Universal conductance in quantum multi-wire junctions

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Phys. Rev. Lett. 105, 226803 (2010).

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Outline

- Introduction and motivation
- Formulation of the problem as a BCFT
- Universal conductance in the BCFT
- Lattice model implementation: a new method
- Numerical benchmarks
- Application to an interacting Y-Junction
- Summary and conclusions

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Introduction and motivation

Device miniaturization is approaching atomic scales...

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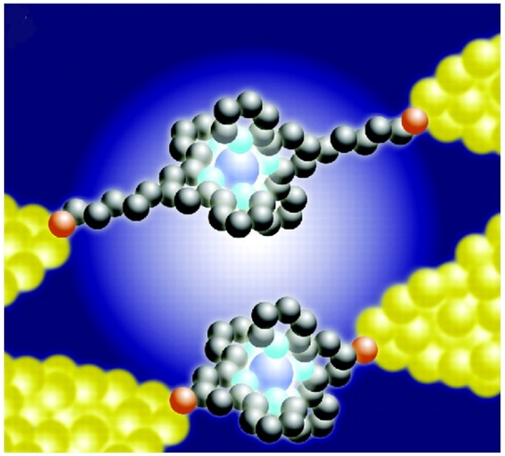
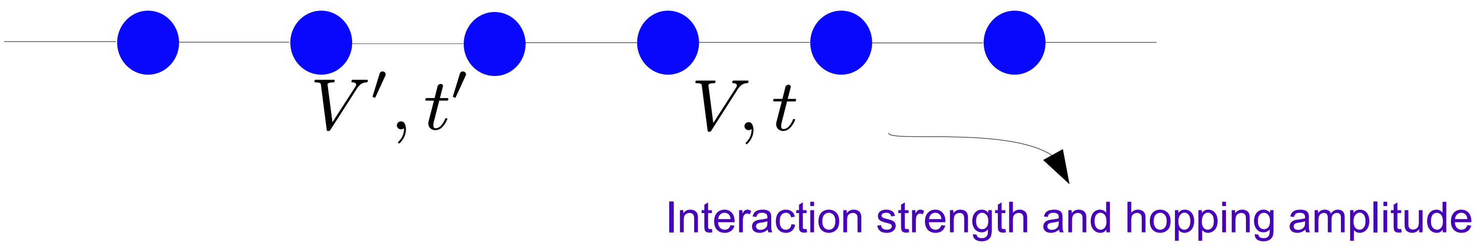


A. Nitzan and M. A. Ratner, Science 300, 1384 (2003).

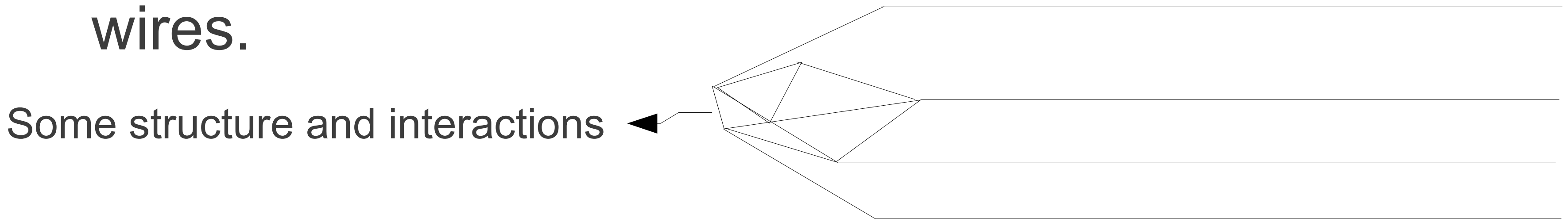
Electrical current passing through molecular structures

Introduction and motivation

At molecular length scales quantum mechanics is important. A simple theoretical description of such structures is based on the tight-binding model.



Any electrical circuit made with molecular building blocks must involve junctions of three or more wires.

