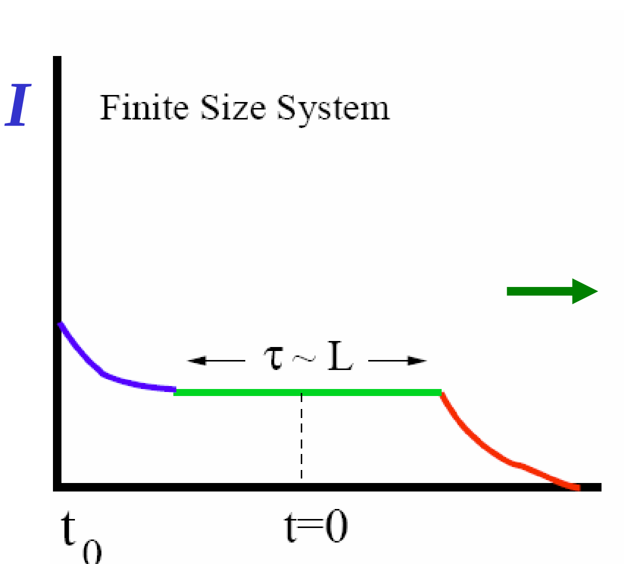
$\Rightarrow \exists \lim_{t_o \to -\infty}$, **no *IR* divergences,** $\frac{1}{L} \ll \frac{1}{|t_0|} \ll \eta \to 0$ **(B Doyon, NA,** *PRB* ‘05)

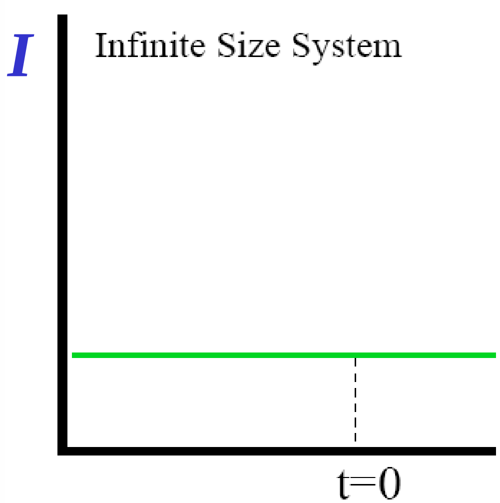
(order by order in P.T.)

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 $\frac{1}{L} \ll \frac{1}{|t_o|} \ll \eta \to 0$:

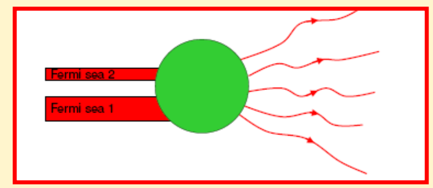
$$\longrightarrow \quad \boxed{|\psi, V\rangle_s = U(0, -\infty)|\phi_o, V\rangle}$$ **a well defined state.**

Properties:

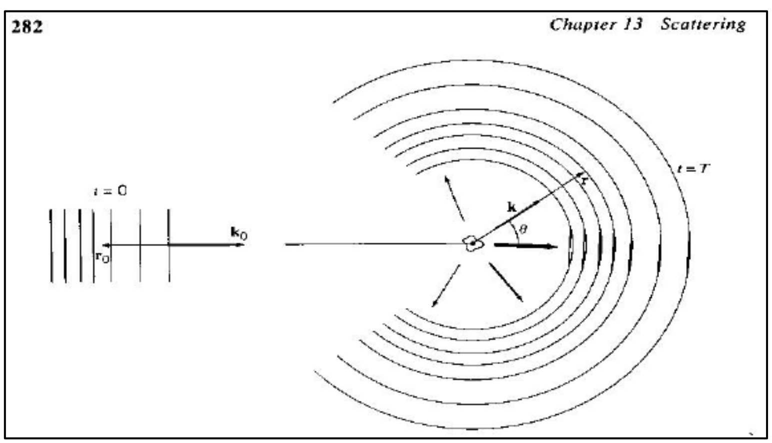
P. Mehta, N.A. *PRL 96*, '06

- $|\psi, V\rangle_s$ **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 $\to$ boundary condition
- $|\psi, V\rangle_s$ **scattering state** - eigenstate on the **infinite line**



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

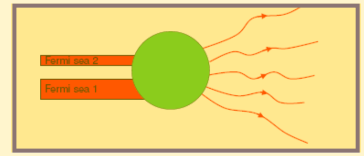
$$H = \frac{1}{2m} p^2 + V(x)$$

with incoming boundary condition

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

(Both H, H_o enter description)

The Non-equilibrium Steady State

- Non-equilibrium T=0 steady state is described by: $|\psi, V\rangle_s =$ 

- Non-equilbrium value: $\boxed{\langle O \rangle_s = \langle \psi, V | O | \psi, V \rangle_s}$

- ***For T=0,*** $|\phi_o, V\rangle \xrightarrow{\text{L-S}} |\psi, V\rangle_s$ $\quad |\phi_o, V\rangle$ ***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*** $|\phi_n\rangle \in \mathcal{H}_o^{\perp, V}$

- ***For T>0,*** "free leads" boundary conditions: $p_n^o = e^{-\beta E_n^o}/Z_o$

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

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

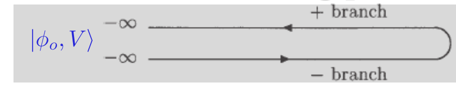
In steady state - $\exists$ "non-thermal" density operator! **cf. Hershfield '93**

- In equilibrium: $\rho_0 \rightarrow \rho_s = \frac{1}{Z} e^{-\beta H}$ **(Keldysh $\longrightarrow$ Boltzmann)** **Doyon, N.A. '05**

