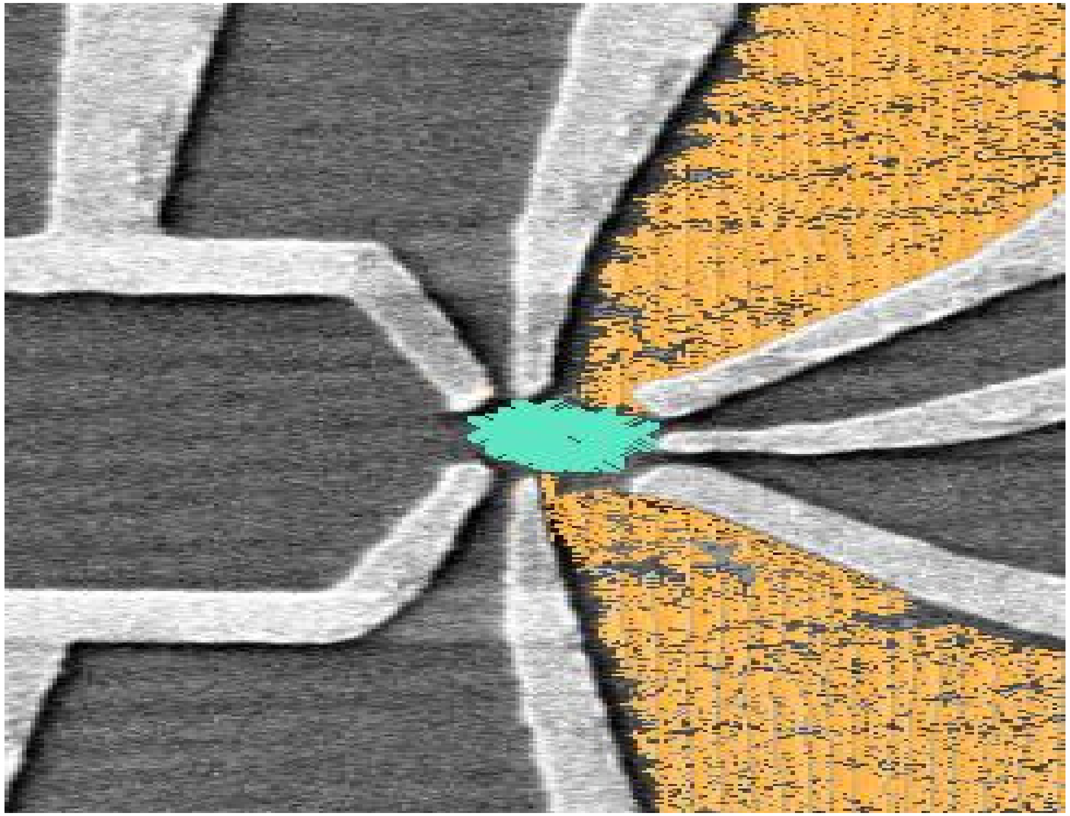
Quantum Impurities Out of Equilibrium



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Outline

- **Non-equilibrium and Steady State (Quantum impurities)**
  - *Time dependent description*
  - *The steady State - open systems*
  - *Time independent description*
    - **Scattering theory, Lippmann-Schwinger equation**
  - *Scattering eigenstates and Non-equilibrium Steady State Dynamics*
- **Scattering States in integrable Impurity Models**
  - *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**
    - **Equilibrium, Thermodynamics**
- **The Interacting Resonance Level Model (*SBA*)**
- **The Kondo Model (*SBA*)**
- **Conclusions**

