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Non-equilibrium transport in quantum impurity models (Bethe-Ansatz for open systems)

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Non-equilibrium Transport in Quantum Impurity Model
(Bethe-Ansatz for open systems)

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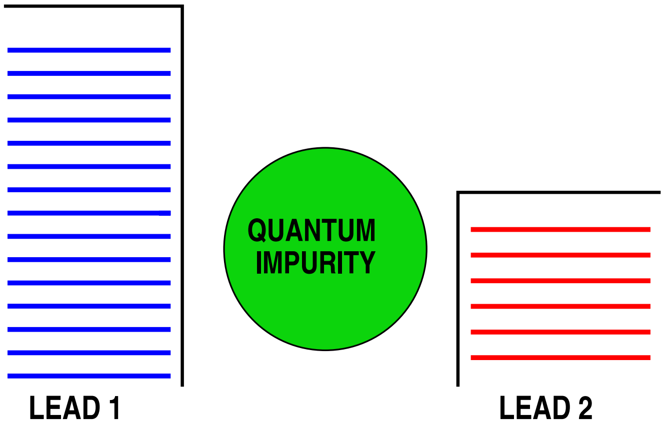
- Non-equilibrium and Steady State (Quantum Impurities)
  - Time-dependent Description
  - The steady state
  - Time-independent Description:
    Scattering Theory, Lippmann-Schwinger equation
- Scattering in Impurity Models
  - ⋆ *Scattering states of electrons off magnetic impurities*
    - Relaxation processes in metallic wires
  - ⋆ *Scattering states and the non-equilibrium steady state*
    - Non-eqilibrium Bethe-Ansatz (*NEBA*)
    - Traditional Bethe-Ansatz (equilibrium, closed system)
- The Interacting Resonance Level model - *NEBA*
- The steady state current and dot occupation
- Conclusions

Quantum Impurity - out of equilibrium



Typical models:

$$H_{\text{Kondo}} = \sum_{i=1,2,\vec{k}} \epsilon_k c^\dagger_{ia\vec{k}} c_{ia\vec{k}} + \sum_{i=1,2,\vec{k}} J_{ij}\, c^\dagger_{ia\vec{k}} (\vec{\sigma})_{ab} c_{ib\vec{k}} \cdot \vec{S}$$

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

Non-equilibrium: time-dependent Description

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

At $T > 0$:

1. initial condition: ρ_0

2. evolution: $U(t_o, t) = T\{e^{-i \int_{t_o}^{t} dt' H(t')}\}$

- $\rho(t) = U^{\dagger}(t_o, t)\ \rho_0\ U(t_o, t)$

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

At $T = 0$:

1. initial condition: $|\phi\rangle_{baths}$

2. evolution: $U(t_o, t) = T\{e^{-i \int_{t_o}^{t} dt' H(t')}\}$

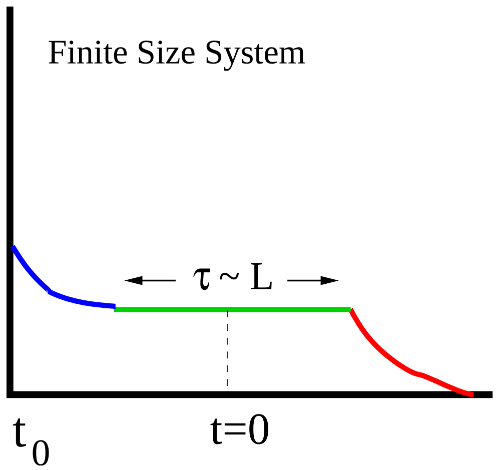
- $|\psi(t)\rangle = U(t_o, t)\ |\phi\rangle_{baths}$

