Interacting impurity out-of-equilibrium: an exact solution

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Outline

- Non-equilibrium in impurity models:
    - Background
    - General framework
- Introduction of the IRL model
- Analytical approach: TBA
- Numerical approach: td-DMRG

Background

Out-of-equilibrium in quantum impurities

- Keldysh approach: perturbative / hard to resum

- Dressed TBA (Quantum Hall edge states tunneling)
  (P.Fendley, A.W.W.Ludwig, H.Saleur 1995)

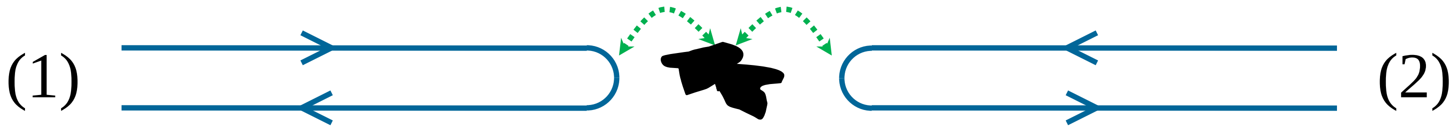
- Map to equilibrium problem (boundary sine Gordon model)
  (V.Bazhanov, S.Lukyanov, A.B.Zamolodchikov 1999)

- Effectively non-interacting system (Toulouse point)
  (A. Komnik, O. Gogolin 2003)

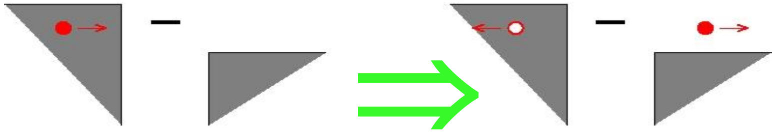
- Scattering Bethe Ansatz (IRLM, Anderson model)
  (P.Mehta, N.Andrei 2006)

- “Impurity conditions” (IRLM)
  (B.Doyon 2007)

General framework



- No interaction: Landauer Büttiker formula



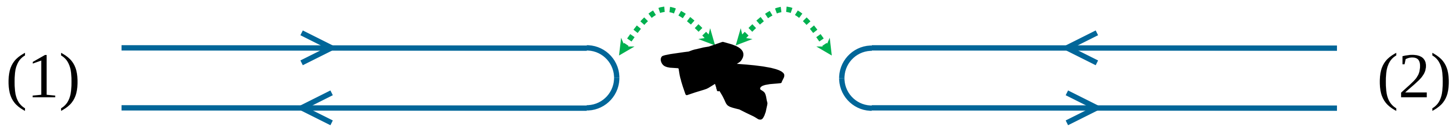
$$I = \int dE \left(f_1(E) - f_2(E)\right) T(E)$$

scattering approach:
Landauer-Büttiker formula

Fermi functions
for **electrons**
in wires (1) and (2)

transmission probability

General framework



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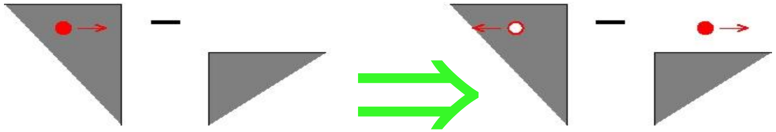
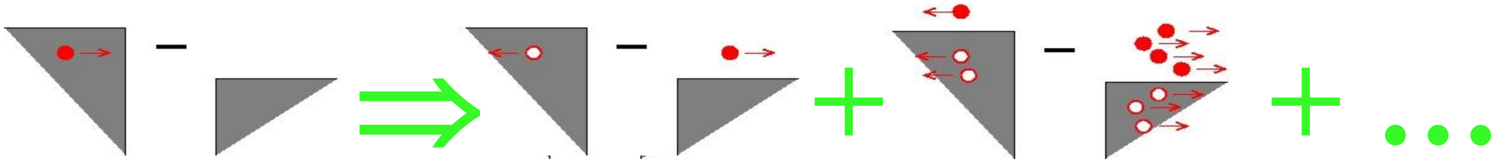
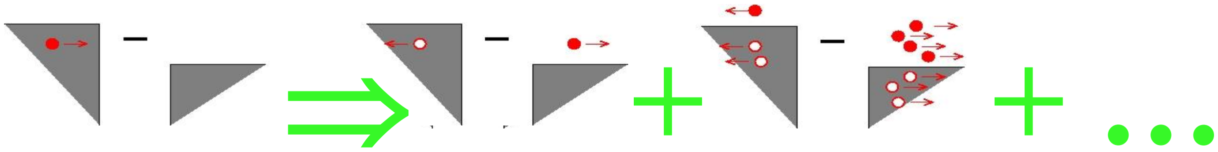


$$I = \int dE \left(f_1(E) - f_2(E)\right) T(E)$$

- Interaction: **particle production !**



General framework



Approach:

- describe the baths (Hilbert space of the wires) in terms of quasiparticles with the following properties:

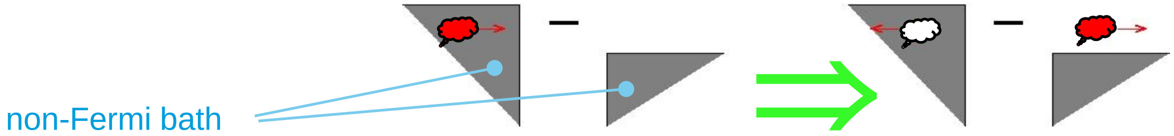
  (i) they **diagonalize the scattering** on the impurity, → **“equilibrium” integrability**

  no particle production (diagonal boundary scattering)

  (ii) they **survive out of equilibrium.** → **further (severe) requirement**

  not destroyed by the voltage

- use the Landauer Büttiker formula for this gas of (interacting) quasiparticles to compute the current.

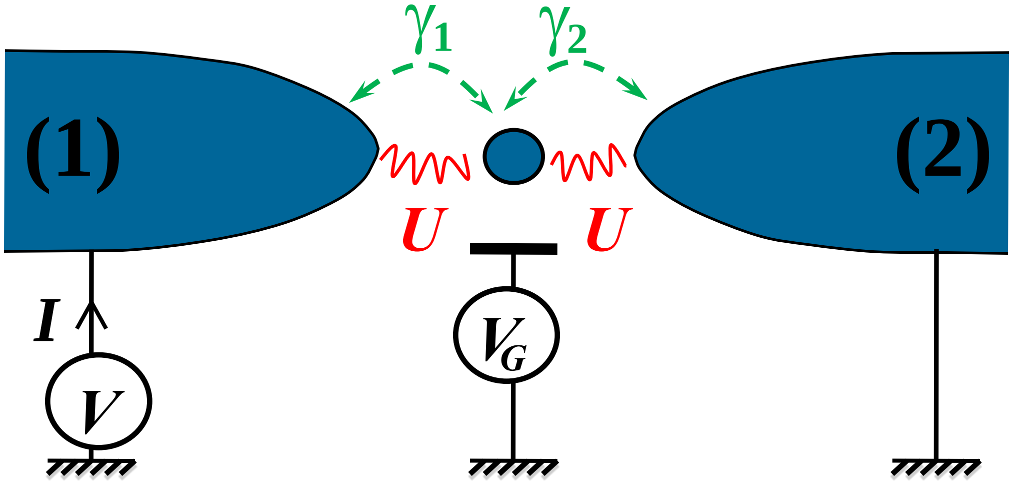


Impurity model: IRLM

Interacting Resonant Level Model

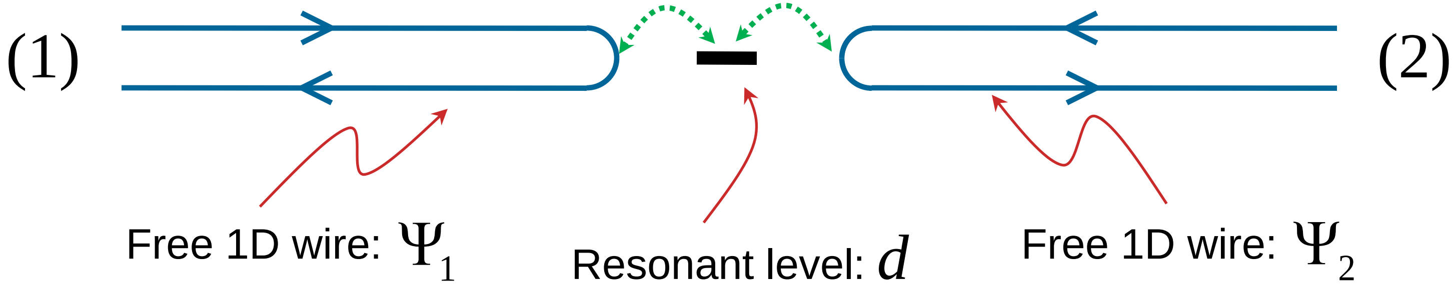
- Simplest quantum impurity model supporting both interactions and non-equilibrium
- Describes strongly polarized electrodes (*spinless*) coupled to nanostructure via:
  - tunnelling: γ_1, γ_2
  - Coulomb repulsion: U