Steady-states & Scattering States

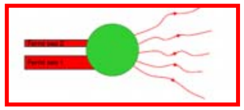
- **Time-dependent (Keldysh) vs. time-independent approach (Scattering)**

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



-Keldysh approach

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



-Scattering approach

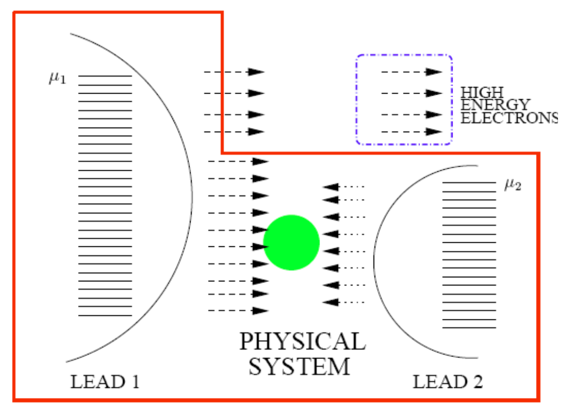
- Scattering approach: $|\psi, V\rangle_s \longleftrightarrow$ *non-perturbative Keldysh*

- **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* <u>and</u> *environment (open system)***

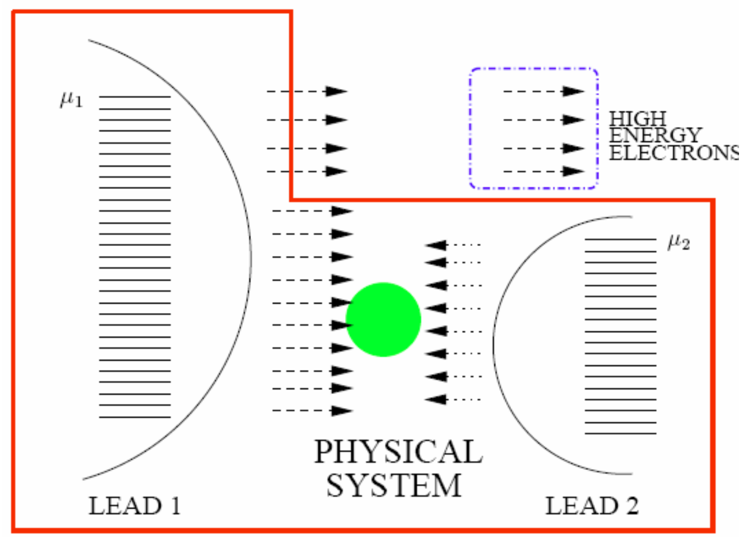


Entropy production and Dissipation

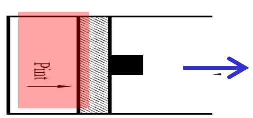
Non-equilibrium currents dissipate heat into environment:

- **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 ~ L → 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 and Dissipation

- **"Thermodynamic" approach:** (discontinuous system - defined w.r.t. quasi-equil , L ~ infty)

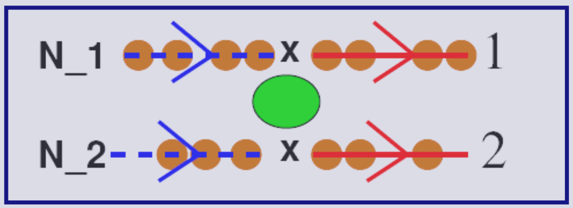
$$\sigma \equiv \frac{dS}{dt} = \frac{1}{T_1}\frac{\delta Q_1}{dt} + \frac{1}{T_2}\frac{\delta Q_2}{dt} = \left(\frac{1}{T_1} - \frac{1}{T_2}\right)\langle I_E\rangle_s + \left(\frac{\mu_1}{T_1} - \frac{\mu_2}{T_2}\right)\langle I_N\rangle_s$$

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

- **"Boltzmannian" approach – (distributions)**

  scattering $\longrightarrow$ change of distribution:

$\{f_i^- \ \mathrm{in}\}$
equilibrium distributions



$\{f_i^+ \ \mathrm{out}\}$
nonequilibrium distributions

$$\sigma = \sum_i \int dp\, v_F (f_i^+(p) - f_i^-(p)) \frac{p - \mu_i}{T_i}$$
$$f_i^+(p) = f_i^-(p)|R(p)|^2 + f_{\bar{i}}^-(p)|T(p)|^2$$

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

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

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

mixing ***relaxation***

Mixing + Relaxation

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

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

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

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

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

- 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:

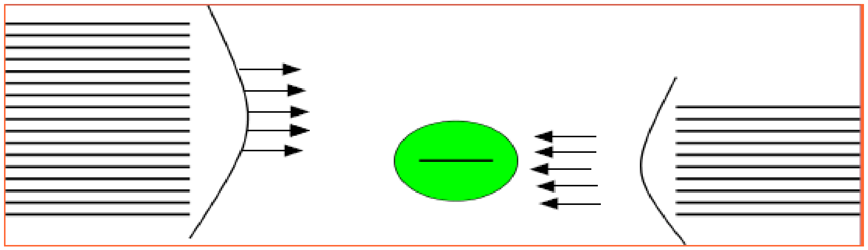
- **Traditional Bethe-Ansatz - inapplicable** $H|\psi\rangle = E|\psi\rangle \quad (+PBC)$
  - Periodic boundary conditions
  - **Closed System**: Equilibrium, Thermodynamics
- **New technology $\longrightarrow$ Scattering States**
  - Asymptotic Boundary conditions on the infinite line
  - **Open System**: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