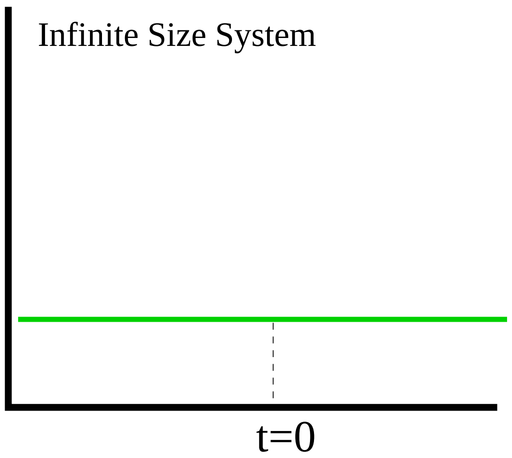
$$\langle \hat{O}(t) \rangle = \langle \psi(t) | \hat{O} | \psi(t) \rangle_s$$

Steady State

When will a steady state occur?

- Leads good thermal baths, size $L \to \infty$
- $\Rightarrow \quad \exists \lim_{t_o \to -\infty}$, (Doyon, N.A. 2005)





- Hence

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

$$|\psi\rangle_s = |\psi(0)\rangle = U(-\infty, 0)\ |\phi\rangle_{baths}$$

Gellman- Low theorem:

- $|\psi\rangle_s$ *eigenstate of* $\quad H = H_0 + H_1 \quad$ (Gellman- Low thm)
- $|\psi\rangle_s$ *scattering state - BC imposed asymptotically*

Non-equilibrium: time-independent Description

- *steady states are time independent*
- *time independent scattering formalism*

• $|\psi\rangle_s$ eigenstate: $H = H_0 + H_1,$

initial condition $\Rightarrow$ *boundary condition*

• $\begin{cases} \text{Lippmann Schwinger equation} \\ \text{Boundary condition } \; |\phi\rangle_{\text{baths}} \end{cases}$

$$|\psi\rangle_s = |\phi\rangle_{baths} + \tfrac{i}{E - H_0 \pm i\eta} H_1 |\psi\rangle_s$$

• $|\psi\rangle_s$ scattering state

scattering states describe Non-equilibrium

- *extends Landauer's approach to interacting models*

– *How to construct the scattering eigenstates?*

– *How to impose appropriate boundary conditions?*

– *For integrable impurity models?*

Integrable **Quantum Impurity Models**

- *Use Bethe-Ansatz to construct scattering states ?*
- *Traditional Bethe-Ansatz:*
  - *Equilibrium, Closed Systems*
  - *Eigenstates with Periodic Boundary Conditions (PBC)*
  - *Thermodynamics*
- *Need new technology:*
  - *Scattering eigenstates*