Resonance: $V_G = V/2$



IRLM (2)

Single channel → mapping to 1D



Free 1D wire: Ψ_1

Resonant level: d

Free 1D wire: Ψ_2

$$\boxed{H = H_0 + H_B + H_V}$$

$$H_0 = -i v_{\mathrm{F}} \sum_{a=1,2} \int_{-\infty}^{\infty} dx \;\; \Psi_a^\dagger \partial_x \Psi_a(x)$$

$$H_V = \frac{V}{2} \int_{-\infty}^{\infty} dx \;\left(\Psi_1^\dagger \Psi_1 - \Psi_2^\dagger \Psi_2 \right)(x)$$

$$H_B = \left(\gamma_1 \Psi_1^\dagger(0) + \gamma_2 \Psi_2^\dagger(0) \right) d \; + \; U \left(: \Psi_1^\dagger \Psi_1 : (0) + : \Psi_2^\dagger \Psi_2 : (0) \right) \left(d^\dagger d - \tfrac{1}{2} \right) \; + \; \varepsilon_d \, d^\dagger d$$

$\varepsilon_d = 0$ at resonance

Mapping to Kondo

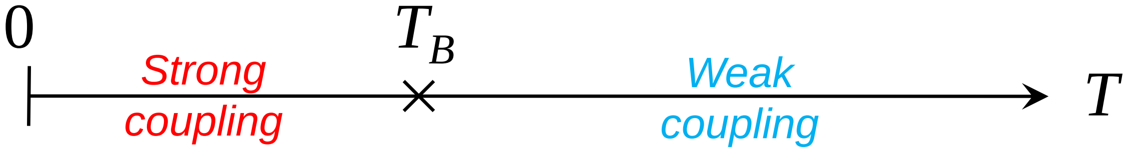
Integrable (in equilibrium)

(V.Filyov, P.Wiegmann 1978)

Mapping to anisotropic Kondo model (P.Wiegmann, A.M.Finkel'stein 1980)

$$\begin{aligned} d^{\dagger} &\leftrightarrow \eta\, S^{+} \\ d^{\dagger} d - \tfrac{1}{2} &\leftrightarrow S^{z} \end{aligned}$$

Kondo temperature T_K ↔ Hybridization temperature T_B



Question: out-of-equilibrium + strong coupling?

Bosonization (I)

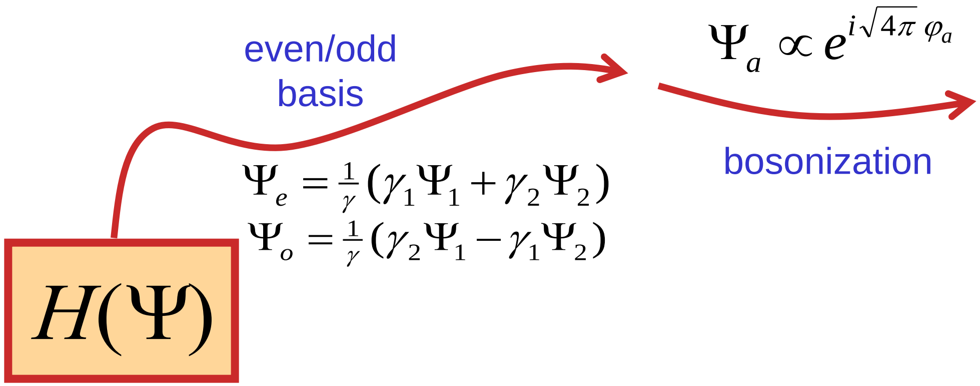
$$\boxed{H(\Psi)}$$

even/odd basis

$$\Psi_e = \tfrac{1}{\gamma}(\gamma_1\Psi_1 + \gamma_2\Psi_2)$$

$$\Psi_o = \tfrac{1}{\gamma}(\gamma_2\Psi_1 - \gamma_1\Psi_2)$$

Bosonization (I)



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bosonization

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bosonization

unitary transformation: cancels interaction along S^z

$$\mathcal{U} = e^{i\left(U/\sqrt{\pi}\right) S^z (\varphi_e+\varphi_o)(0)}$$

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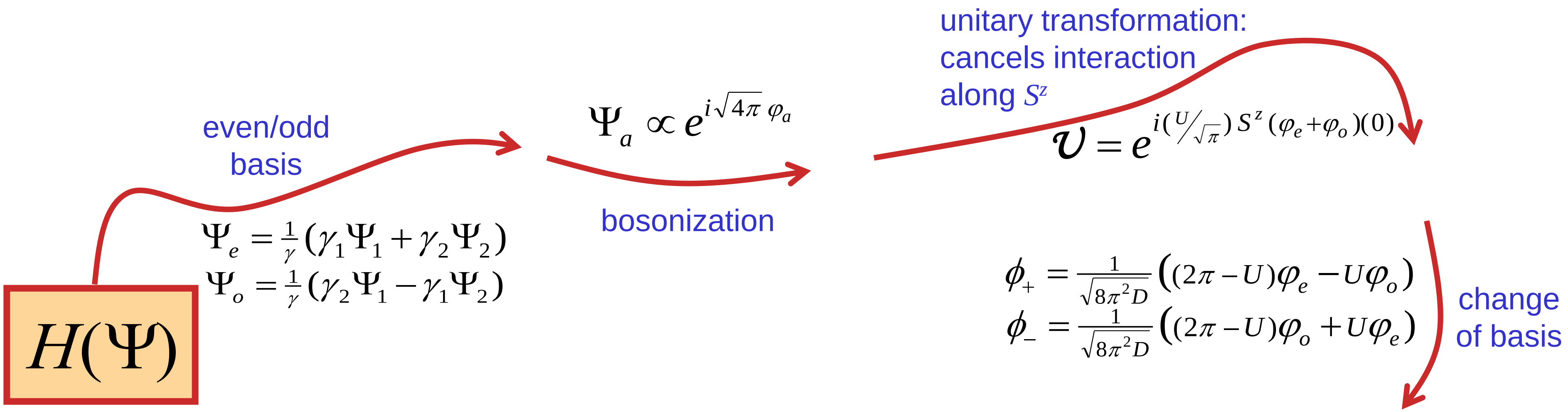
change of basis

$$\phi_+ = \frac{1}{\sqrt{8\pi^2 D}}\big((2\pi - U)\varphi_e - U\varphi_o\big)$$
$$\phi_- = \frac{1}{\sqrt{8\pi^2 D}}\big((2\pi - U)\varphi_o + U\varphi_e\big)$$

Bosonization (I)



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- ϕ_- decouples
- scaling dimension

$$D = \tfrac{1}{4} + \tfrac{1}{4}\left(1 - \tfrac{U}{\pi}\right)^2 \quad \left(\geq \tfrac{1}{4}\right)$$

$$\longrightarrow \quad T_B \propto (\gamma)^{\frac{1}{1-D}}$$

- duality $U \leftrightarrow 2\pi - U$

(A.Schiller, N.Andrei 2007)

anisotropic Kondo model

$$H = H_0(\phi_+) + H_0(\phi_-) + H_B$$

$$H_B = \gamma\, e^{i\sqrt{8\pi D}\,\phi_+(0)} S^+ + \text{h.c.}$$

Voltage operator (1)