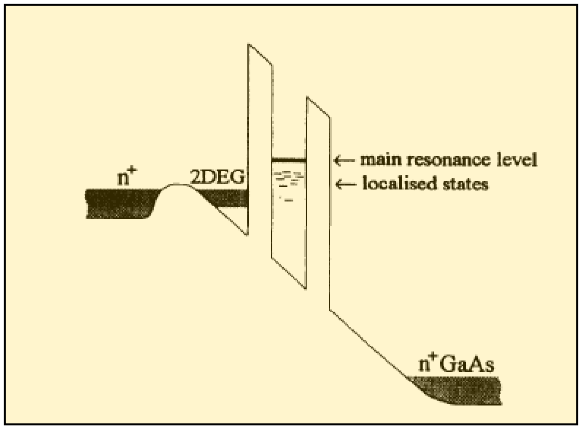
Scattering (Open) Bethe-Ansatz: $H|\psi\rangle_s = E|\psi\rangle_s$ scattering BC on ∞-line

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'

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

- **The 1-d Field Theory**

Thermodynamic BA *Filyov, Wiegman 80'*

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

***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**

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

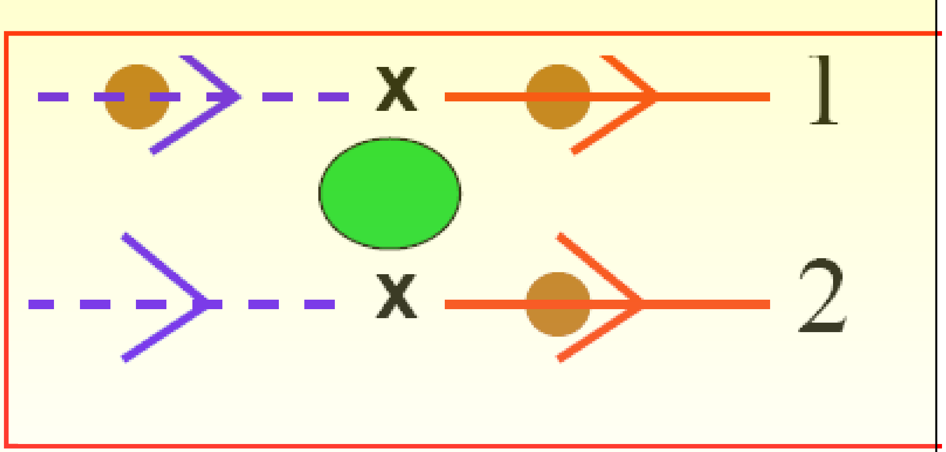
IRL: The Scattering State

Single-particle scattering eigenstates -

Level width: $\Delta = \frac{1}{2}t^2$

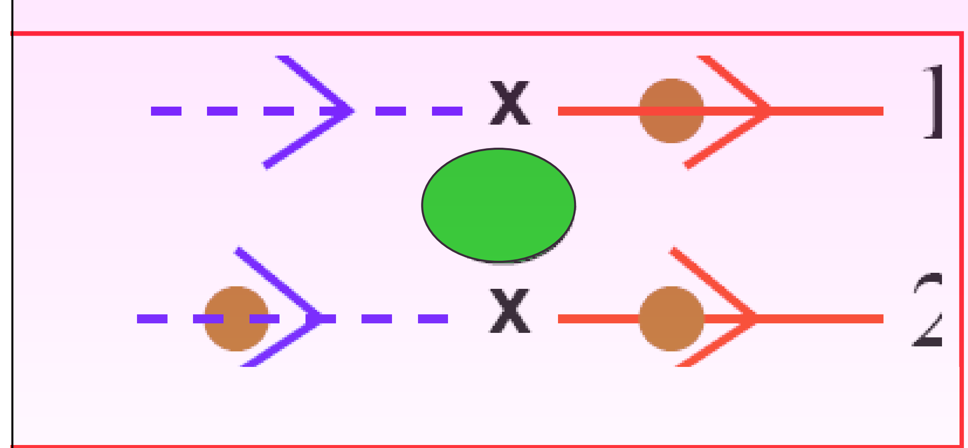
Phase shift : $e^{i\delta_p} = \dfrac{p-\epsilon_d-\Delta}{p-\epsilon_d+i\Delta}$

$|1p\rangle$



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

$|2p\rangle$



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

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

Renormalization prescription

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

Local discontinuity

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

constant - consistent with prescription

Boundary condition

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

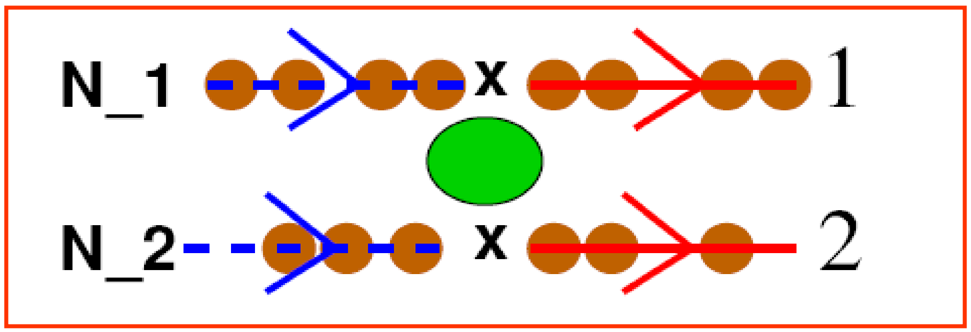
IRL: The Scattering State

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

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

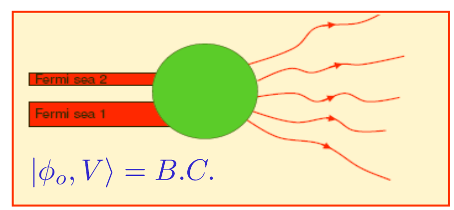
with

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



- $|\{p\}, N_1, N_2\rangle_s$ **eigenstate of** H **for any choice of Bethe momenta** $\{p\}$.