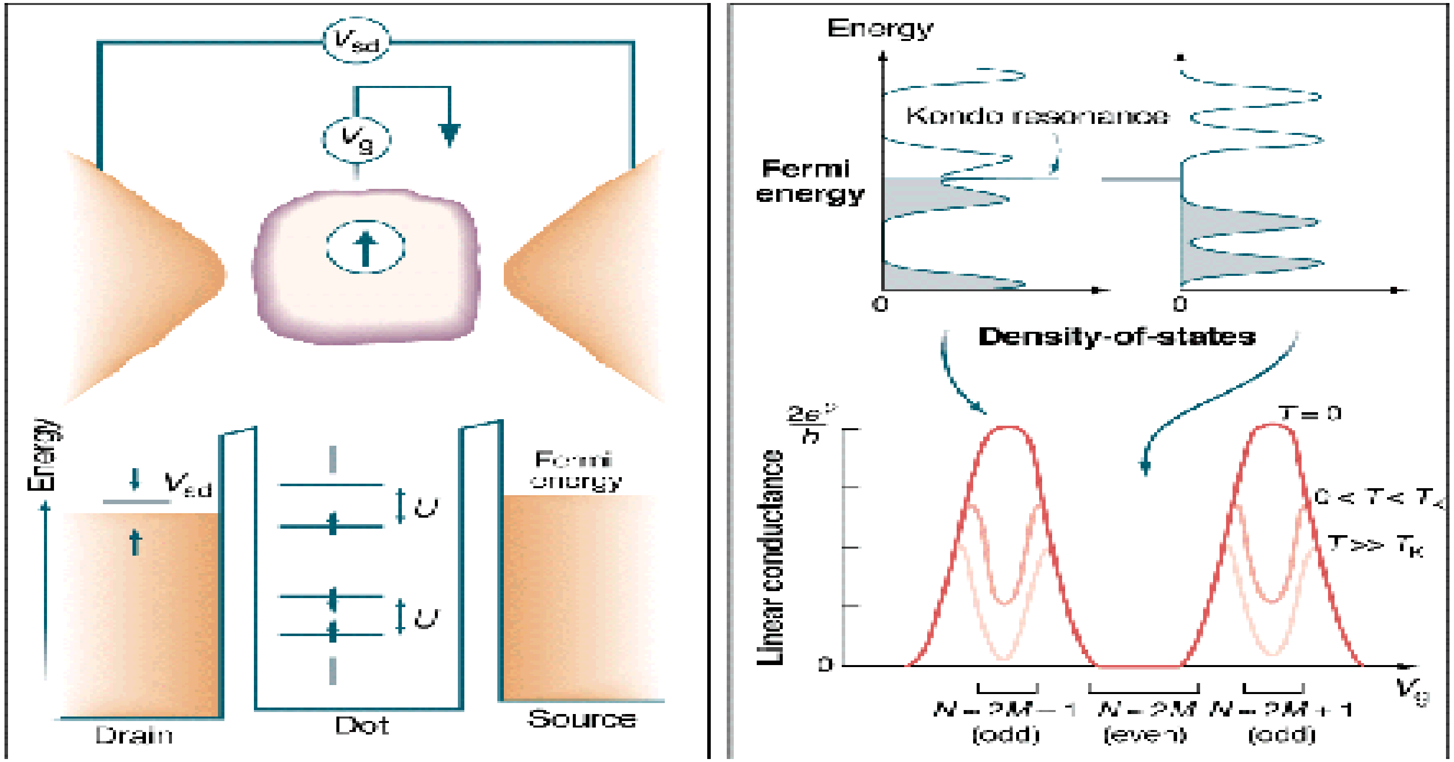
Non-equilibrium and Strong Correlations

- **Nonequilibrium systems are relatively poorly understood compared to their equilibrium counterpart.**

- 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 systems are -in general- poorly understood.**
  - Perturbative approaches fail
  - New degrees of freedom emerge
  - New collective Behavior