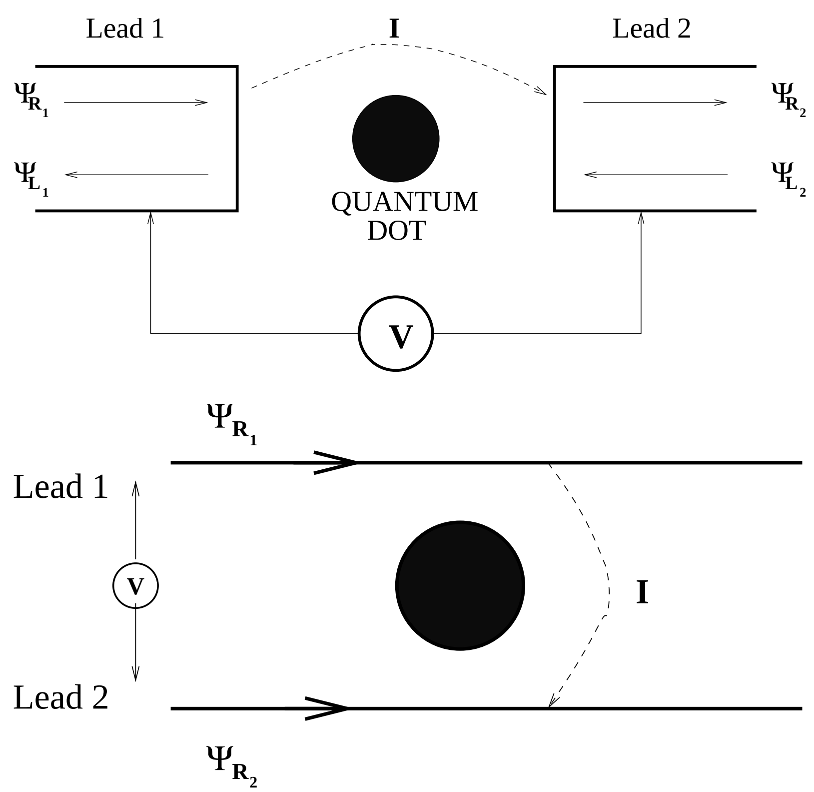
Scattering Bethe-Ansatz

then:

- T-matrix elements, cross-sections
- *Scattering States with BC imposed by leads (non-eq BC)*
- *Non-equilibrium Bethe-Ansatz (NEBA)*
  - ⋆ *Consistency of non-eq BC and integrability (YBE)?*
  - ⋆ *Integrability out-of-quilibrium?*

Quantum Impurity Models (equilibrium) I

Standard manipulations: mode expansion, unfolding



- The Kondo Model:

$$H_K = \sum_{i=1,2} \int dx\, \psi^\dagger_{ia}(x)\partial\psi_{ia}(x) + \sum_{i,j=1,2} J_{ij}\psi^\dagger_{ia}(0)\vec{\sigma}_{ab}\psi_{jb}(0)\cdot\vec{S}$$

- The Anderson Model:

$$H_A = \sum_{i=1,2} \int dx\, \psi^\dagger_{ia}(x)\partial\psi_{ia}(x) + \epsilon_d d^\dagger_a d_a +$$

$$+ V\sum_{i=1,2}(\psi^\dagger_{ia}(0)d_a + h.c.) + U n_{d\uparrow}n_{d\downarrow}$$

Quantum Impurity Models (equilibrium) II

- *The Interacting Resonance Level Model (IRL model):*
  - *level d coupled to leads*
  - *Coulomb interaction between leads and dot*

$$H_{\rm IRL} = \sum_{i=1,2} \int dx \psi_i^\dagger(x) \partial \psi_i(x) + \epsilon_d d^\dagger d$$

$$+ \frac{V}{\sqrt{2}} \left(\sum_{i=1,2} \psi_i^\dagger(0) d + h.c. \right) + 2U \sum_{i=1,2} \psi_i^\dagger(0) \psi_i^\dagger(0) d^\dagger d$$

  - *related to anisotropic Kondo model:*

    $n_d = 0, 1 \;\Leftrightarrow\; \sigma_z = \pm 1$ *(Wiegmann, Finkelstein 1979)*
  - *local magnetic field ϵ_d*

- Want to show:

$$\boxed{H_{\rm IRL} \text{ - } \textit{integrable out of equilibrium}}$$

The *Interacting Resonance Level model* Out-of-equilibrium

- The model:

$$H_{\mathrm{IRL}} = \sum_{i=1,2} \int dx \psi_i^\dagger(x)\partial\psi_i(x) + \epsilon_d d^\dagger d$$
$$+\frac{V}{\sqrt{2}}(\sum_{i=1,2}\psi_i^\dagger(0)d + h.c.) + 2U\sum_{i=1,2}\psi_i^\dagger(0)\psi_i(0)d^\dagger d$$

- The *non-equilibrium* Boundary Conditions (non-eq BC):
  $|scattering\ state\rangle \to |\phi\rangle_{baths}$

- The space of states? separate into: $\mathcal{H}_{e/o}$
  - $\psi_{e/o}(x) = \frac{1}{\sqrt{2}}(\psi_1(x) \pm \psi_2(x))$
  - $H_{\mathrm{IRL}} = H_e + H_o$

$$\begin{cases} H_e = -i\int dx\, \psi_e^\dagger(x)\partial\psi_e(x) + U\psi_e^\dagger(0)\psi_e(0)d^\dagger d + \\ \qquad + V(\psi_e^\dagger(0)d + h.c.) + \epsilon_d d^\dagger d \\ H_o = -i\int dx\, \psi_o^\dagger(x)\partial\psi_o(x) + U\psi_o^\dagger(0)\psi_o(0)d^\dagger d \end{cases}$$