- **<u>Choose distributions</u>** $\rho_i(p)$ **<u>to impose non-eq BC:</u>**
  - incoming particle 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

$$
\begin{aligned}
2\rho(p) &= \frac{1}{2\pi} - \int_{-D}^{B_2} 2\rho(k)\mathcal{K}(k,p)dk - \int_{B_2}^{B_1} \rho(k)\mathcal{K}(k,p)dk \\
\rho_2(p) &= \rho(p) \quad p \le B_2 \\
\rho_1(p) &= \rho(p) \quad p \le B_1
\end{aligned}
$$

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

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: $\epsilon_d \ge B_j$ (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: $|\{p\}\rangle_{L\to\infty}^{\mu_1,\mu_2}$

$$\boxed{\Delta = t^2/2}$$

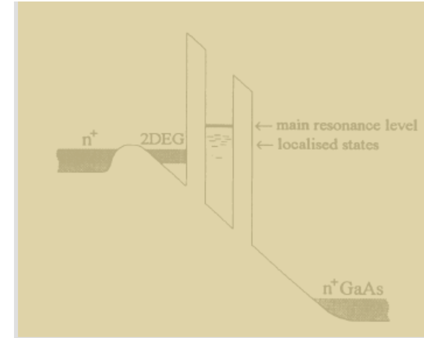
Hybridization width

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

- **For U=0, Landauer-Buttiker formulas** $\boxed{\rho_i(p) \to f_i(p)}$
- **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:**



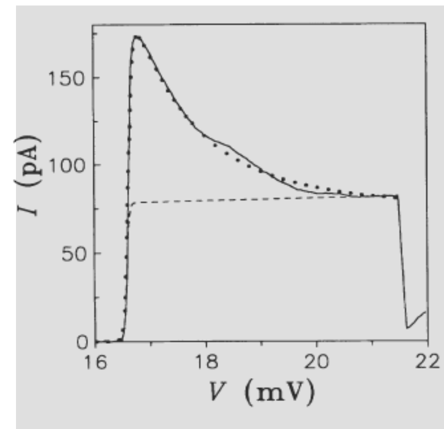
Non-monotonicity in U

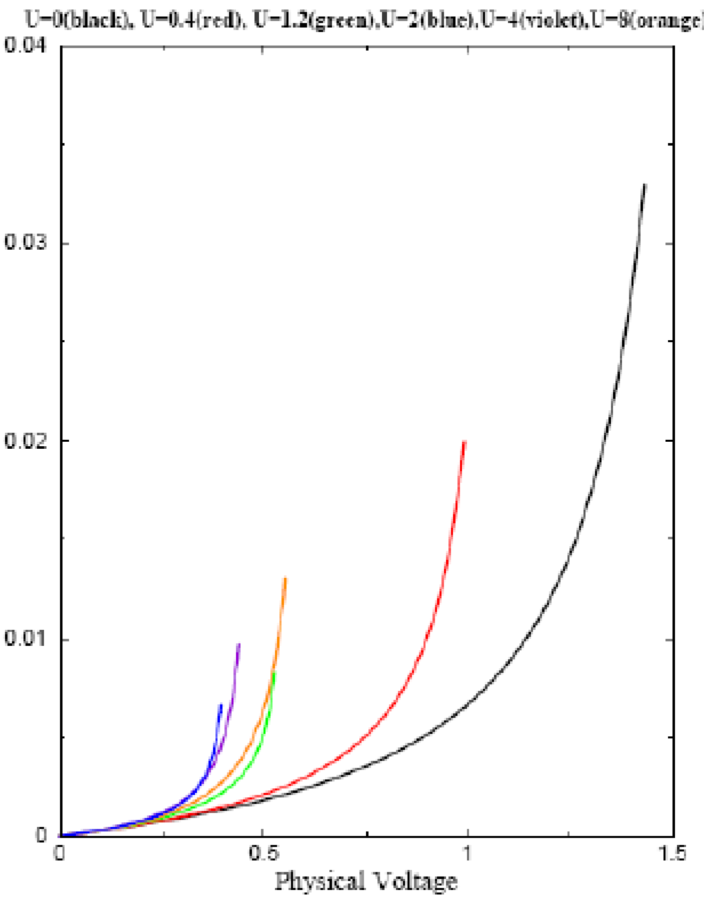
- **FES :** repulsion vs IR Catastrophe (*Borda et al*)
- **Duality :** $U/2 \to 1/(U/2)$ (*Schiller NA)*