Kondo Impurities –
Strong Correlations out of Equilibrium

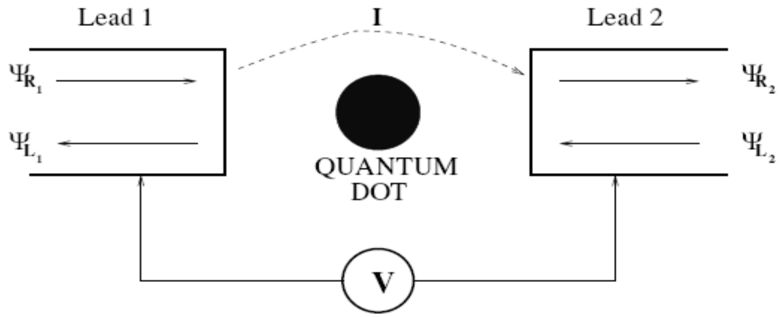


Inoshita:Science 24 July 1998: Vol. 281. no. 5376, pp. 526 - 527

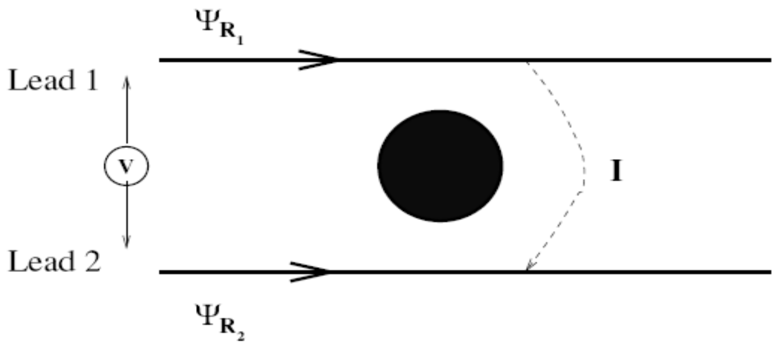
- Can control the number of electrons on the dot using gate voltage
- For odd number of electrons- quantum dot acts like a quantum impurity (Kondo, Interacting Resonant Level Model)
- Quantum impurity models exhibit new collective behaviors such as the Kondo effect

Quantum Impurities out of Equilibrium

The Quantum Impurity:



The Quantum Impurity unfolded:



Preview:

- **Describe:** *Steady State*
- **Construct:** *Scattering states eigenstates - Boundary conditions set by leads:* $x_i \rightarrow -\infty$
- **Compute:** *Current in scattering states*

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

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

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

At $T = 0$:

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

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

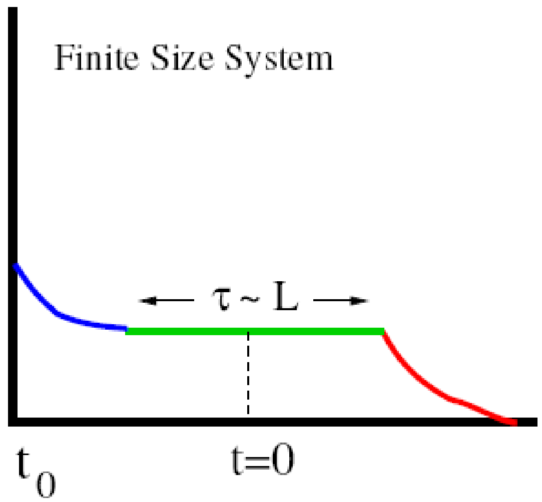
- $|\psi(t)\rangle = U(t,t_o)\ |\phi\rangle_{baths}$

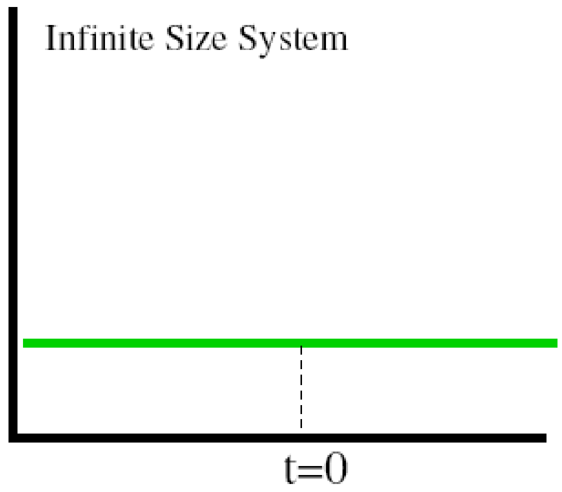
$$\langle \hat{O}(t) \rangle = \langle \psi(t)|\hat{O}|\psi(t)\rangle_s$$

The Steady State

When will a steady state occur?

- **Leads good thermal baths, size $L \to \infty$**
- $\Rightarrow$ $\exists \lim_{t_o \to -\infty}$, *no IR div.* **(Doyon, N.A. 2005)**





- **Hence**

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

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

- $|\psi\rangle_s$ *eigenstate of:* $H = H_0 + H_1$ *(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*