  - H_o trivial, H_e integrable (Filyov, Wiegmann 1980)
- Hilbert spaces $\mathcal{H}_{e/o}$ couple in equilibrium only via d
- non-eq BC recouple two spaces

The Scattering States I

- Solve the Schrödinger equation (sector by sector)
- Single-particle eigenstate:

$$\int dx\,[A(g_p(x)\psi_e^\dagger(x) + e_p d^\dagger) + B h_p(x)\psi_o^\dagger(x)]|0\rangle$$

$$\begin{aligned}
g_p(x) &= \frac{2e^{ipx}}{1+e^{i\delta_p}}\left[\theta(-x)+e^{i\delta_p}\theta(x)\right], \quad (g_p(0)=1) \\
h_p^\pm(x) &= \frac{2e^{ipx}}{1+e^{i\delta_p}} \qquad x \neq 0 \\
h_p^\pm(0) &= \pm\frac{(p-\epsilon_d)e_p e^{ipx}}{V} = \pm g_p(0)e^{ipx} \qquad x = 0 \\
e_p &= V g_p(0)/(p-\epsilon_d) \\
\delta_p &= 2\arctan\left[\frac{V^2}{2(p-\epsilon_d)}\right].
\end{aligned}$$

- Single-particle scattering state:
  choose A, B to impose non-eq BC

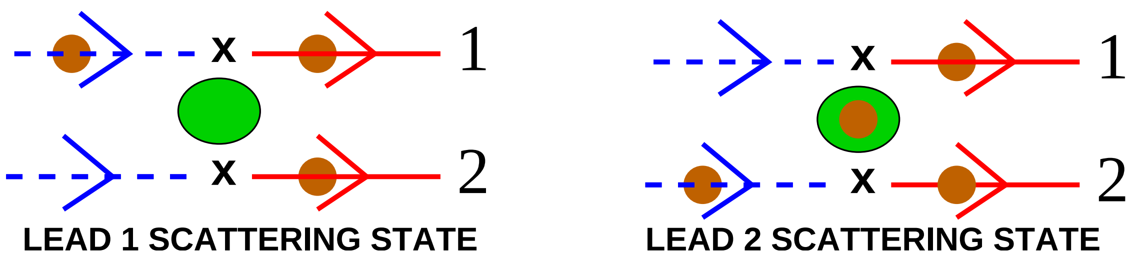
The Scattering States II

- Single-particle scattering states
  - choosing $A = B$:

$$|1p\rangle = \int dx\, e^{ipx} \left[\frac{2}{1+e^{i\delta_p}} \Big([2\theta(-x) + (e^{i\delta_p}+1)\theta(x)]\psi_1^\dagger(x) + [(e^{i\delta_p}-1)\theta(x)]\psi_2^\dagger(x) \Big) + \sqrt{2} e_p d^\dagger \delta(x) \right] |0\rangle$$

  - choosing $A = -B$:

$$|2p\rangle = \int dx\, e^{ipx} \left[\frac{2}{1+e^{i\delta_p}} \Big([2\theta(-x) + (e^{i\delta_p}+1)\theta(x)]\psi_2^\dagger(x) + [(e^{i\delta_p}-1)\theta(x)]\psi_1^\dagger(x) \Big) + \sqrt{2} e_p d^\dagger \delta(x) \right] |0\rangle$$



  - $|1/2p\rangle = \int dx e^{ipx} \alpha^\dagger_{1/2p}(x)|0\rangle$
  - $\alpha^\dagger_{1/2p}(x) = g_p(x)\psi_e^\dagger(x) \pm h_p^\pm(x)\psi_o^\dagger(x) + e_p\delta(x)d^\dagger$