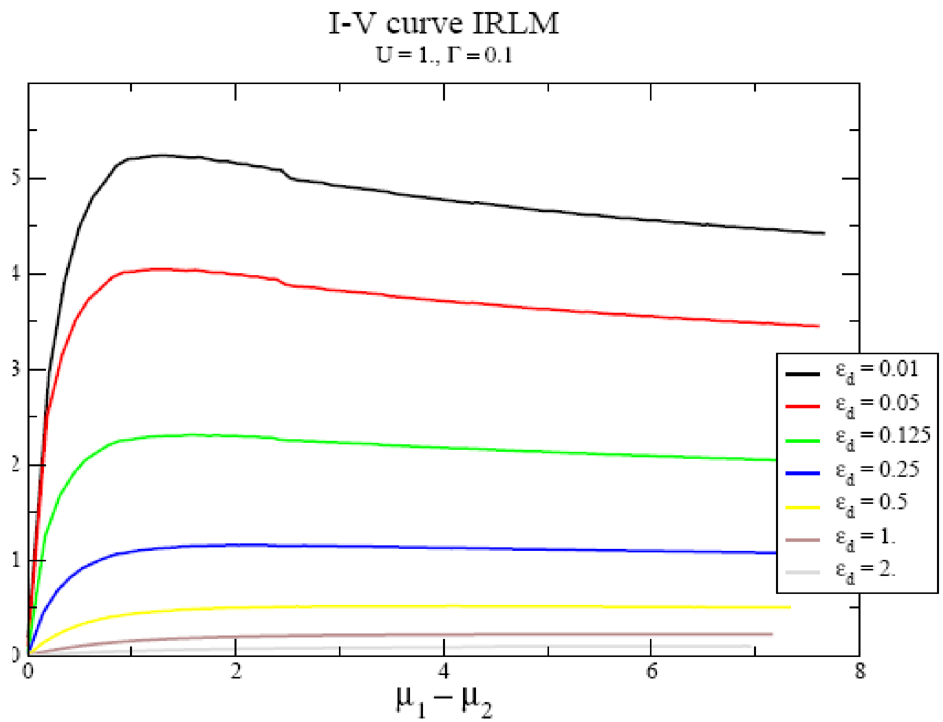
Fermi Edge Singularity out of equilibrium

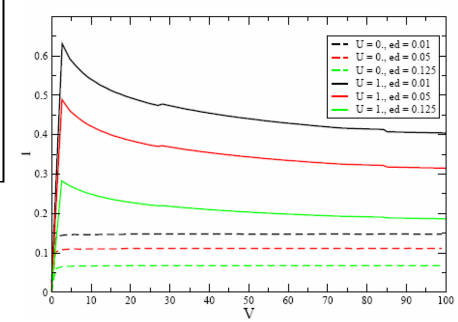
(Matveev & Larkin, Levitov, Abanin..)

(Geim et al '93)







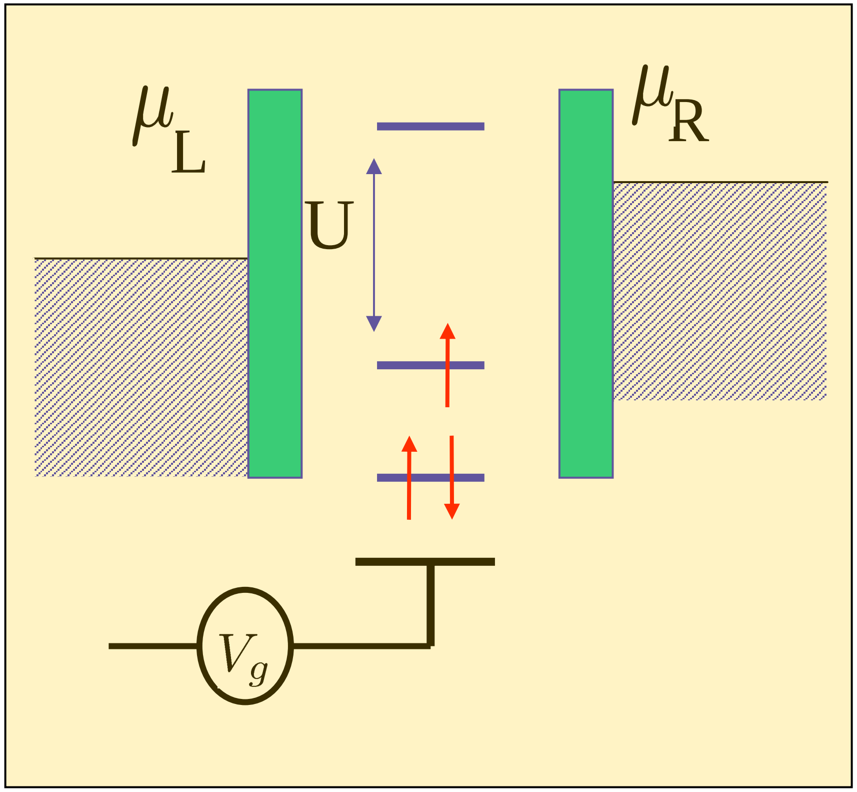


Other approaches:

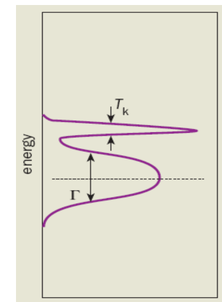
1. Perturbative RG Borda, Zawadowski 06' **2. Perturbative expansion** Doyon 07' **3. DMRG** Scmitteckert 07'

4. Model at self-dual point (U=2) → **BSG : BA + *dressed* Landauer**: Boulat, Saleur (08') **cf** Fendley, Ludwig, Saleur 95'