- Lippmann Schwinger equation; Boundary condition $|\phi\rangle_{\text{baths}}$

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

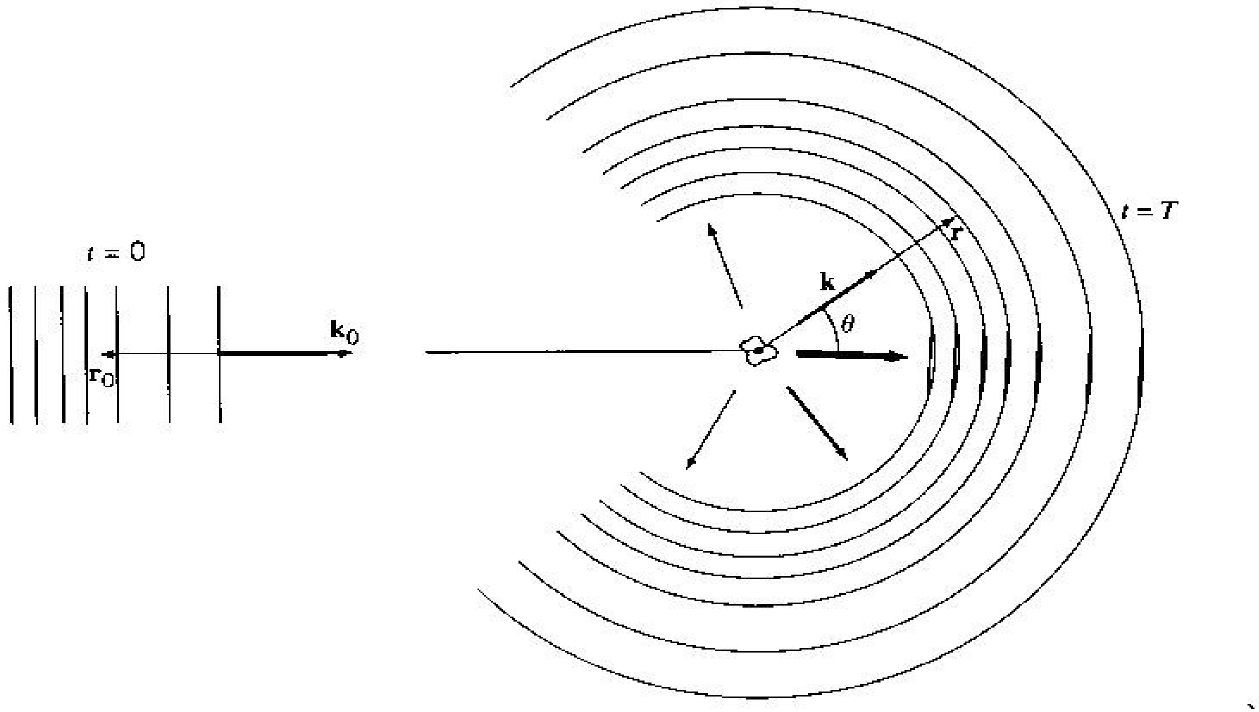
- $|\psi\rangle_s$ scattering state

scattering states describe Non-equilibrium

Scattering States (QM)

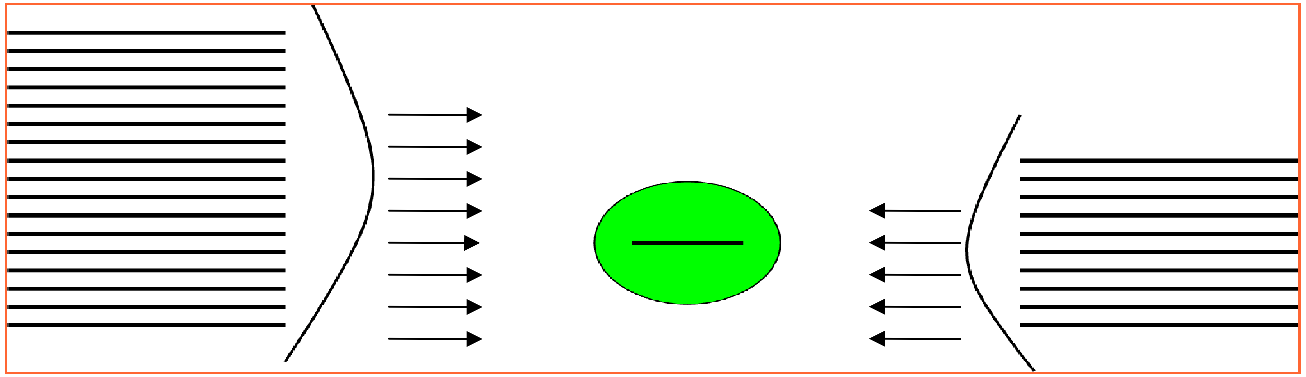
- Since we are in a steady-state, can go to a time-independent picture.
- Scattering by a localized potential is given by the Lippman-Schwinger equation:

$$|\psi_p^{\pm} > = |\phi_p > + \frac{H_1}{E - \hat{H}_o \pm i\epsilon} |\psi_p^{\pm} >$$