The Scattering States III

- Multi-particle states

$\int\int[Ag(x_1,x_2)\psi_e^\dagger(x_1)\psi_e^\dagger(x_2)+Ch(x_1,x_2)\psi_o^\dagger(x_1)\psi_o^\dagger(x_2)$
$+\int\int Bj(x_1,x_2)\psi_e^\dagger(x_1)\psi_o^\dagger(x_2)]|0\rangle$
$+\int[Ae(x)\psi_e^\dagger(x)d^\dagger+Bf(x)\psi_0^\dagger(x)d^\dagger]|0\rangle$

with:

$$
\begin{aligned}
2g(x_1,x_2) &= g_p(x_1)g_k(x_2)Z(x_1-x_2)-(1\leftrightarrow 2)\\
2h(x_1,x_2) &= h_p(x_1)h_k(x_2)Z(x_1-x_2)-(1\leftrightarrow 2)\\
j^{ab}(x_1,x_2) &= g_p(x_1)h_k^a(x_2)Z(x_1-x_2)\\
&\quad +(-1)^{ab}g_k(x_1)h_p^b(x_2)Z(x_2-x_1)
\end{aligned}
$$

- Same S-matrix between any two particles

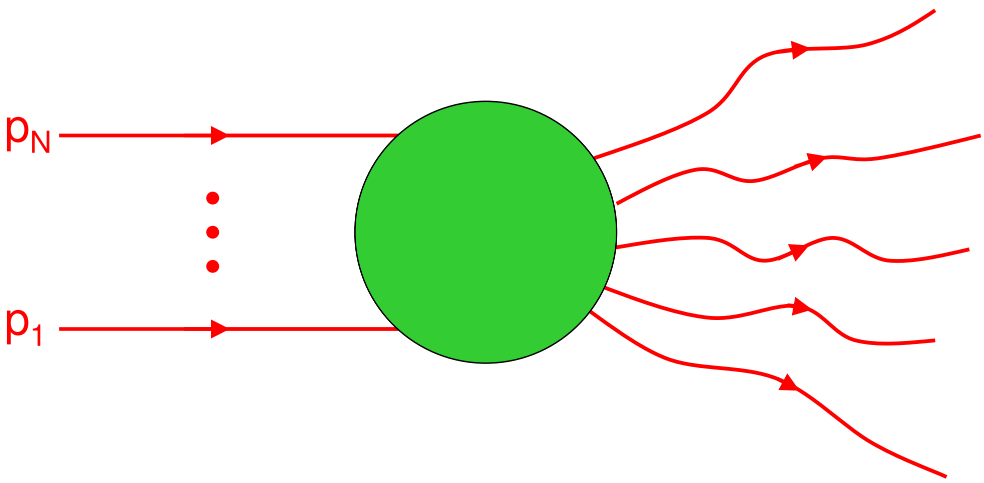
$$
\begin{aligned}
Z(x_1-x_2) &= e^{i\Phi(p,k)\mathrm{sgn}(\mathrm{x}_1-\mathrm{x}_2)}\\
e^{2i\Phi(p,k)} &= \frac{i+\frac{U}{2}\frac{p-k}{k+p-2\epsilon_d}}{i-\frac{U}{2}\frac{p-k}{k+p-2\epsilon_d}}
\end{aligned}
$$

- Scattering states: A,B,C determined by BC
- **In general, a state with N_1 *lead-1*, N_2 *lead-2* particles:**

$$
|\{p\}\rangle_s=\int dx e^{i\sum_j p_j x_j}e^{i\sum_{s<t}\Phi(p_s,p_t)sgn(x_s-x_t)}
\prod_{u=1}^{N_1}\alpha_{1p_u}^\dagger(x_u)\prod_{v=N_1+1}^{N_2}\alpha_{2p_v}^\dagger(x_v)|0\rangle
$$