- Simple theory: ***diagonal*** boundary scattering

$$\mathcal{H} = \mathcal{H}_+ \otimes \mathcal{H}_-$$

Kondo scattering

trivial scattering

- BUT: quasiparticles ***DESTROYED*** by the voltage

$$H_V = \tfrac{V}{2} \int \frac{\cos\theta}{\sqrt{2\pi D}} \left(\partial_x \phi_+ + (1-\tfrac{U}{\pi})\partial_x \phi_-\right) + \frac{\sin\theta}{\pi} \sin\sqrt{\tfrac{2\pi}{D}} \left(\phi_+ + (1-\tfrac{U}{\pi})\phi_-\right)$$

$$\boxed{\gamma_1 + i\gamma_2 = \gamma e^{i\theta/2}}$$

$\rightarrow$ {
- mixes $\mathcal{H}_+$ and $\mathcal{H}_-$
- worse: non-local wrt. the Kondo soliton creation operator

(exceptions: $D = 1/2$, $D = 1/4$)

Bosonization (II)

$$(\text{wire }1)\otimes(\text{wire }2) = \mathrm{U}(1)\otimes\mathrm{SU}(2)_1$$

total charge

iso-spin →

$$\begin{cases} J^z = \tfrac{1}{2}(\Psi_1^\dagger\Psi_1 - \Psi_2^\dagger\Psi_2) & \text{relative charge} \\ J^+ = \Psi_1^\dagger\Psi_2 & \text{mix the wires} \end{cases}$$

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iso-spin ⟶

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$$\boxed{H(\Psi)}$$

bosonization

$$\Psi_{1(2)} \propto e^{i\sqrt{4\pi}\,\varphi_{1(2)}}$$

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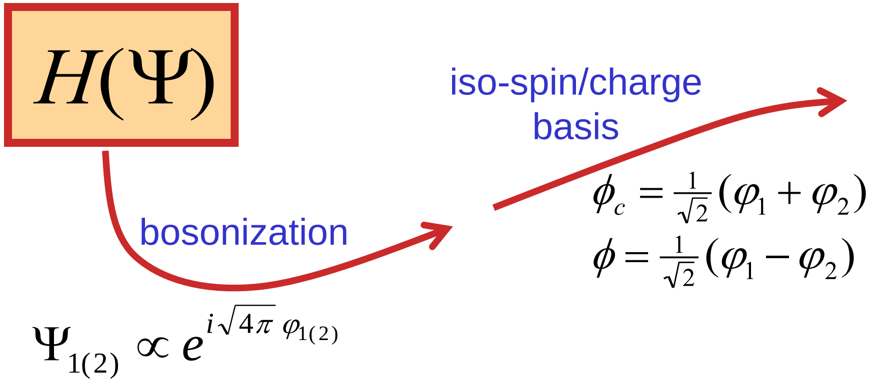

$$H(\Psi)$$

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iso-spin/charge basis

$$\phi_c = \tfrac{1}{\sqrt{2}}(\varphi_1 + \varphi_2)$$

$$\phi = \tfrac{1}{\sqrt{2}}(\varphi_1 - \varphi_2)$$

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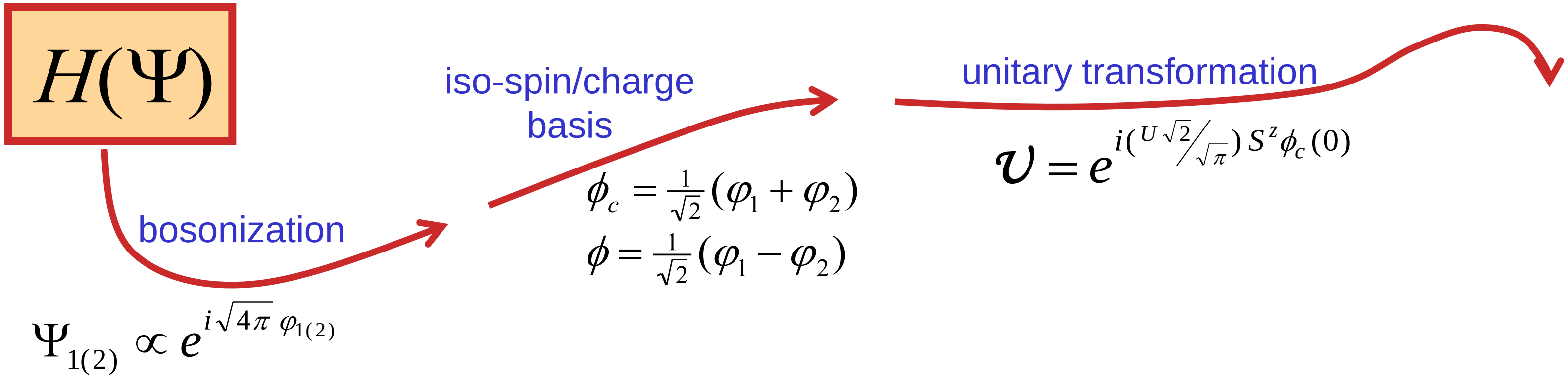

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$$\phi_c=\tfrac{1}{\sqrt{2}}(\varphi_1+\varphi_2)$$

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unitary transformation

$$\mathcal{U}=e^{i(U\sqrt{2}/\sqrt{\pi})\,S^z\phi_c(0)}$$

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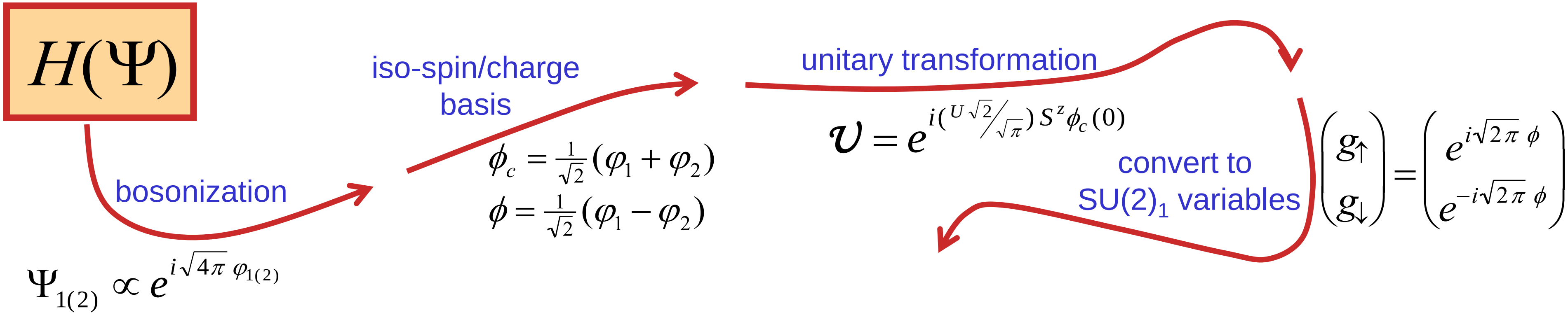

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$$\mathcal{U} = e^{i\left(U\sqrt{2}/\sqrt{\pi}\right)S^z\phi_c(0)}$$

convert to SU(2)$_1$ variables

$$\begin{pmatrix} g_\uparrow \\ g_\downarrow \end{pmatrix} = \begin{pmatrix} e^{i\sqrt{2\pi}\,\phi} \\ e^{-i\sqrt{2\pi}\,\phi} \end{pmatrix}$$

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$$\boxed{\begin{array}{c} H = H_0(\phi) + H_0(\phi_c) + H_B \\ H_B = \left(\gamma_1\, g_\uparrow(0) + \gamma_2\, g_\downarrow(0)\right) e^{i\beta_c\phi_c(0)} S^+ + \text{h.c.} \end{array}}$$

scaling dimensions : $\frac{1}{4}$ $\qquad$ $(\frac{1}{2} - \frac{U}{2\pi})^2 = D - \frac{1}{4}$