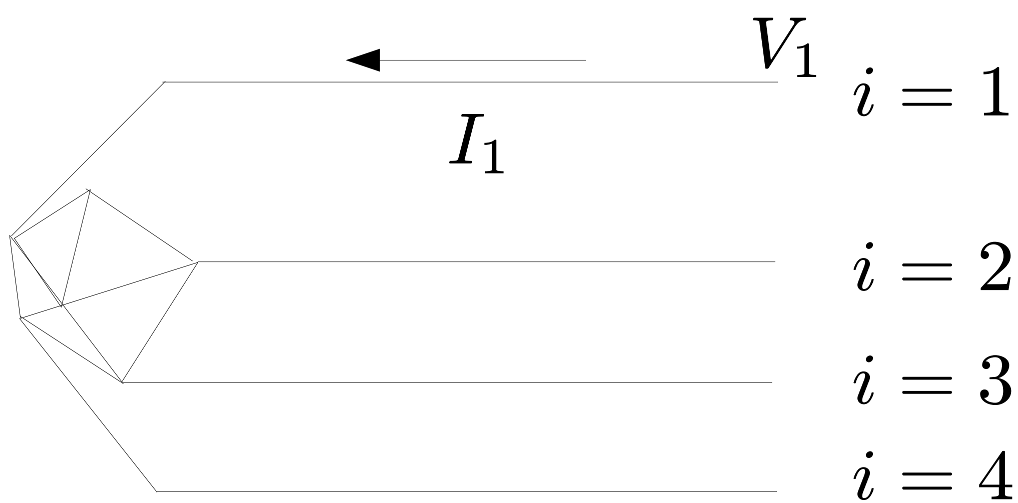


Introduction and motivation

Question: How does a junction conduct electricity?

$$I_i = f(V_1, V_2 \ldots V_n)$$

Linear response regime: $I_i = \sum_j G_{ij} V_j$



Introduction and motivation

Universality

Many different junctions, i.e. with different structure and interactions, can have the same linear conductance.

Challenge: given an arbitrary junction with some structure and interactions, determine the universal conductance of the junction?

Difficult because 1) conductance is related to *dynamical* correlation functions and 2) conductance is a property of an *open* quantum system. Do we need to do *time-dependent* calculations in *infinitely large* systems?

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Formulation of the problem as a BCFT

Let us consider one wire and take the continuum limit of the lattice quantum wire. The low energy effective description of the quantum wire is a Luttinger liquid, which is a critical theory of bosons.

$$H = \sum_j \left[-t c_j^\dagger c_{j+1} + \mathrm{h.c.} + V(n_j - \frac{1}{2})(n_{j+1} - \frac{1}{2}) \right]$$

$$n_j = c_j^\dagger c_j$$

$$H_{\mathrm{LL}} = \int dx \frac{v}{4\pi} \left[g(\partial_x \varphi)^2 + \frac{1}{g}(\partial_x \theta)^2 \right]$$

$$\rho(x) = \partial_x \theta(x)/(\sqrt{2}\pi)$$

$$[\varphi(x), \theta(x')] = i\pi \mathrm{sgn}(x' - x)$$

Formulation of the problem as a BCFT

At half-filling we have from the Bethe ansatz:

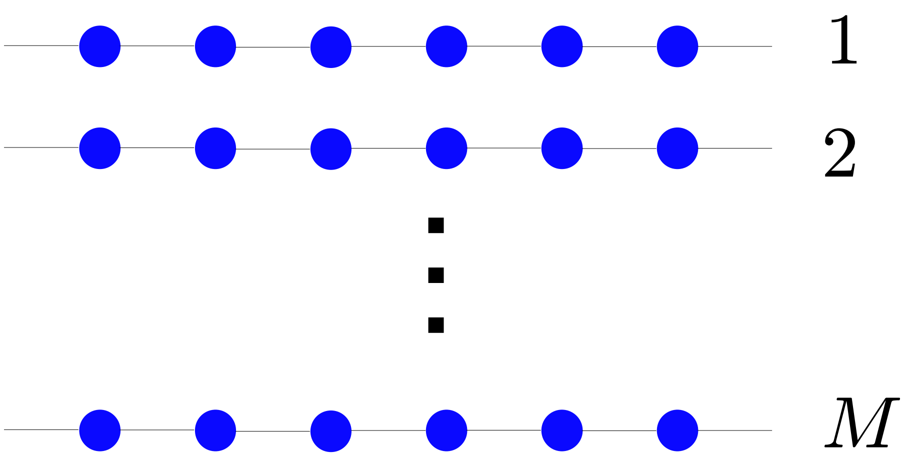
$$g = \frac{\pi}{2\,\mathrm{arccos}\,(-V/2t)}, \qquad v = \pi t \frac{\sqrt{1-(V/2t)^2}}{\mathrm{arccos}\,(V/2t)}.$$