Open boundary conditions I

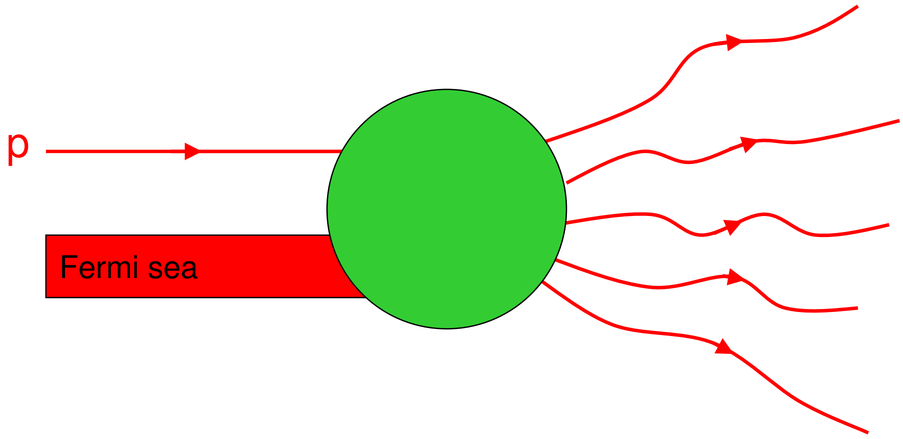
- Eigenstate for any $p_1 \cdots p_N$



- **Choice of momenta: determined by problem**

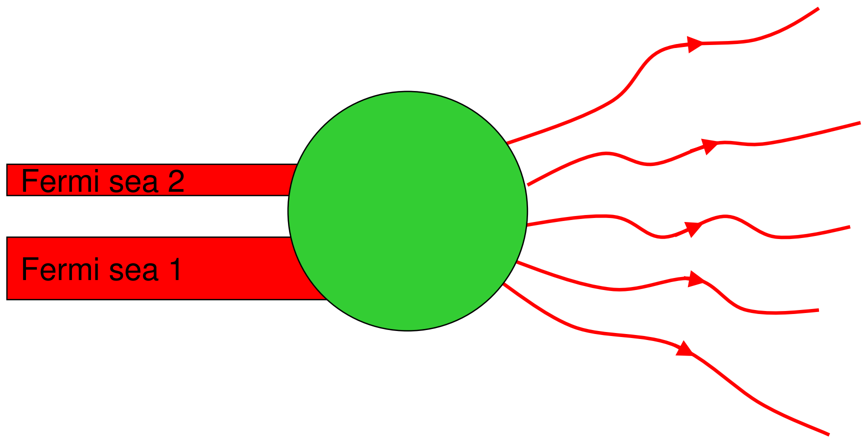
Open boundary conditions II

Scattering BC: electron with momentum p above Fermi-sea



- exact computation of *(in)elastic* scattering amplitudes of electron off the impurity
- exact cross-sections at $T = 0$, $T > 0$
- energy, phase relaxation processes in metallic wires

Non-eq BC: *far from impurity* $\rightarrow$ *free leads*



- Nonequilibrium physics

Steady State Current and Dot Occupation - I

1. *Non-interacting model, $U=0$, (RLM)*

- Multi-particle scattering states

$$
\begin{aligned}
|\{p\}\rangle_s &= \int dx e^{i\sum_j p_j x_j} \prod_{u=1}^{N_1} \alpha^\dagger_{1p_u}(x_u) \prod_{v=N_1+1}^{N_2} \alpha^\dagger_{2p_v}(x_v)|0\rangle \\
&= \prod_{u=1}^{N_1} |1p_u\rangle \prod_{v=N_1+1}^{N_1+N_2} |2p_v\rangle
\end{aligned}
$$

- Expectation values of

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

- Calculation in $\lim L \to \infty$.
  - Steady state
  - Orthogonality

Steady State Current and Dot Occupation - II

- Expectation values: $\hat{I}, \hat{n}_d$ in *Scattering State* $|\{p\}\rangle$

$$\langle I \rangle_s = \sum_{u=1}^{N_1} \frac{\Delta^2}{(p_u - \epsilon_d)^2 + \Delta^2} - \sum_{v=N_1+1}^{N_1+N_2} \frac{\Delta^2}{(p_v - \epsilon_d)^2 + \Delta^2}$$

$$\langle n_d \rangle_s = \sum_{u=1}^{N_1} \frac{\Delta}{(p_u - \epsilon_d)^2 + \Delta^2} + \sum_{v=N_1+1}^{N_1+N_2} \frac{\Delta}{(p_v - \epsilon_d)^2 + \Delta^2}$$