Voltage operator (2)

$$H = H_0(\phi) + H_0(\phi_c) + H_B$$
$$H_B = \left(\gamma_1\, g_{\uparrow}(0) + \gamma_2\, g_{\downarrow}(0)\right) e^{i\beta_c \phi_c(0)} S^+ + \text{h.c.}$$

Voltage operator: $\boxed{H_V = V \int J^z}$ SU(2) generator

¿ Quasiparticle basis with

(i) diagonal boundary scattering **?**

(ii) simple action of H_V **?**

➡ **Self-dual point** $\beta_c = \sqrt{2\pi}(1 - \tfrac{U}{\pi}) = 0$

Self-dual point

- Universal characterization: $D=\frac{1}{4}$ ($U=\pi$ in our scheme)
- Total charge ϕ_c decouples $\longrightarrow$ interaction only in $\mathrm{SU}(2)$ sector

"interacting Toulouse point"

- Full Hamiltonian:

$$H = \underbrace{H_0(\phi)+H_B+H_V}_{\mathrm{SU}(2)\text{ iso-spin sector}} + \underbrace{H_0(\phi_c)}_{\text{Total charge sector}}$$

$$H_B = \left(\gamma_1\, g_\uparrow(0) + \gamma_2\, g_\downarrow(0)\right) S^+ + \mathrm{h.c.} \qquad H_V = V\int J^z$$

(massless) spectrum

- Rotate to Kondo

$$H_B = \left(\gamma_1\, g_\uparrow(0) + \gamma_2\, g_\downarrow(0)\right) S^+ + \text{h.c.} \xrightarrow{\mathcal{R}^y_{-\theta}} \boxed{\gamma\, g_\uparrow(0)\, S^+ + \text{h.c.}}$$

Kondo

$$(\mathcal{R}^y_\theta = e^{i\theta \int J^y} \quad \text{and} \quad \gamma_1 + i\gamma_2 = \gamma e^{i\theta/2})$$

- Fold the system $\Phi(x) = \phi(x) + \phi(-x)$
- Quasiparticle basis inherited from bulk sine Gordon model defined on the half-line, at $\beta = \sqrt{2\pi}$:

$$\lim_{\Lambda \to 0} \left(H_0(\Phi) + \Lambda \int_{-\infty}^{0} dx \cos\left(\sqrt{2\pi}\Phi\right) + H_B \right)$$

The bulk theory has a global SU(2) symmetry (generators: $\int J^a$)

(massless) spectrum

Spectrum: soliton/antisoliton $A_\pm$

first breather A_1

$S = 1$ triplet

second breather A_0

$S = 0$ singlet

parametrize momentum by rapidity λ: $p = \frac{m}{2} e^{\lambda}$

⇒ incoming Hilbert space spanned by the basis states:

$$\left|\alpha_1,\alpha_2,....,\alpha_n;\lambda_1 > \lambda_2 > .... > \lambda_n > 0\right\rangle = A_{\alpha_1}(\lambda_1)\, A_{\alpha 2}(\lambda_2)\ ...\ A_{\alpha_n}(\lambda_n)\left|0\right\rangle$$

⇒ outcoming Hilbert space:

$$\left|\alpha_1,\alpha_2,....,\alpha_n;\lambda_1 < \lambda_2 < .... < \lambda_n < 0\right\rangle = A_{\alpha_1}(\lambda_1)\, A_{\alpha 2}(\lambda_2)\ ...\ A_{\alpha_n}(\lambda_n)\left|0\right\rangle$$

Remark: each such state has a **finite-dimensional** orbit under the global $\mathrm{SU}(2)$ action.

Bulk scattering

$$\boxed{\lambda\lambda' > 0: \quad A_\alpha(\lambda)A_\beta(\lambda') = S_{\alpha\beta}(\lambda - \lambda')\, A_\beta(\lambda')A_\alpha(\lambda)}$$

$$\alpha, \beta \neq 0: \quad S_{\alpha\beta}(\lambda) = S_1(\lambda) = \frac{2\sinh\lambda + i\sqrt{3}}{2\sinh\lambda - i\sqrt{3}}$$

$$\alpha \neq 0: \quad S_{0\alpha}(\lambda) = S_{\alpha 0}(\lambda) = S_0(\lambda) = \frac{\sinh\lambda + i}{\sinh\lambda - i}\,\frac{2\sinh\lambda + i}{2\sinh\lambda - i}$$

$$S_{00}(\lambda) = \left(S_1(\lambda)\right)^3$$

Boundary scattering

- Incoming and outcoming states are related through the boundary scattering matrix R

$$\boxed{A_\alpha(\lambda) = R_{\alpha\beta}(\lambda)\, A_\beta(-\lambda)}$$

- R depends on rapidity λ and boundary temperature $\Box T_B = \frac{m}{2} e^{\lambda_B}$

Kondo:

$$R^K = \left(\begin{array}{cccc} P^K & 0 & 0 & 0 \\ 0 & P^K & 0 & 0 \\ 0 & 0 & R_1^K & 0 \\ 0 & 0 & 0 & R_0^K \end{array}\right)\begin{array}{c} + \\ - \\ 1 \\ 0 \end{array}$$

$$P^K = \tanh\left(\tfrac{\lambda-\lambda_B}{2} - \tfrac{i\pi}{4}\right)$$

$$R_1^K = \frac{\tanh\left(\frac{\lambda-\lambda_B}{2} - \frac{i\pi}{12}\right)}{\tanh\left(\frac{\lambda-\lambda_B}{2} + \frac{i\pi}{12}\right)}$$

$$R_0^K = \frac{\tanh\left(\frac{\lambda-\lambda_B}{2} - \frac{i\pi}{6}\right)}{\tanh\left(\frac{\lambda-\lambda_B}{2} + \frac{i\pi}{6}\right)}$$

$$\mathcal{R}_\theta^y$$

IRLM:

$$R^{IRLM} = \left(\begin{array}{cccc} P^K + \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & 0 \\ \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & P^K + \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & 0 \\ \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & \cos^2\theta\, R_1^K + \sin^2\theta\, P^K & 0 \\ 0 & 0 & 0 & R_0^K \end{array}\right)\begin{array}{c} + \\ - \\ 1 \\ 0 \end{array}$$

Boundary scattering

$$\boxed{A_\alpha(\lambda) = R_{\alpha\beta}(\lambda)\, A_\beta(-\lambda)}$$

$$R^{IRLM} = \begin{array}{cc} \begin{pmatrix} P^K + \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & 0 \\ \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & P^K + \frac{\sin^2\theta}{2}\,(R_1^K - P^K) & \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & 0 \\ \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & \frac{\sin 2\theta}{2\sqrt{2}}\,(R_1^K - P^K) & \cos^2\theta\, R_1^K + \sin^2\theta\, P^K & 0 \\ 0 & 0 & 0 & R_0^K \end{pmatrix} & \begin{array}{c} + \\ - \\ 1 \\ 0 \end{array} \end{array}$$

Soliton → breather 1 : charge transfered $\Delta Q = -2e$

Relative charge $Q_1 - Q_2 = \int J^z$ carried by quasiparticles:

$$(Q_1 - Q_2)\, A_\alpha(\lambda)|0\rangle = q_\alpha\, A_\alpha(\lambda)|0\rangle \qquad q_\pm = \pm 2e \qquad q_0 = q_1 = 0$$

Recollection

- The quasiparticle basis diagonalizes the boundary scattering (i.e. no quasiparticle production)
- The quasiparticle basis diagonalizes the voltage operator (i.e. quasiparticles survive out of equilibrium)

$\Rightarrow$ compute charge transfer rate

$\Rightarrow$ do the thermodynamics for the gas of incoming states subject to a finite bias

Current

Charge transfer rate:

$$\tau_{\alpha\beta}^{-1}(\lambda) = (q_\alpha - q_\beta)\left|R_{\alpha\beta}(\lambda)\right|^2$$

$$I = \int d\lambda \sum_{\alpha\beta} \tau_{\alpha\beta}^{-1}(\lambda)\, n_\alpha n_\beta f_\beta (1 - f_\alpha) = \ldots = \int d\lambda\, n_+ (f_+ - f_-) \frac{2}{1 + e^{6(\lambda - \lambda_B)}}$$