g<1, repulsive
g=1, non-interacting
g>1, attractive

The action for one wire can then be written as:

$$S = \frac{g}{4\pi}\int d^2x\,\partial_\mu\varphi\partial^\mu\varphi = \frac{1}{4\pi g}\int d^2x\,\partial_\mu\theta\partial^\mu\theta$$

Formulation of the problem as a BCFT



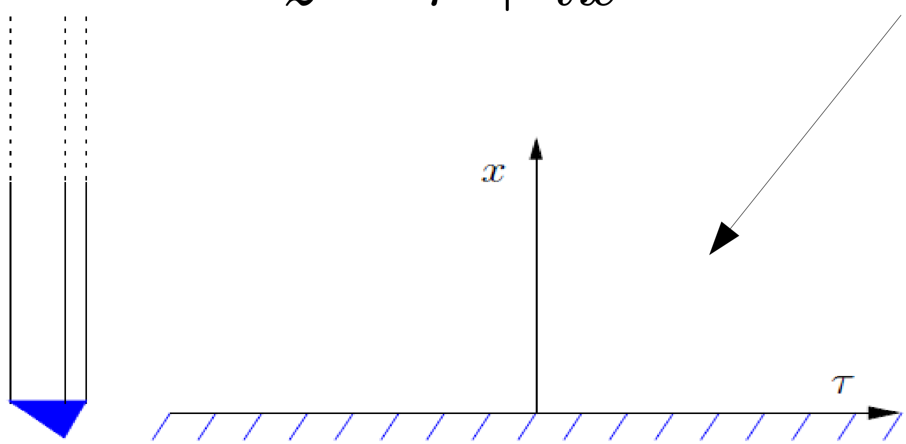
M wires with no connection (no junction) can be described by a conformal field theory with M species of bosonic fields living on the infinite plane.

Hypothesis:
The universal behavior of a junction, i.e. at the renormalization group fixed point, can be generically described by a conformally invariant boundary condition.

Formulation of the problem as a BCFT

$$z = \tau + ix$$

$$\theta_j, \quad j = 1 \ldots M$$



$$|\mathcal{B}\rangle$$

The junction modeled as a boundary conformal field theory with M species of bosonic fields living on the upper half-plane.

$$\partial \equiv \partial_z = \frac{1}{2}(\partial_\tau - i\partial_x)$$

$$\bar{\partial} \equiv \partial_{\bar{z}} = \frac{1}{2}(\partial_\tau + i\partial_x)$$

J. L. Cardy, Nucl. Phys. B 324, 581 (1989).

Primary fields are the vertex operators and

$$J_L^j(z) = \frac{i}{\sqrt{2\pi}}\,\partial\,\theta^j(z,\bar{z})$$

$$J_R^j(\bar{z}) = -\frac{i}{\sqrt{2\pi}}\,\bar{\partial}\,\theta^j(z,\bar{z})$$

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Universal conductance in the BCFT

Where in this BCFT is the conductance of the junction hiding?