- Momenta $\{p\}$ not specified - part of imposition of BC
- Imposing BC in thermodynamic limit:
  - momenta in *each lead* have F-D distribution $\rho_i(p) = \frac{1}{2\pi} f_{T_i,\mu_i}(p)$.
  - $\rho_i(p) = \frac{1}{2\pi}\theta(k_o^i - p)$ at $T = 0$, with k_o^i set by μ^i
- Standard RL results (Landauer):

$$\langle I \rangle_s = \int dp\,[f_1(p) - f_2(p)]\,\frac{\Delta^2}{(p - \epsilon_d)^2 + \Delta^2}$$

$$\langle n_d \rangle_s = \int dp\,[f_1(p) + f_2(p)]\,\frac{\Delta}{(p - \epsilon_d)^2 + \Delta^2}$$

Steady State Current and Dot Occupation - II

2. *Interacting model,* $U \neq 0$*, IRLM*

- Same structure (result of $L \to \infty$ limit, orthogonality):

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

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

- What are the distributions $\rho_i(p)$? No longer Fermi-Dirac.

- Non-trivial S-matrix

$$S(p,k) = e^{2i\Phi(p,k)} = \frac{i + \frac{U}{2} \frac{p-k}{k+p-2\epsilon_d}}{i - \frac{U}{2} \frac{p-k}{k+p-2\epsilon_d}}$$

- **New basis** of states in free leads

  example: $e^{ik_1 x_1 + k_2 x_2}[A\theta(x_1 - x_2) + (SA)\theta(x_2 - x_1)]$

  eigenfunction of: $h_0 = -i(\partial_1 + \partial_2)$ for any S (infinite egeneracy)

- In the new basis the require momenta satisfy:

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

- Distribution $\rho_i(p)$ determined by TBA equations

Steady State Current and Dot Occupation - IV

- Determine momentum destributions: $e^{ip_jL} = \prod_{l=1}^{N} S(p_j, p_l)$
  $\Rightarrow$ TBA equations:

$$\rho_1(p) + \rho_2(p) = \frac{1}{2\pi}\theta(k_o^1 - p) - \sum_{j=1,2}\int_{-D}^{k_o^j} \mathcal{K}(p,k)\rho_j(k)\, dk$$

$$2\rho_2(p) = \frac{1}{2\pi}\theta(k_o^2 - p) - \sum_{j=1,2}\int_{-D}^{k_o^j} \mathcal{K}(p,k)\rho_j(k)\, dk$$

  with

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

  – Upper cut-off k_o^i in each lead, set by μ^i, (here $k_o^1 > k_o^2$)
  – Lower cut-off D - common to both leads

- Here $T = 0$ TBA equations
- For $T > 0$, *finite temperature* TBA equations
  (sum over Boltzmann weighted scattering states
  corresponding to non-eq BC of excited lead states.)

Steady State Current and Dot Occupation - V

- Solve TBA equations for distributions: Wiener-Hopf metho
- $\rho_i(p)$ parametrized by D - lower cut-off (bandwidth)
- For Universality: ($physical\ scales \ll D$)
  - lower cut-off: $D \to \infty$
  - vary U, keeping low-E physics unchanged
  - $U \to$ *uv fixed point*, on RG trajectory
  - Δ does not renormalize
- New scale emerges T_k characterizing RG trajectory
- Universality out-of-equilibrium

Steady State Current and Dot Occupation - VI

- Solve TBA eqn:
  - $p = \alpha m_o e^{\lambda} + \tilde{\epsilon}_d$: $\rho_\pm(p)$, correspond to $p \geq \tilde{\epsilon}_d$, $p \leq \tilde{\epsilon}_d$
  - Lower cut-off, $\Lambda \leq \lambda$, Λ determined by bandwidth D