$\Rightarrow$ do the thermodynamics for the gas of incoming states subject to a finite bias

(bulk) TBA

Determine the occupation functions f_α ,
and density of allowed states n_α :

$$f_\alpha(\lambda, {}^V\!/_T) = \left(1 + e^{\varepsilon_\alpha - q_\alpha V/T}\right)^{-1} \qquad n_\alpha(\lambda, V/T) = \frac{T}{2\pi}\frac{\partial \varepsilon_\alpha}{\partial \lambda}$$

→ Pseudo energies ε_α: determined by the bulk scattering of quasi-particles

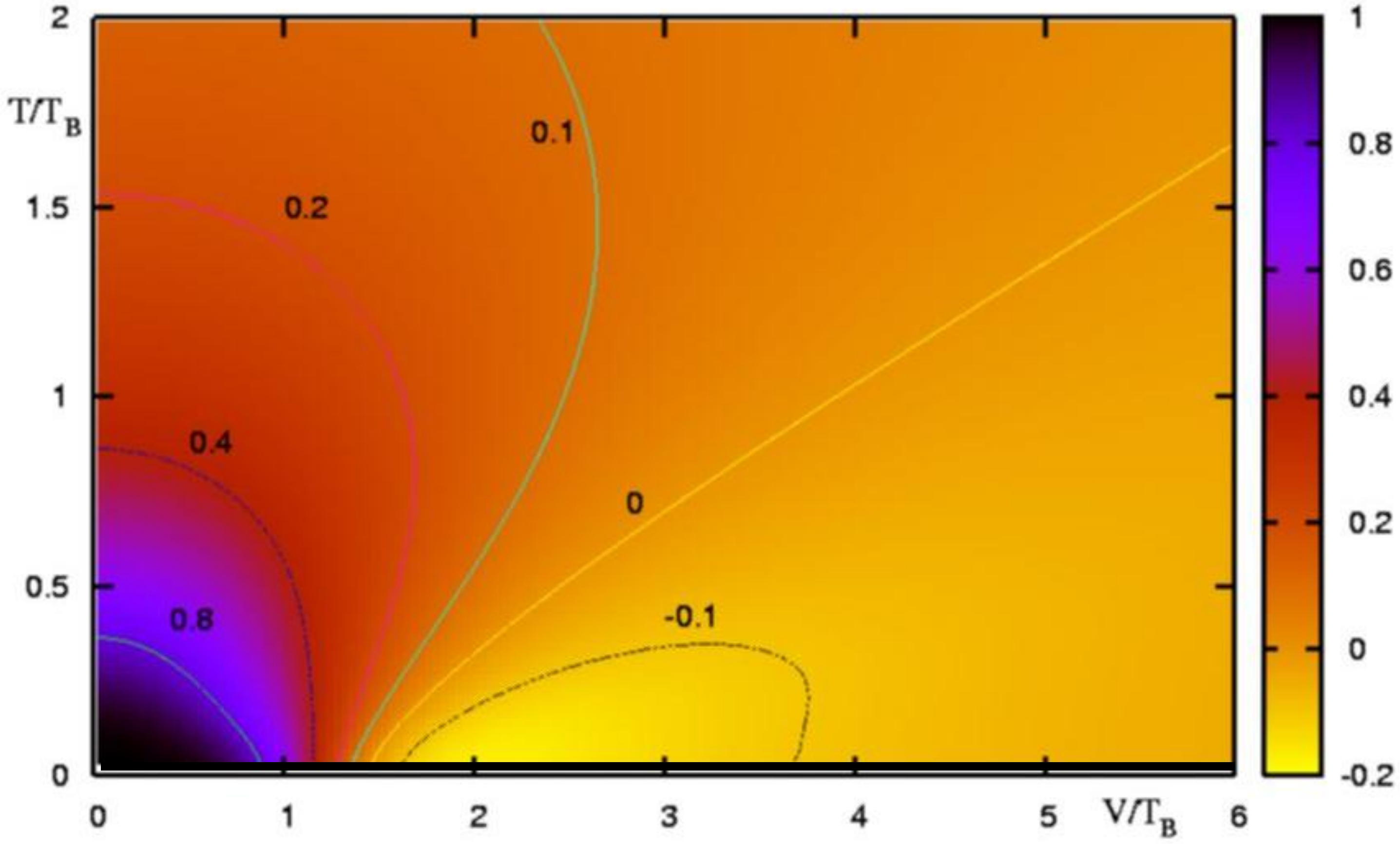
TBA equations:

$$\varepsilon_\alpha(\lambda, V/T) = \mu_\alpha e^\lambda \; - \; \frac{1}{2\pi}\left[-i\partial_\lambda \ln(S_{\alpha\beta}) * \ln\left(1 + e^{q_\beta V/T} e^{-\varepsilon_\beta}\right)\right](\lambda)$$

I-V curve (finite T)

Numerical integration of the TBA equations ⟶ current

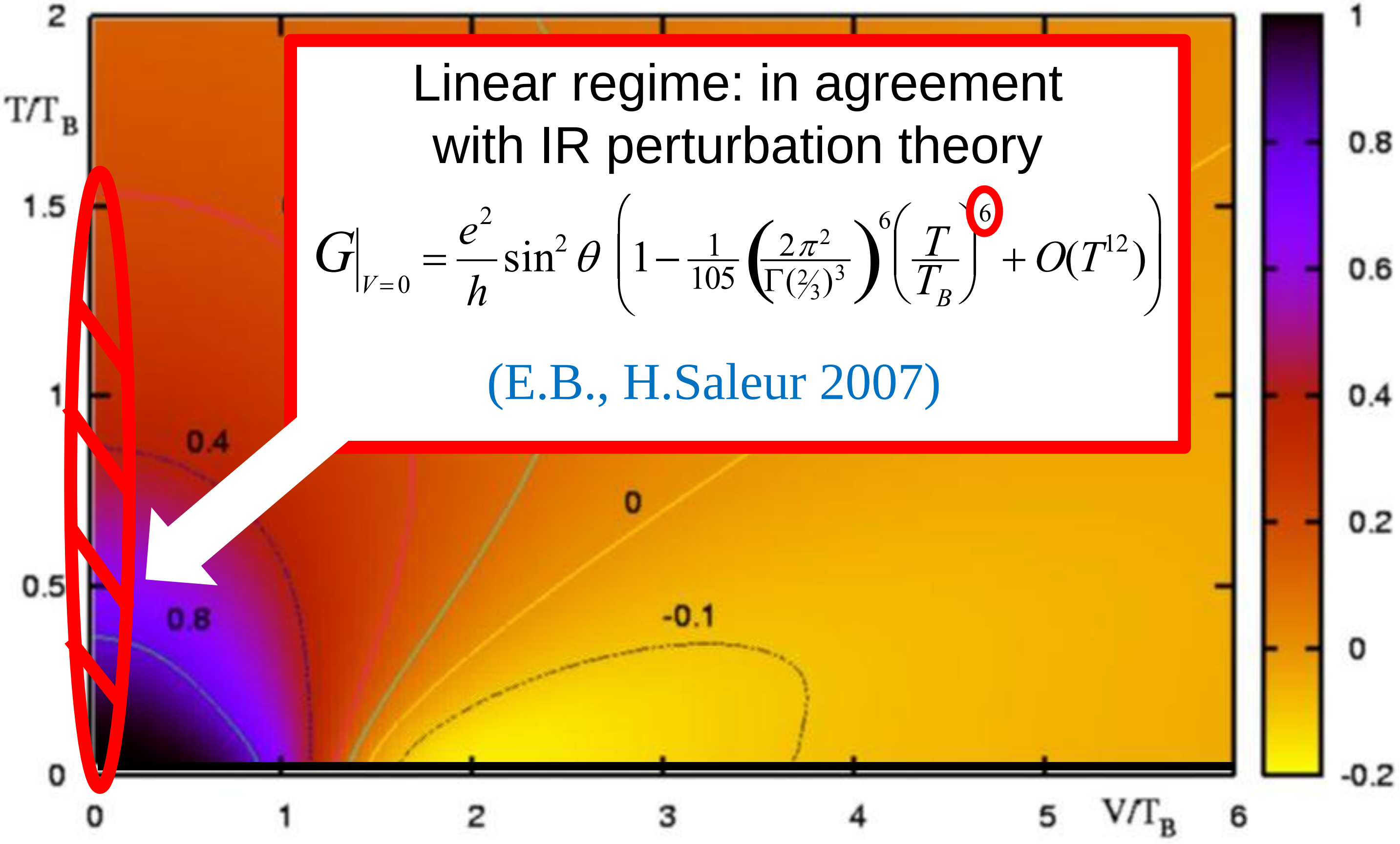
Differential conductance $G = \partial I / \partial V$