Consider the Kubo formula

$$G_{ij} = \lim_{\omega\to 0_+} -\frac{e^2}{\hbar}\frac{1}{\omega L}\int_{-\infty}^{\infty} d\tau\, e^{i\omega\tau}\int_0^L dx\, \langle \mathcal{T}_\tau J^i(y,\tau) J^j(x,0)\rangle .$$

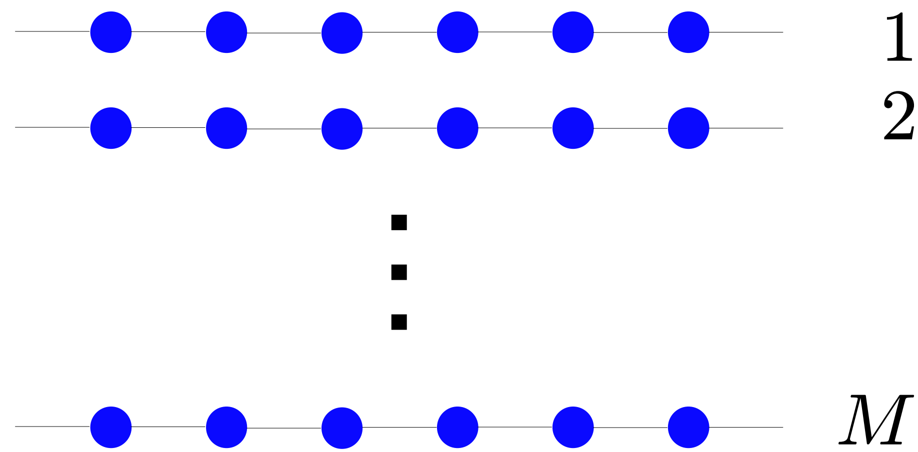
First, we need to figure out how the current-current correlation functions behave.

Let us write the currents in terms of the chiral ones:

$$J^j = J^j_R - J^j_L$$

Universal conductance in the BCFT

Let us forget about the boundary for now and consider the CFT in the infinite plane.



Different wires do not talk to each other and neither do the right-movers to the left-movers.

$$\langle \mathcal{T}_\tau J_L^i(z_1) J_L^j(z_2) \rangle = -\frac{g}{4\pi^2} \frac{\delta_{ij}}{(z_1 - z_2)^2}$$

$$\langle \mathcal{T}_\tau J_R^i(\bar{z}_1) J_R^j(\bar{z}_2) \rangle = -\frac{g}{4\pi^2} \frac{\delta_{ij}}{(\bar{z}_1 - \bar{z}_2)^2}$$

Universal conductance in the BCFT

Important observation:

Adding a boundary to the theory does not change the correlations between the chiral currents but adds new correlations between left-movers and right-movers.

$$\langle \mathcal{T}_\tau J_L^i(z_1) J_R^j(\bar{z}_2) \rangle = -\frac{g}{4\pi^2} A_{\mathcal{B}}^{ij} \frac{1}{(z_1 - \bar{z}_2)^2}$$

The boundary condition does not change the scaling dimension of the operators. The information about the boundary state is encoded in the coefficient.

J. L. Cardy and D. C. Lewellen, Phys. Lett. B 259, 274 (1991).

Universal conductance in the BCFT

Let us go back to the Kubo formula and do the integrals:

$$\boxed{i \neq j}$$

$$G_{ij} = g\frac{e^2}{h}\frac{1}{L}\int_0^L dx[A^{ij}_{\mathcal{B}}\ H(x+y) + A^{ji}_{\mathcal{B}}\ H(-x-y)] = A^{ij}_{\mathcal{B}}\ g\frac{e^2}{h}$$

Recall the two difficulties of a numerical calculation of conductance:

$$\begin{cases} \text{dynamical correlators} \Rightarrow \text{time-dependent calculations} \\ \text{open quantum system} \Rightarrow \text{infinitely large systems} \end{cases}$$