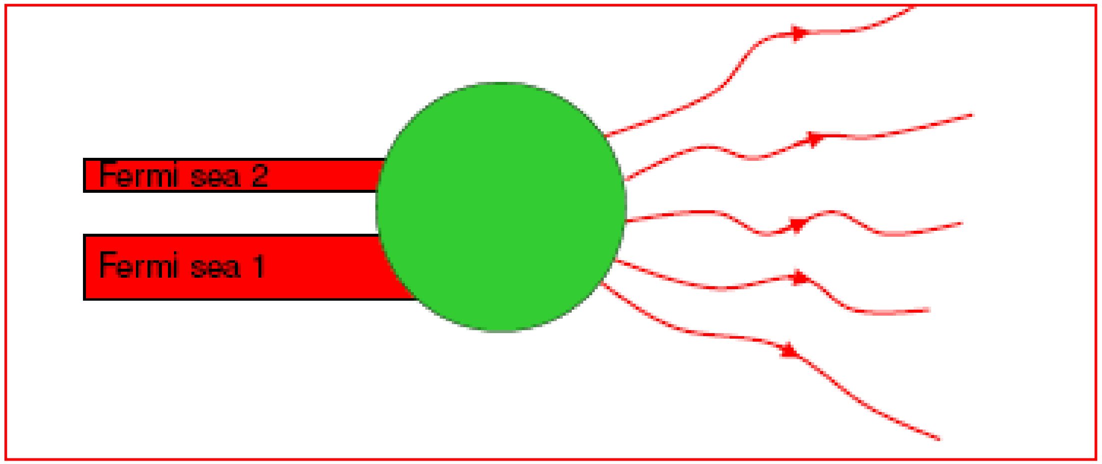


The Scattering state (Many body)

A scattering eigenstate is determined by the *incoming asymptotics*: *the baths*



The scattering eigenstate in unfolded geometry:



How to construct the scattering States?

The Scattering Bethe-Ansatz

- Can we use Bethe-Ansatz for scattering states ?
  - ∗ Traditional Bethe-Ansatz - inapplicable:
  - – *Periodic Boundary Conditions*
  - – *Equilibrium, Closed Systems: Thermodynamics*
  - ∗ New technology $\Rightarrow$ Scattering eigenstates
  - – *Asymptotic Boundary Conditions*

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Scattering Bethe-Ansatz

- ⋆ Consistency of non-eq BC and integrability (YBE)?
- ⋆ Integrability out-of-quilibrium?

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- Explicit construction - the IRL model:

  (integrability: *Filyov-Wiegmann 1980*)

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

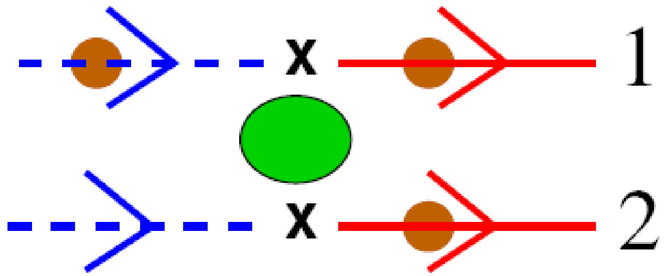
IRL: The Scattering State I

Diagonalize the Hamiltonian by means of **Scattering Bethe-Ansatz:**

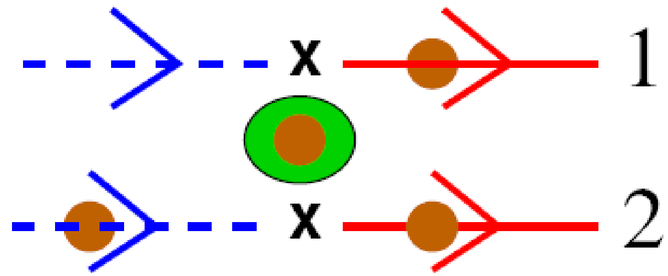
Single-particle scattering states: ($\delta_p = 2\arctan\left[\frac{t^2}{2(p-\epsilon_d)}\right]$, phase-shift)