I-*V* curve (finite *T*)

Numerical integration of the TBA equations ⟶ current

Differential conductance $G = \partial I / \partial V$



Linear regime: in agreement with IR perturbation theory

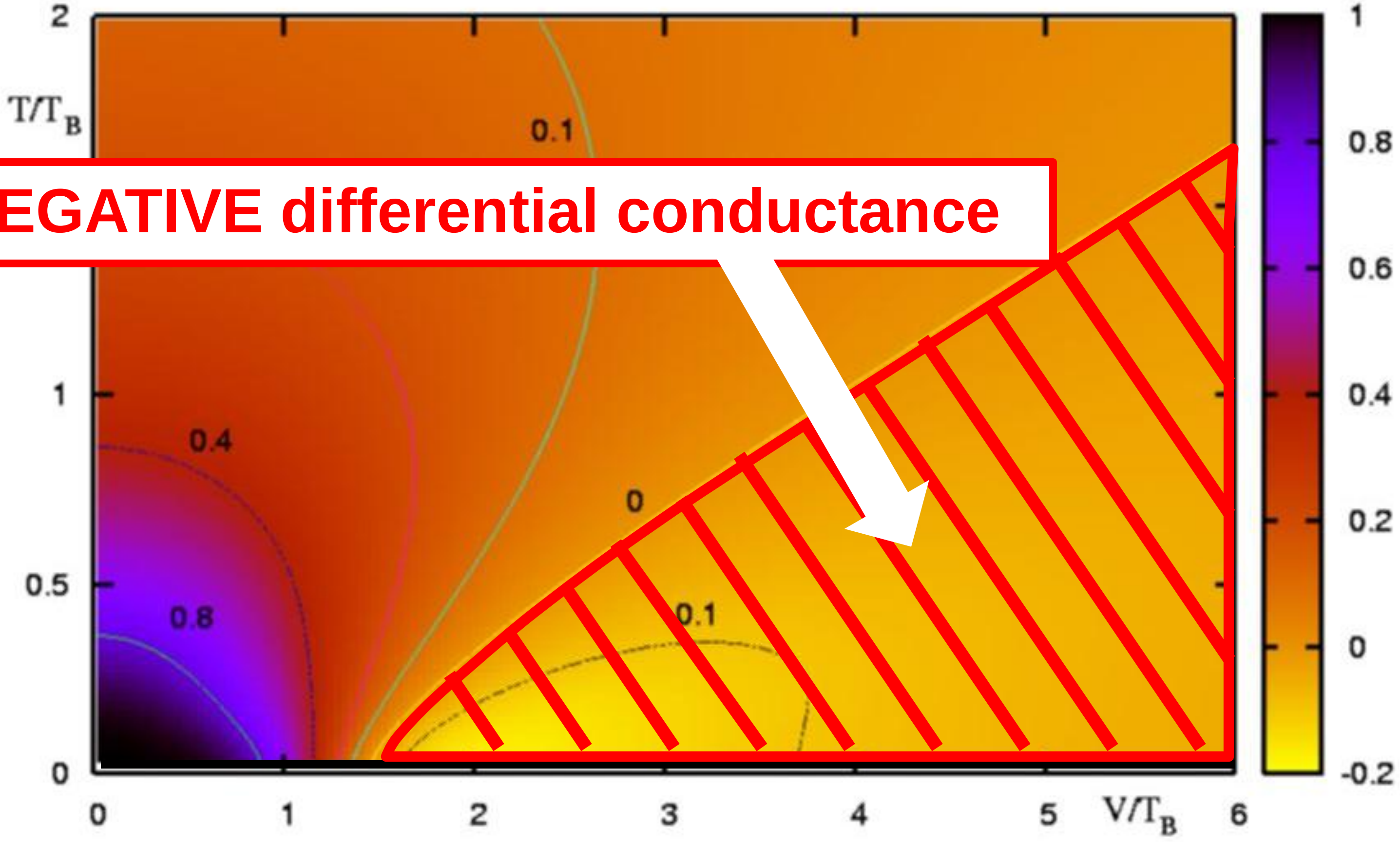
$$G\big|_{V=0} = \frac{e^2}{h}\sin^2\theta\left(1 - \frac{1}{105}\left(\frac{2\pi^2}{\Gamma(\frac{2}{3})^3}\right)^6\left(\frac{T}{T_B}\right)^{6} + O(T^{12})\right)$$

(E.B., H.Saleur 2007)

I-V curve (finite T)

Numerical integration of the TBA equations ⟶ current

Differential conductance $G = \partial I / \partial V$



NEGATIVE differential conductance

I-V curve ($T=0$)

$T=0$: well defined “Fermi” level for antisolitons

$$p_{\mathrm{F}} = \frac{2^{1/3}}{3^{1/2}} \frac{\Gamma(1/6)}{2\sqrt{\pi}\,\Gamma(2/3)} V$$

Wiener-Hopf technique → explicit solution of TBA equations

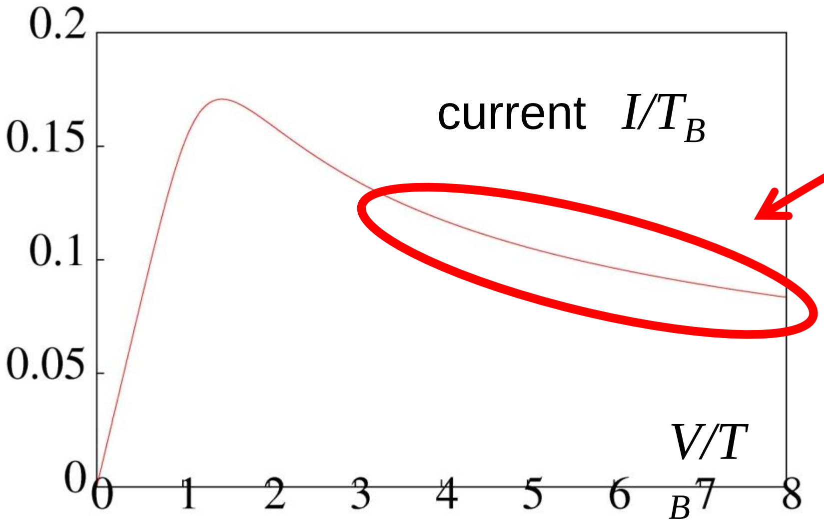
→ closed form for $I(V)$

$$I = V \sum_{n\geq 0} \frac{(-1)^n}{4\sqrt{\pi}} \frac{(4n)!}{n!\,\Gamma(3n+3/2)} \bar{V}^{6n}$$

$$\bar{V} = \frac{\Gamma(1/6)}{4\sqrt{\pi}\,\Gamma(2/3)} \frac{V}{T_B}$$

$$I = V \sum_{n>0} \frac{(-1)^{n+1}}{4\sqrt{\pi}} \frac{\Gamma(1+n/4)!}{n!\,\Gamma(3/2-3n/4)} \bar{V}^{-3n/2}$$