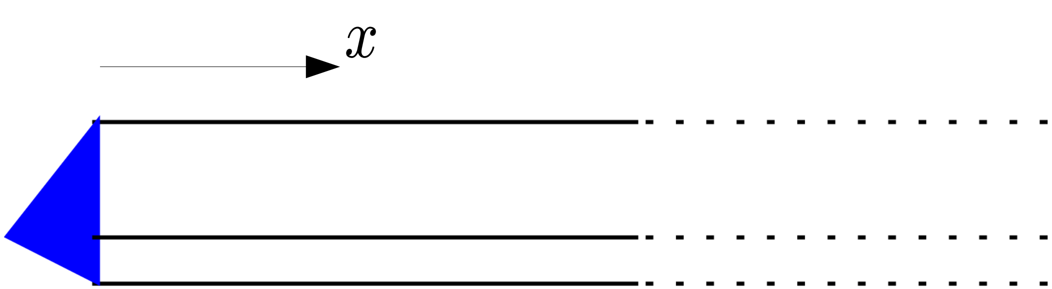
Universal conductance in the BCFT

We have effectively solved the first difficulty. Conformal symmetry ties space and time together. The same coefficient appearing in a dynamical correlation function appears in a static one.

$$\langle \mathcal{T}_\tau J_L^i(z_1) J_R^j(\bar{z}_2)\rangle = -\frac{g}{4\pi^2} A_{\mathcal{B}}^{ij} \frac{1}{(z_1 - \bar{z}_2)^2}$$

$$\langle J_L^i(x) J_R^j(x)\rangle_{\mathrm{GS}} = \frac{g}{4\pi^2} A_{\mathcal{B}}^{ij} \frac{1}{(2x)^2}$$

A static ground state (GS) expectation value



Universal conductance in the BCFT

$\text{dynamical correlators} \Rightarrow \text{time-dependent calculations} \ \surd$

So far, we can obtain the conductance by measuring the ground state expectation value of an operator. But we need a large enough system to faithfully approximate the semi-infinite plane.

$\text{open quantum system} \Rightarrow \text{infinitely large systems ?}$

Universal conductance in the BCFT

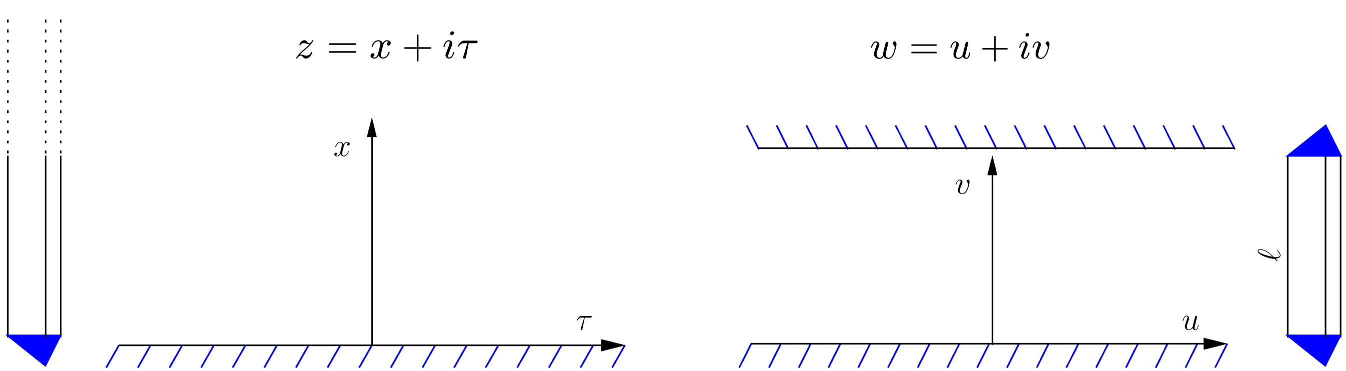
dynamical correlators $\Rightarrow$ time-dependent calculations $\surd$

So far, we can obtain the conductance by measuring the ground state expectation value of an operator. But we need a large enough system to faithfully approximate the semi-infinite plane.

open quantum system $\Rightarrow$infinitely large systems ?