The Quantum Dot - equilibrium

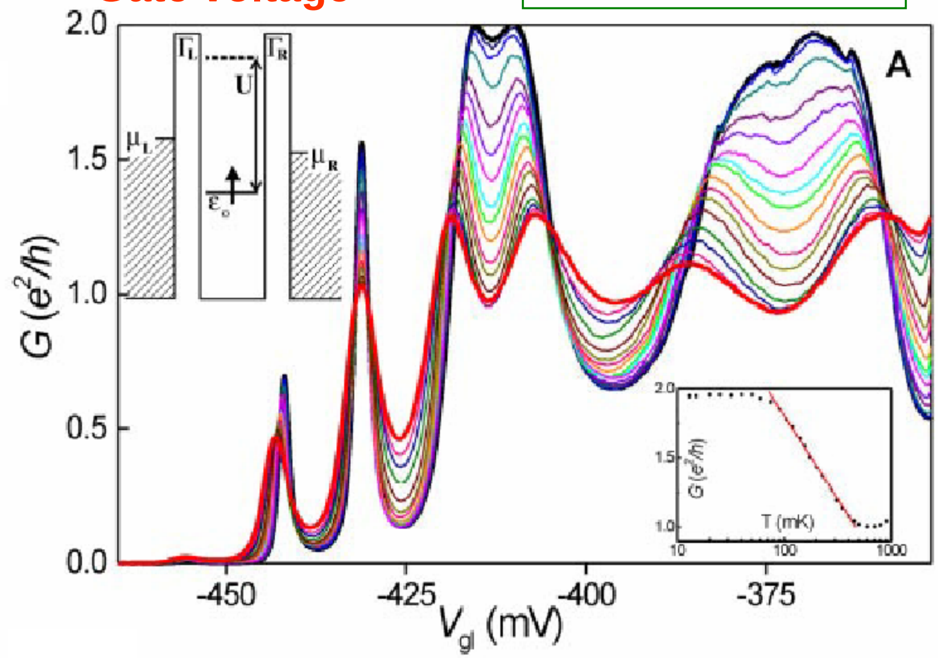


- Can control number of electrons on dot using gate voltage
- For odd number of electrons- quantum dot acts as **quantum impurity**
- New collective behaviours, e.g. **Kondo effect**
  - formation of narrow peak at the Fermi surface as T→ 0



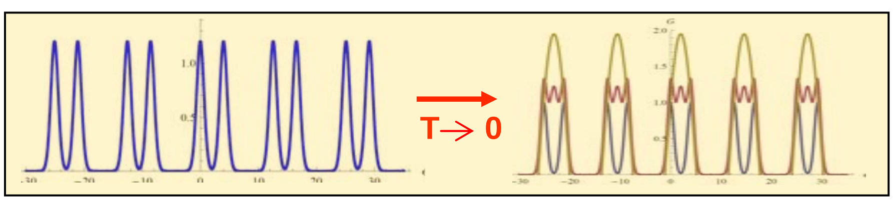
Conductance vs Gate voltage

van der Wiel *et al.* Science 2000



Kondo effect - zero bias (equilibrium):

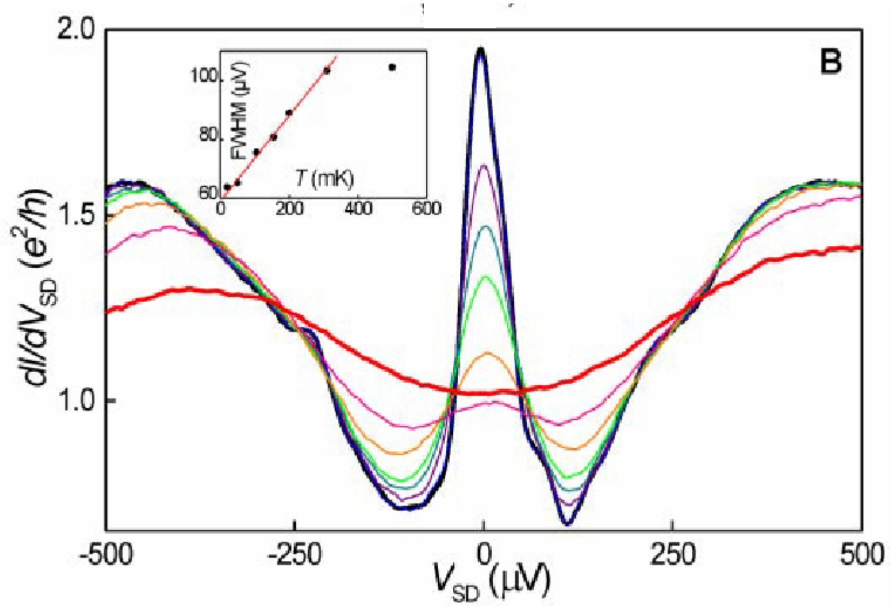
filling of odd valleys of Coulomb Blockade at low T



The Quantum Dot - nonquilibrium

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:

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

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

Equilibrium BA: *Wiegmann & Tsvelik, 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 ~ spinon + holon. No spinon-antispinons, no holon-antiholons.

- **Approximation invalid** in general - except for for **V=0, (cf N.A. '82)**

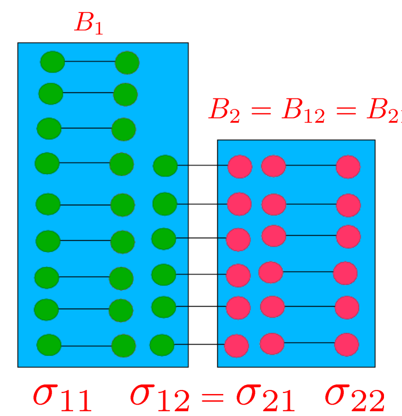
Anderson Model of the single-level Quantum Dot

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**

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

$$\sigma_{12}(\lambda) = \sigma_{21}(\lambda) = \sigma_{22}(\lambda) = \sigma(\lambda), \qquad B_2 \le \lambda \le \infty$$

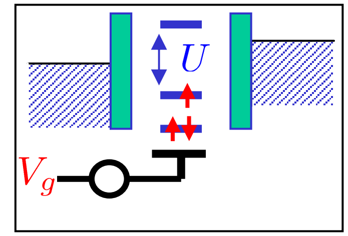
$$\sigma_{11}(\lambda) = \sigma(\lambda), \qquad B_1 \le \lambda \le \infty$$