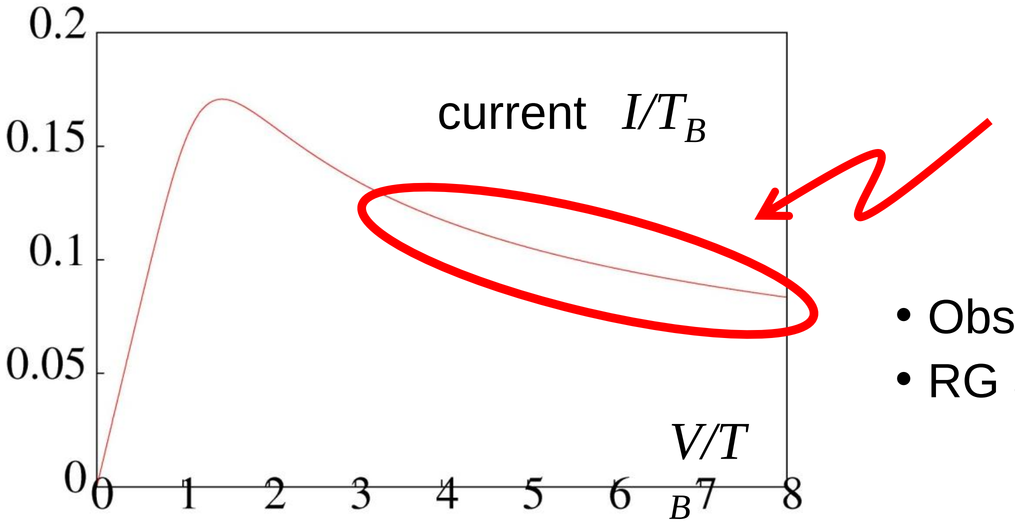
I-V curve (T=0)



$$I \propto T_B^{3/2}\, V^{\underbrace{-1/2}_{2D-1}}$$

- Observed at small U (B.Doyon 2007)
- RG argument: V cuts off the flow

I-V curve ($T=0$)



$$I \propto T_B^{3/2}\ V^{-1/2}$$

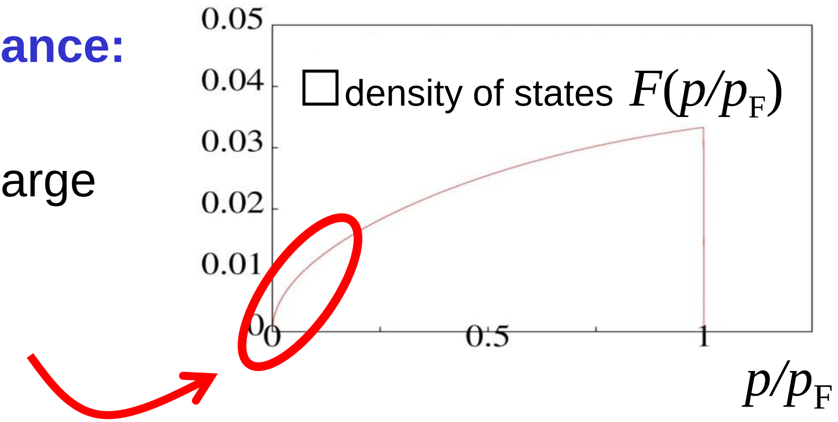
$2D$-1

- Observed at small U (B.Doyon 2007)
- RG argument: V cuts off the flow

Origin of Negative Differential Conductance:

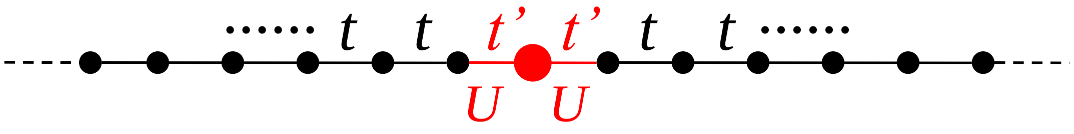
→ Density of states for current carriers (antisolitons) vanishes as a power law at large voltage and small momentum

$$\rho_-(p) = F(p/p_F)\ \Theta(p_F - p) \underset{p<<V}{\propto} \sqrt{p/V}$$



Numerical approach

- Lattice model



- Time-dependent DMRG

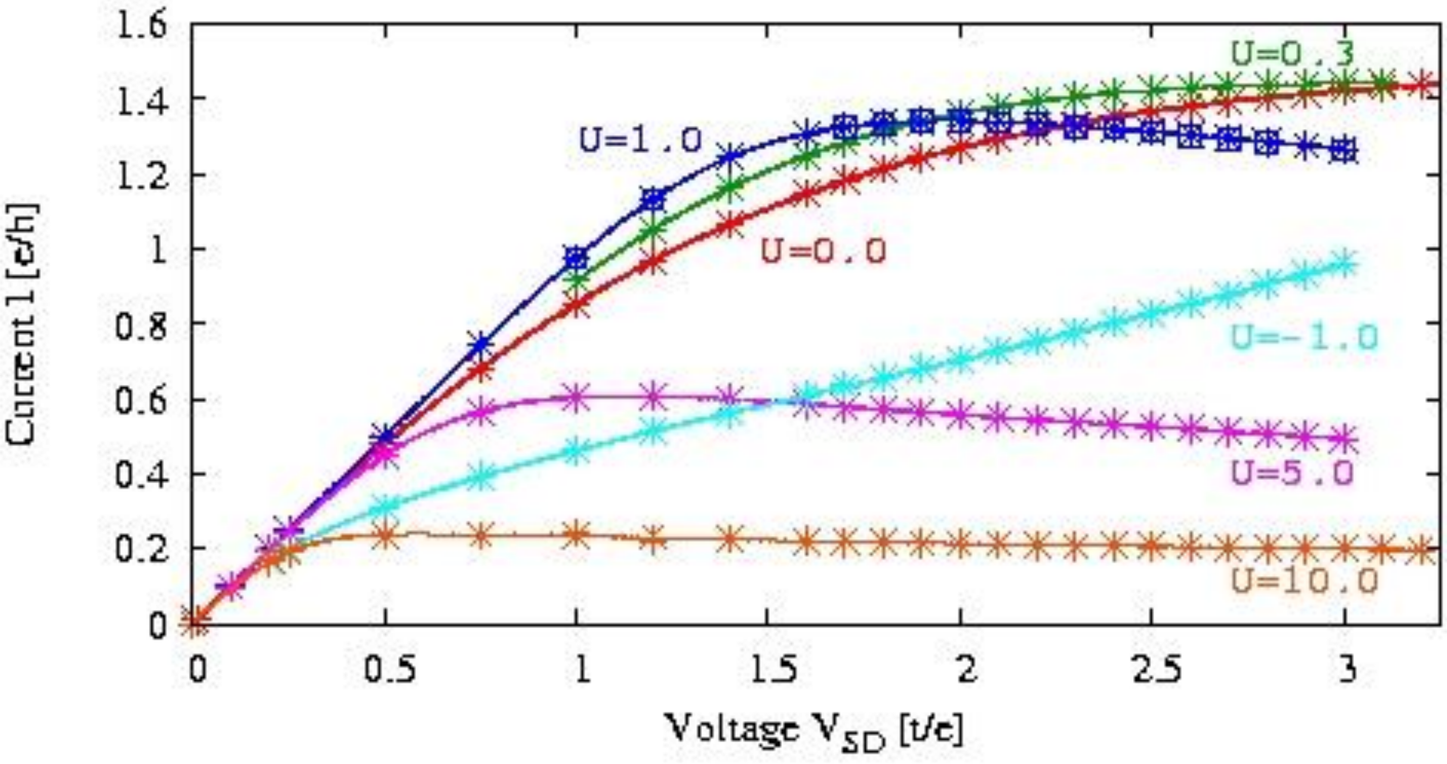
  (S.White, A.Feiguin 2004, P.Schmitteckert 2004)

  - Initial state ($t<0$): prepare the electrodes at different chemical potentials $\pm V/2$
  - Switch off the voltage at $t=0$
  - Time-evolve using interacting Hamiltonian

    (duration $\Delta t < L_{\mathrm{lead}} / v_{\mathrm{F}}$)
  - Extrapolate to infinite size