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

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



LEAD 1 SCATTERING STATE



LEAD 2 SCATTERING STATE

IRL: The Scattering State II

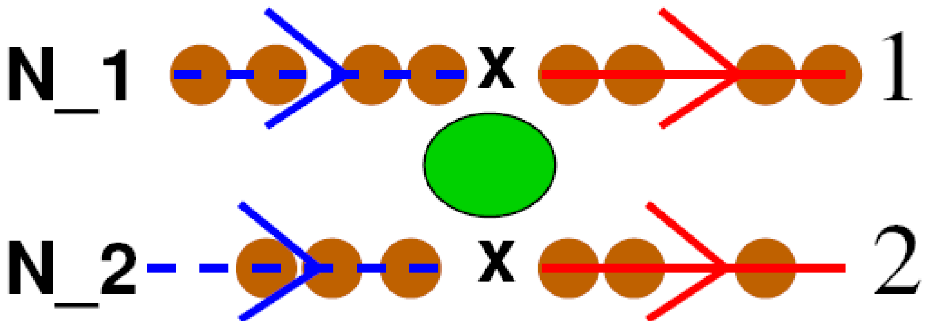
Multi-particle scattering state: N_1 *lead-1*, N_2 *lead-2*:

$$|\{p\}\rangle_s = \int dx\; e^{i\Sigma_j p_j x_j}\; e^{i\Sigma_{s<t}\Phi(p_s,p_t)sgn(x_s-x_t)}$$

$$\Pi_{u=1}^{N_1}\alpha^{\dagger}_{1p_u}(x_u)\Pi_{v=N_1+1}^{N_1+N_2}\alpha^{\dagger}_{2p_v}(x_v)|0\rangle$$

with:

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



IRL: Current & Dot Occupation

- Current and dot-occupation:

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

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

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

Apparent simplicity is misleading:

In the Bethe basis:

-Excitations undergo phase shifts only

-Choice of momenta incorporates interactions and boundary conditions

Need determine: $\rho_1(p), \rho_2(p)$

The Boundary Conditions I

Boundary condition: $|\psi\rangle_s \to$ **wave function of two free baths :**

$$|\psi\rangle \to |\phi\rangle_{baths} = \int e^{i\Sigma_j p_j x_j} \Pi_{u=1}^{N_1} \psi_1^\dagger(x_u) \Pi_{v=1}^{N_2} \psi_2^\dagger(x_v)|0\rangle$$

However $|\{p\}\rangle$ **tends to:**

$$|\{p\}\rangle \to |\{p\}\rangle_o = \int e^{i\Sigma_j p_j x_j}\ e^{i\Sigma_{s<t}\Phi(p_s,p_t) sgn(x_s - x_t)} \Pi_{u=1}^{N_1} \psi_1^\dagger(x_u) \Pi_{v=1}^{N_2} \psi_2^\dagger(x_v)|0\rangle$$

Both $|\phi\rangle_{baths}$ **and** $|\{p\}\rangle_o$ **are eigenstates of** H_0. **so**

$$|\phi\rangle_{baths} = \sum_{\{p\}} A_{\{p\}} |\{p\}\rangle_o$$

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: $e^{ik_1x_1+k_2x_2}[A\theta(x_1 - x_2) + (SA)\theta(x_2 - x_1)]$

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

Bethe Anstaz basis vs. Fock basis

S-Matrix	$S=1$	→	$S\neq 1$
Basis	**Fock Basis**	→	**Bethe Basis**
Fermi-sea Momenta	**Fermi – Dirac distribution**	→	**Bethe distribution**