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

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

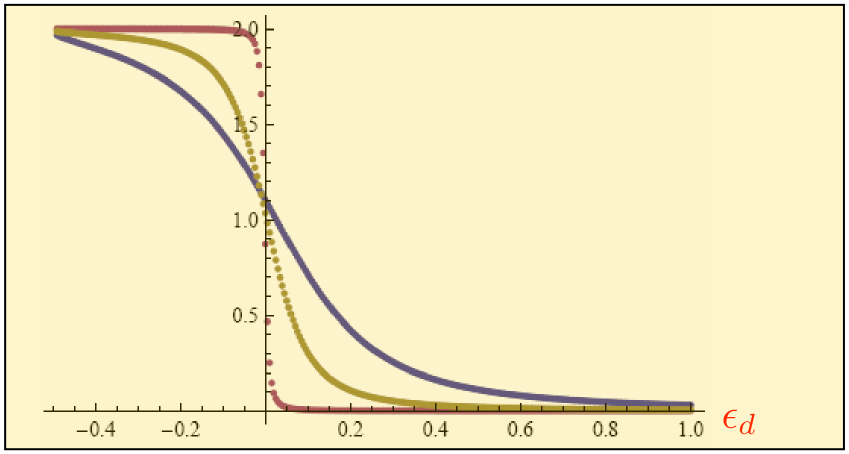
$$F = \int_{B_1}^{\infty} 2(x(\lambda) - \mu_1)\sigma_{11}(\lambda)d\lambda + \int_{B_{12}}^{\infty}(2x(\lambda) - \mu_1 - \mu_2)(\sigma_{12}(\lambda) + \sigma_{21}(\lambda))d\lambda + \int_{B_2}^{\infty} 2(x(\lambda) - \mu_2)\sigma_{22}(\lambda)d\lambda$$

Conductance in and out of equilibrium



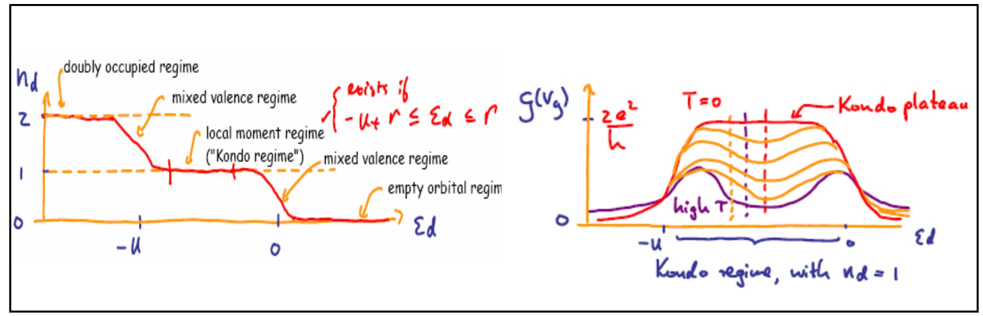
- **Conductance $G(V=0,\epsilon_d)$ vs. gate voltage ϵ_d**

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



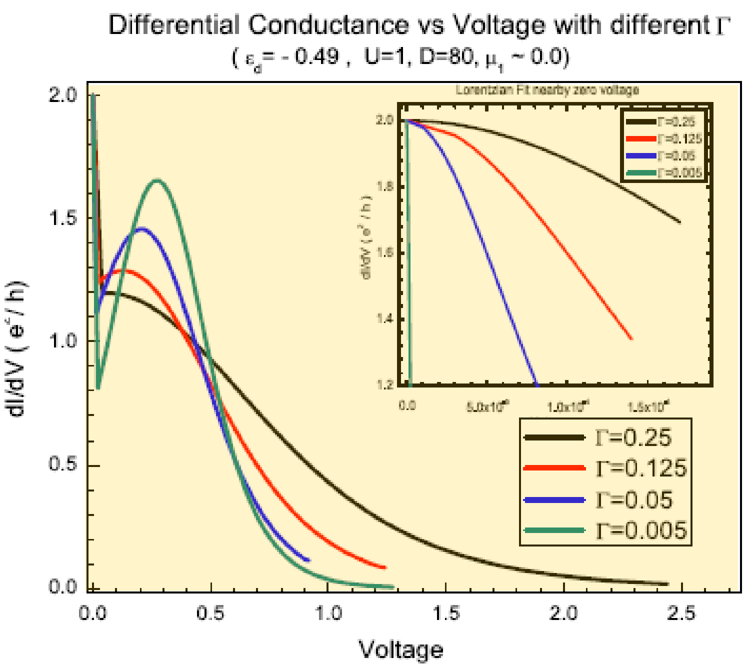
- ***Direct calculation from current.***
- ***Verifies Friedel SR***
- ***TBA vs SBA***