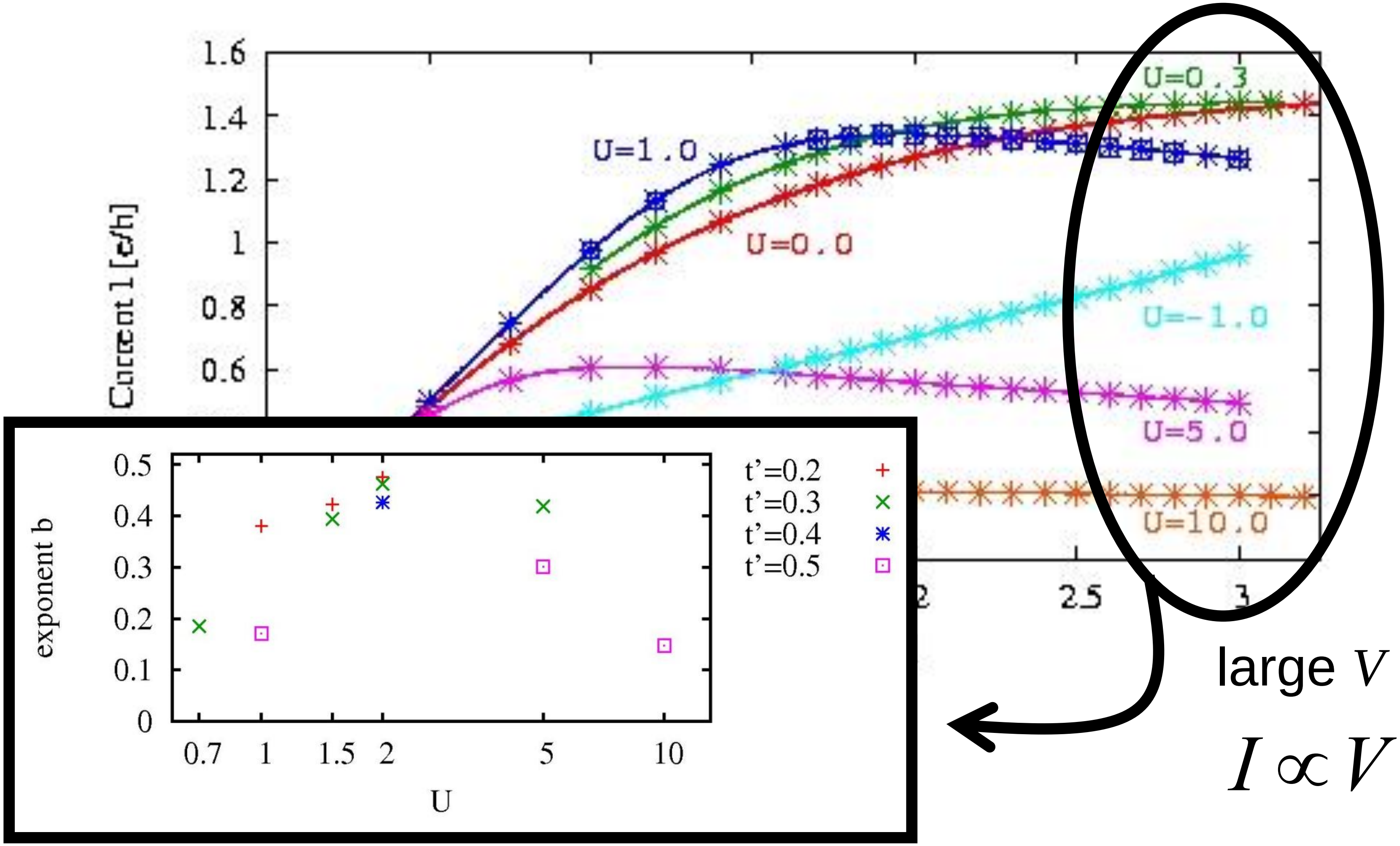
Numerical results

M=96 sites ; N=2000 states kept



Numerical results

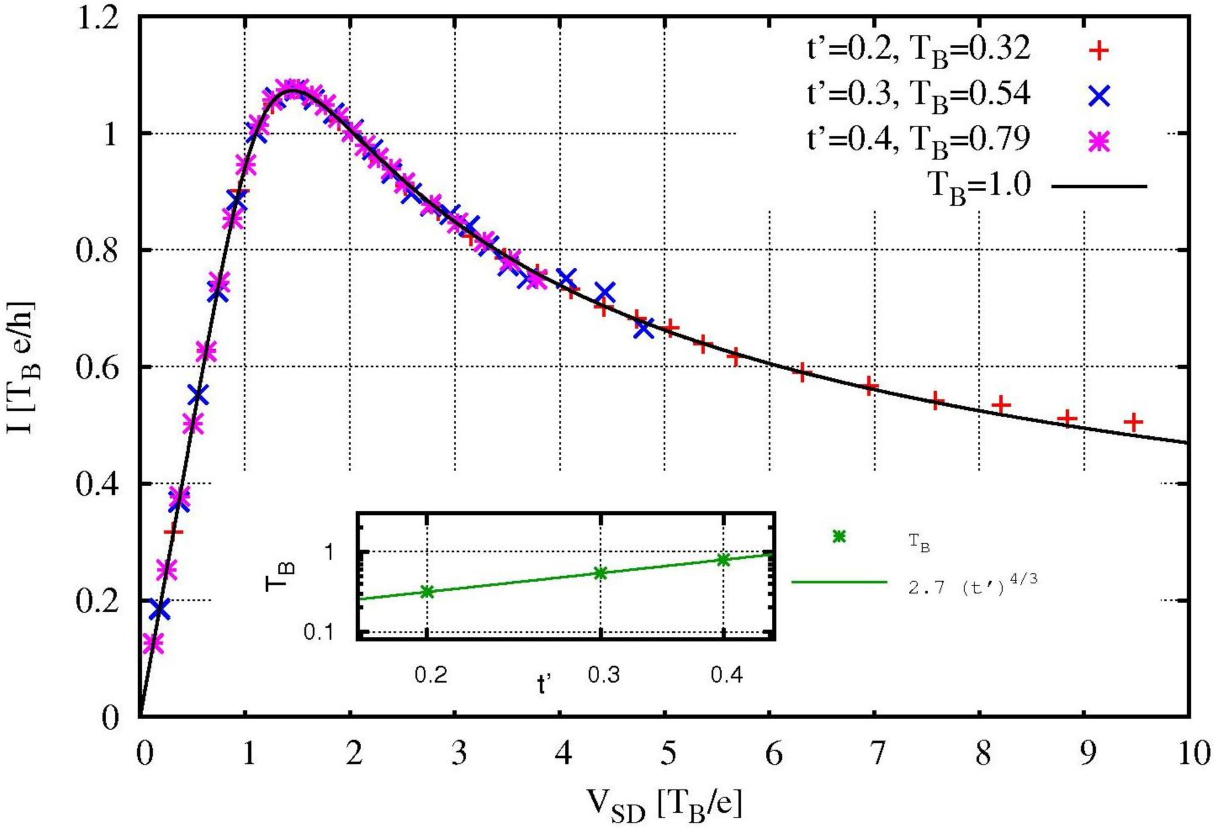
M=96 sites ; N=2000 states kept ; t’=0.5



large *V* fit:

$$I \propto V^{-b}$$

Numerical results



M=96 sites ; N=2000 states kept ; *U=2*

Conclusions

- Dressed TBA approach valid when *both* boundary scattering *and* voltage operator are diagonal.

- This is the case in the self-dual IRLM

  → Carry on with noise, computation of Green’s function (form factors)

- Necessary condition for the existence of such a diagonal basis in general? Relationship to Scattering Bethe Ansatz?

Thank you !

Extra slides

Alternate derivation

- Klein factors cancel out at all order of the Keldysh expansion for the current
- Choose $\gamma_1 = \gamma_2 = \gamma$

$$H_B = \left(\gamma_1 \kappa_1\, e^{i\sqrt{2\pi}\phi(0)} + \gamma_2 \kappa_2\, e^{-i\sqrt{2\pi}\phi(0)}\right) S^+ + \text{h.c.} \quad \Rightarrow \quad 4\gamma \cos\left(\sqrt{2\pi}\phi(0)\right) S^x$$

$\Longrightarrow$ **Out-of-equilibrium Boundary Sine Gordon model**

- Problem equivalent to the tunelling of edge states in the fractionnal quantum Hall effect (P.Fendley, A.W.W.Ludwig, H.Saleur 1995)