-**Energy levels are infinitely degenerate (linear spectrum)**

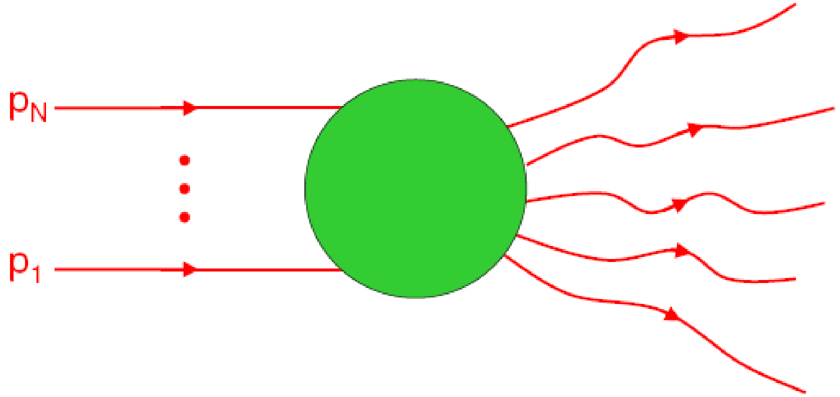
-Choose momenta of incoming particles to look like two free Fermi seas

The Scattering State III

- $|\{p\}\rangle_s$ eigenstate for any $p_1 \cdots p_N$

BC:

$|\{p\}\rangle_o$ ←

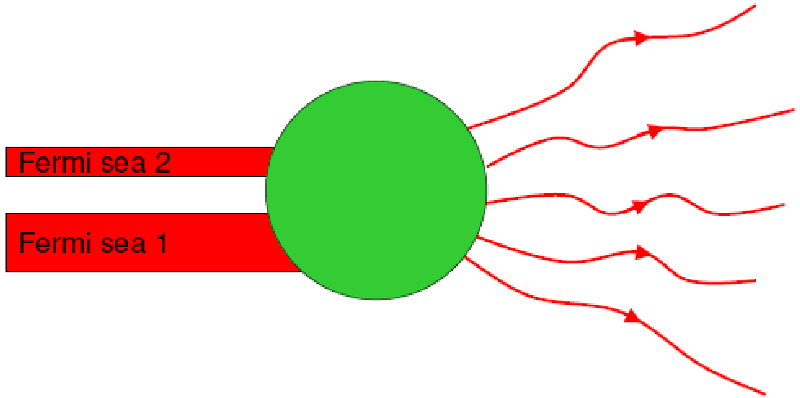


- $\{p\}$ - BA momenta (not Fock momenta)
- Choice of BA momenta: determined by problem.

Non-eq BC: *far from impurity → 2 free leads*

BC:

$|\phi\rangle_{baths}$ ←



- Momentum distributions in leads - need to solve TBA eqns

The Boundary Conditions II

How to choose the momenta $\{p\}$?

Auxiliary problem: **in $\mathcal{H}_o$ match ground state in Fock basis with 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)

The Boundary Conditions III

•Non-eq BC → 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: $\mathcal{K}(p,k) = \frac{U}{\pi} \frac{(k-\tilde{\epsilon}_d)}{(p+k-2\tilde{\epsilon}_d)^2 + \frac{U^2}{4}(p-k)^2}$

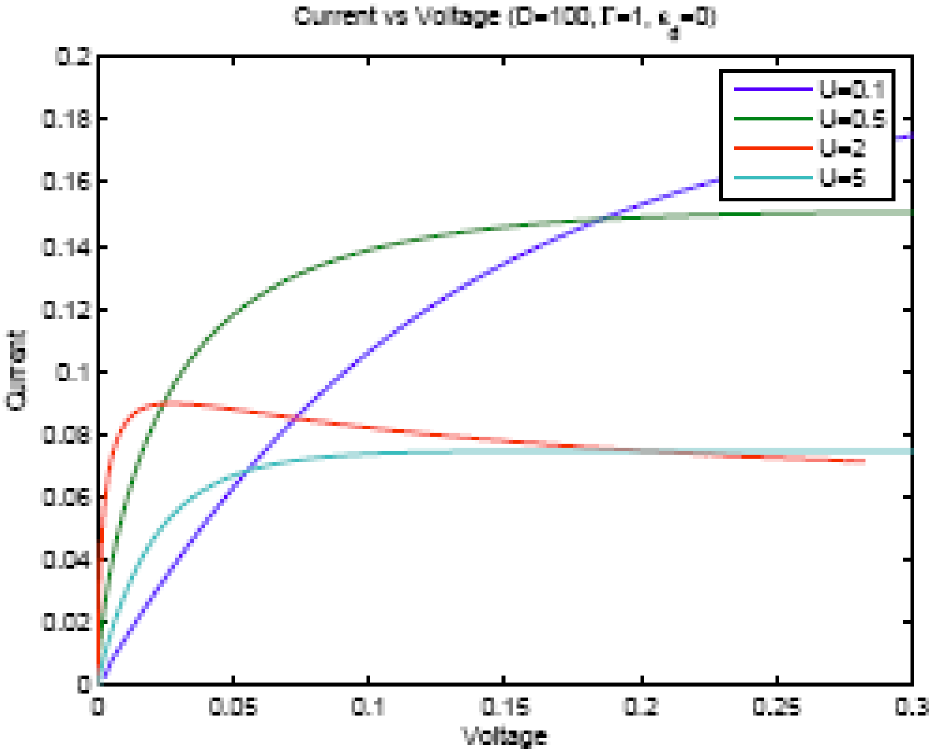
TBA eqns describe the free leads on a ring (in the Bethe basis)