Let us map the semi-infinite plane to a strip.

$$w = \frac{\ell}{\pi} \ln z$$



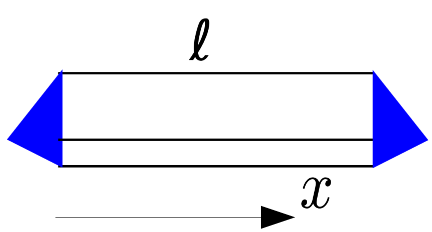
Universal conductance in the BCFT

We know how correlation functions change under a conformal transformation

$$\langle O(z)\rangle = A_{\mathcal{B}}^{O}(2x)^{-X_O} \Rightarrow \langle O(w)\rangle = \left|\frac{dw}{dz}\right|^{-X_O}\langle O(z)\rangle$$

This gives us the conductance in terms of
a ground state expectation value in a finite (closed) system.

$$\langle J_L^i(x) J_R^j(x)\rangle_{\mathrm{GS}} = \frac{g}{4\pi^2} A_{\mathcal{B}}^{ij}\left[2\sin\left(\frac{\pi}{\ell}x\right)/\frac{\pi}{\ell}\right]^{-2}$$



open quantum system $\Rightarrow$ infinitely large systems $\checkmark$

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Lattice model implementation: a new method

Let us go back to the tight-binding lattice model of the junction and make use of the the relationship we just derived to calculate the conductance.

$$G_{ij} = A_{\mathcal{B}}^{ij}\; g\frac{e^2}{h}$$

$$\langle J_L^i(x) J_R^j(x)\rangle_{\mathrm{GS}} = \frac{g}{4\pi^2} A_{\mathcal{B}}^{ij} \left[2\sin(\frac{\pi}{\ell}x)/\frac{\pi}{\ell}\right]^{-2}$$

We can now measure the conductance by measuring a ground state expectation value in a finite system.

$$\begin{cases} \text{How to model chiral currents on the lattice?} \\ \text{What exactly is this finite system?} \end{cases}$$

Lattice model implementation: a new method

How to model chiral currents on the lattice?

In the continuum, the chiral current are related to the physical current and charge density through

$$J^j(x) = v\,(J^j_R(x) - J^j_L(x)), \qquad N^j(x) = J^j_R(x) + J^j_L(x)$$

It turns out that we can use the same relationship on the lattice if we measure the correlation function for two different wires.

c_m $\quad$ c_{m+1}

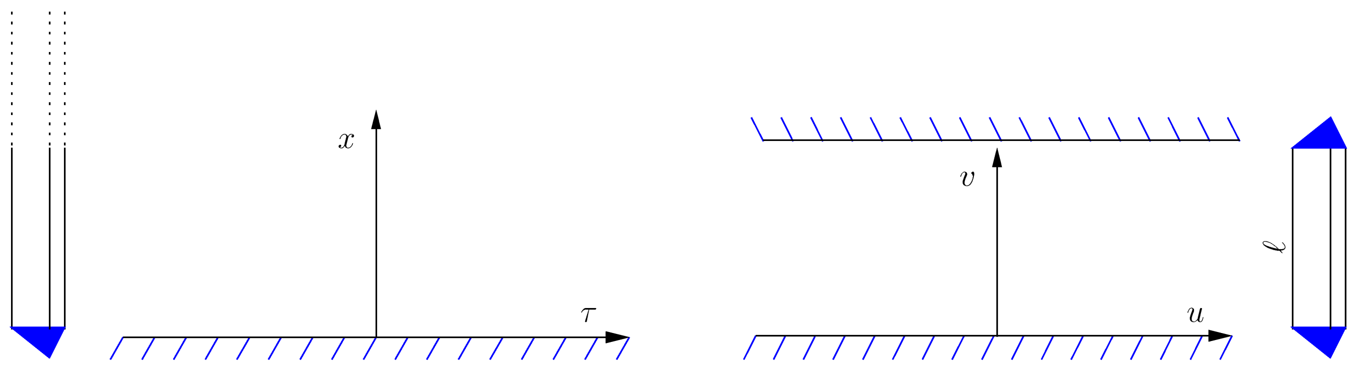
$$J^j_m = i({c^j}^\dagger_{m+1} c^j_m - {c^j}^\dagger_m c^j_{m+1})$$

$$N^j_m = \frac{1}{2}\left(n^j_m + n^j_{m+1} - \langle n^j_m\rangle - \langle n^j_{m+1}\rangle\right)$$

Lattice model implementation: a new method

What exactly is this finite system?