- The solution in each lead :

  $\sigma_+(\lambda) = \rho_+(\lambda + \lambda_o)$, $\sigma_+^-(\lambda) = \sigma_+(\lambda)\theta(-\lambda)$

$$\tilde{\sigma}_+^-(\omega) = \sum_{n=1}^{\infty} \frac{i(-1)^n m_o e^{\Lambda} e^{-\frac{2n\pi(\Lambda-\lambda_o)}{\pi+\zeta}} \sin\frac{n\pi(\pi-\zeta)}{\pi+\zeta} \tilde{K}_+(-\frac{2in\pi}{\pi+\zeta})}{2\pi \tilde{K}_-(\omega)(1-\frac{2n\pi}{\pi+\zeta})(\frac{(\pi+\zeta)\omega}{2}+in\pi)}$$

$$\tilde{\rho}_-(\omega) = \frac{1}{2\sinh\frac{(\pi+\zeta)}{2}\cosh\frac{(\pi-\zeta)}{2}} \left[\frac{m_o e^{\Lambda} e^{-i\omega\Lambda}\sinh\pi\omega}{2\pi(1-i\omega)} + e^{-i\omega\lambda_o}\sinh\left((\pi-\zeta)\omega\right)\tilde{\sigma}_+^-(\omega)\right]$$

with ($b = \zeta/\pi$)

$$\tilde{K}_+(\omega) = \frac{\sqrt{2\pi}\Gamma(\frac{1}{2} + \frac{i(1-b)\omega}{2})\Gamma(1+ib\omega)e^{\chi(\omega)}}{\Gamma(1+\frac{i(1+b)\omega}{2})}$$

$$\tilde{K}_-(\omega) = \left(\frac{4\pi b}{1+b}\right)\frac{\sqrt{2\pi}\Gamma(1-\frac{i(1+b)\omega}{2})e^{\chi(\omega)}}{\Gamma(\frac{1}{2}-\frac{i(1-b)\omega}{2})\Gamma(1-ib\omega)}$$

$$\chi(\omega) = -i\omega\left[\frac{1}{2}\ln\frac{1-b}{1+b} + b\ln\frac{2b}{\sqrt{1-b^2}}\right]$$

and

$$e^{i\zeta(U)} = \frac{(1-\left[\frac{U}{2}\right]^2) + 2i\frac{U}{2}}{1+\left[\frac{U}{2}\right]^2}, \quad 0 \leq \zeta(U) \leq \pi$$

Steady State Current and Dot Occupation - VI

- The current and dot occupation for $L \to \infty$

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

- In the universality limit, $\Lambda \to \infty$, we find: (miraculously..)

$$\langle I \rangle_s = \frac{\Delta}{2\pi} \left(\frac{T_k}{\Delta} \right) \left[\tan^{-1} \frac{\mu_1 - \epsilon_d}{T_k} - \tan^{-1} \frac{\mu_2 - \epsilon_d}{T_k} \right]$$
$$\langle n_d \rangle_s = \frac{1}{2} + \frac{1}{2\pi} \left(\frac{T_k}{\Delta} \right) \left[\tan^{-1} \frac{\mu_1 - \epsilon_d}{T_k} + \tan^{-1} \frac{\mu_2 - \epsilon_d}{T_k} \right]$$

- New low-energy scale

$$T_k = m_o e^{\Lambda} \left(\frac{\Delta}{m_o e^{\Lambda}} \right)^{\frac{2\pi}{\pi + \zeta(U)}}$$

- Scaling limit T_k held fixed: $\Lambda \to \infty$, $\zeta \to \pi$ ($U \to \infty$)
- Results resemble RL: *interactions renormalize* Δ *into* T_k.

Conclusions

- **Showed:**
  Scattering States with non-eq BC describe Steady State
- **Computed:**
  The current and dot occupation in Steady State: 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 $T > 0$, $T_1 \neq T_2$, $B_0 > 0$, $B_1 \neq B_2$
  - 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 integrable *bulk* systems
  - Non-equilibrium RG