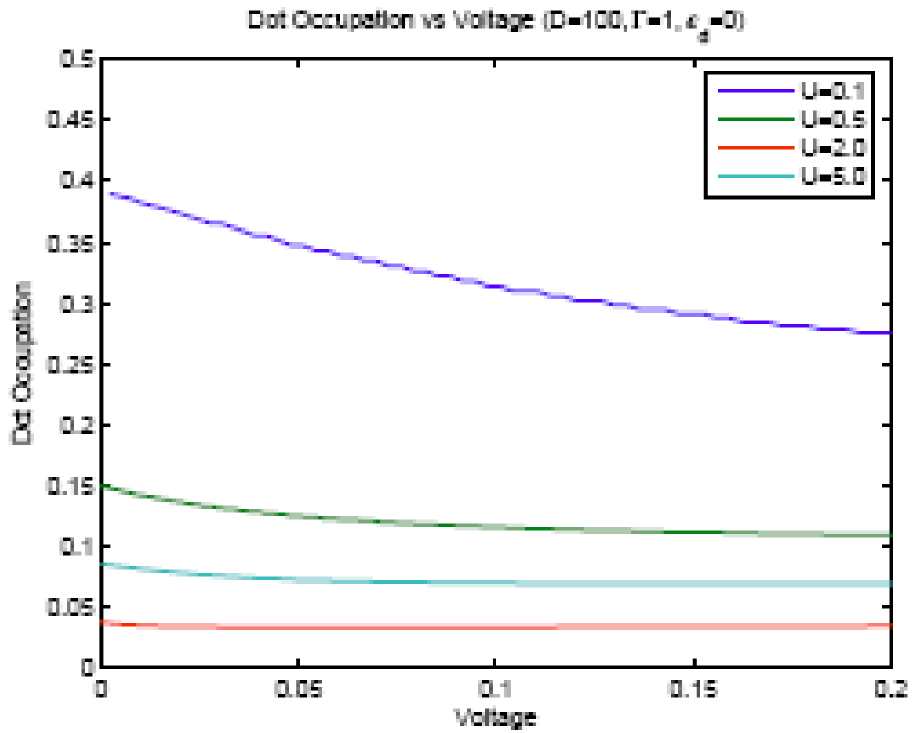
Comment:

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

IRL: Current vs. Voltage

- **Solve the TBA equations (numerically, analytically)**
- **Compute Exactly current 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 Δ

IRL: Current vs. Voltage

- **TBA eqns for momentum distributions: Non-eq BC**
- $\rho_i(p)$ **parametrized by** D **- lower cut-off (bandwidth)**
- **For Universality:** ($physical\ scales \ll D$)
  - **lower cut-off:** $D \to \infty$
  - **vary** U, Δ**, keeping low-E physics unchanged**
  - U, Δ **on RG trajectory**
- **New scale emerges** T_k **characterizing RG trajectory**
- **Universality out-of-equilibrium**

Explicitly, for $U \to \infty$, we find: (Wiener-Hopf..)

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

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

Low-energy scale: $T_k = D\left(\frac{\Delta}{D}\right)^{\frac{2\pi}{\pi+\zeta(U)}}$ held fixed in scaling limit:

$$D \to \infty,\ \zeta = -i \ln \frac{(1 - [\frac{U}{2}]^2) + 2i\frac{U}{2}}{1 + [\frac{U}{2}]^2} \to \pi$$

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

Many applications:

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