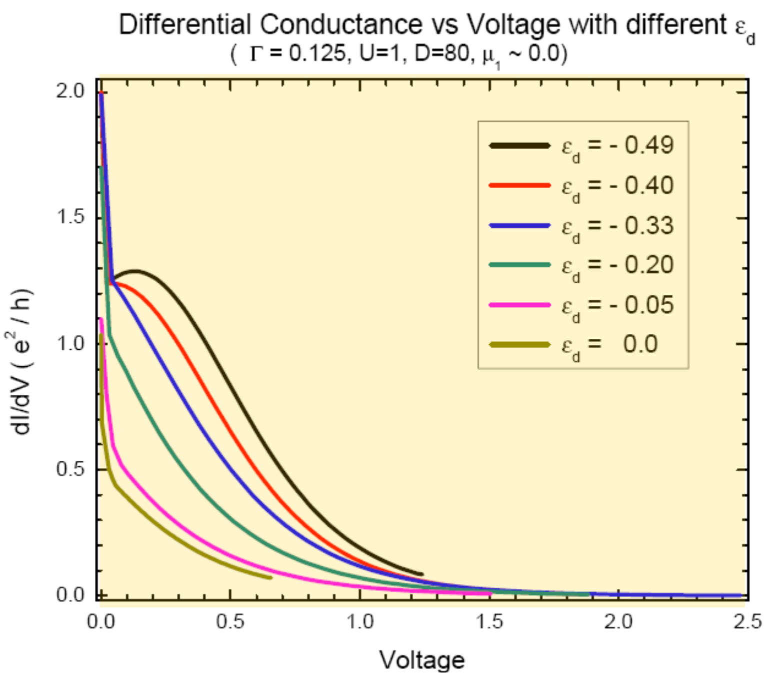
$$G = \frac{e^2}{h}\sum_\sigma \sin^2(\pi n_{d,\sigma})$$



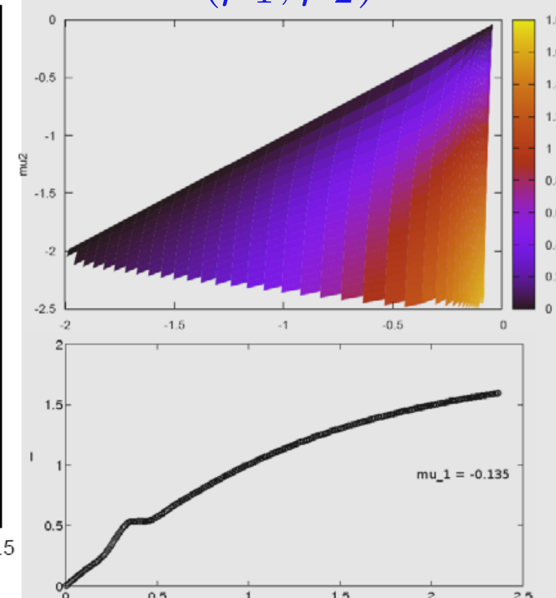
Von Delft, notes

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





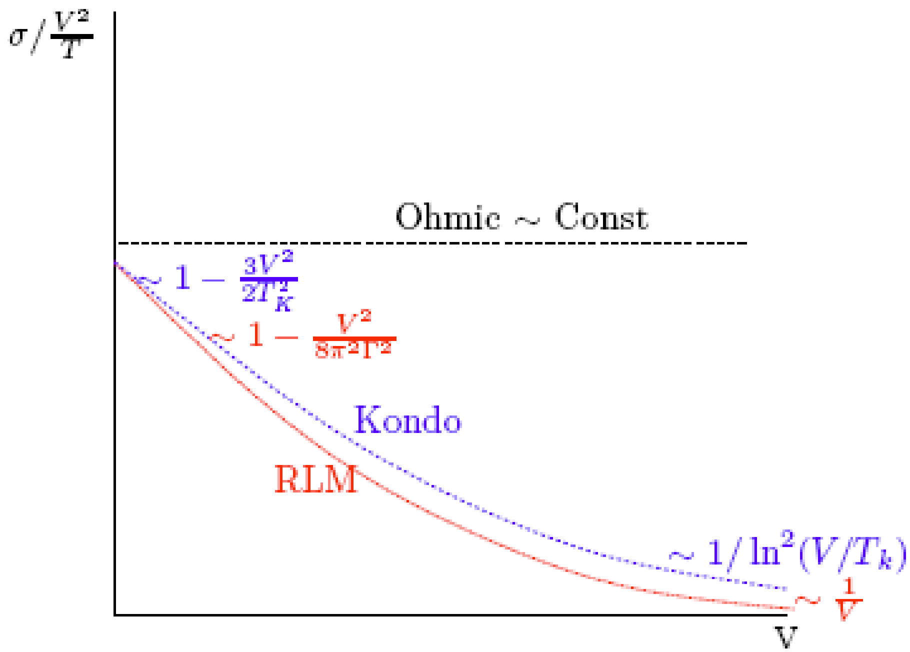
Full descrption:
$I(\mu_1,\mu_2)$



- **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 (<u>resistance minimum</u>)*

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 $H_o - \sum_i \mu_i N_i$ in the Bethe - basis**
- **Choose momenta so incoming state consists of two free Fermi seas in the Bethe - basis**

S-Matrix	$\boxed{\textbf{S=1}}$	$\boxed{\textbf{S}\neq\textbf{1}}$
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 $H_o - \sum_i \mu_i N_i$ in the Bethe basis?***
- ***Not a scattering problem! Solve on the ring $\longrightarrow$ Bethe Anzatz equations.***

The Boundary Conditions III

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

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

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

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:*** $I_{j+1} = I_j + 1$

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 $F_{\rm fock}(x_1, \cdots, x_N) = e^{i\Sigma_j^N p_j x_j}$ eigenstates of leads $H_o = -i\sum_j \partial_j$
- The wave functions on the left of the impurity (using $\alpha_{ip}(x) \to \psi_i(x)$)

$$F_{\rm bethe}(x_1, \cdots, x_N) = e^{i\Sigma_j^N p_j x_j} \; e^{i\Sigma_{s<t}^N \Phi(p_s, p_t) sgn(x_s - x_t)}$$

- 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 degenarate space.
- $e^{ik_1x_1 + ik_2x_2}[A\theta(x_1 - x_2) + (SA)\theta(x_2 - x_1)]$ 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

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