Let us go back to the conformal transformation.

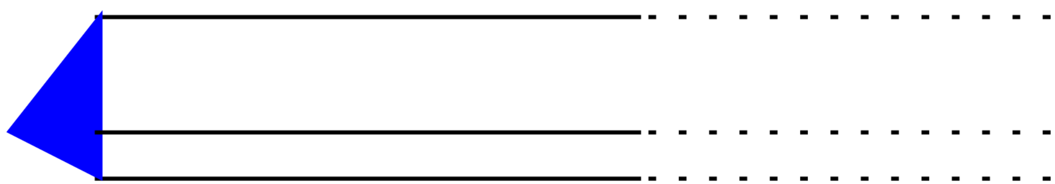


$$w = \frac{\ell}{\pi} \ln z \Rightarrow \begin{cases} v = 0 \sim x = 0, \tau > 0 \\ v = \ell \sim x = 0, \tau < 0 \end{cases}$$

Same boundary condition at both ends of the finite system.

Lattice model implementation: a new method

At $v = 0$ place the same junction as $x = 0$.



$$H = H_{\text{boundary}} + H_{\text{bulk}}$$

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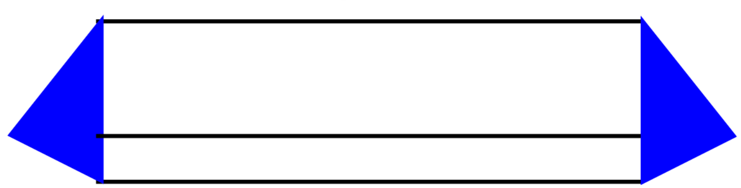

$$H' = H_L + H'_{\text{bulk}} + H_R$$

$$\boxed{H_L = H_{\text{boundary}}}$$

What about H_R?

Lattice model implementation: a new method

Let us consider a non-interacting system for which the boundary condition can be written as an S-matrix. Having the same boundary condition means:

$$\Psi_R(0) = S\Psi_L(0)$$

$$\Psi_R(\ell) = S\Psi_L(\ell)$$

Lattice model implementation: a new method

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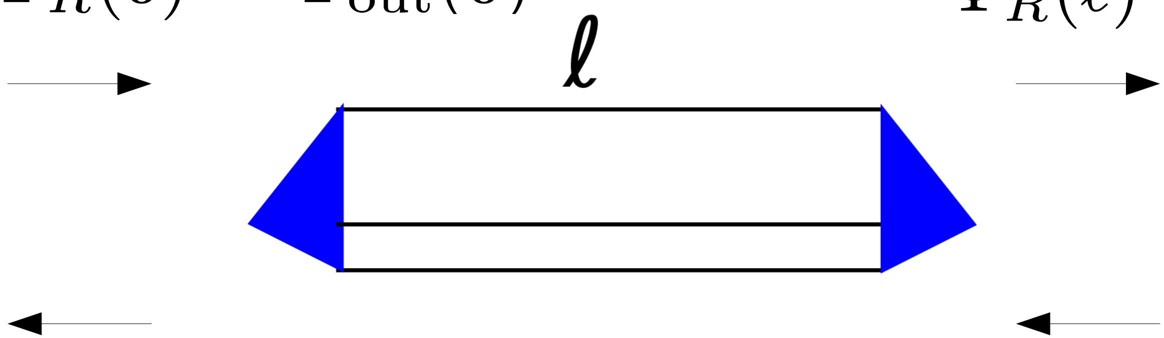
$$\Psi_R(0) = S\Psi_L(0)$$

$$\Psi_R(\ell) = S\Psi_L(\ell)$$

$$\Psi_R(0) = \Psi_{\mathrm{out}}(0) \qquad \Psi_R(\ell) = \Psi_{\mathrm{in}}(\ell)$$



$$\Psi_L(0) = \Psi_{\mathrm{in}}(0) \qquad \Psi_L(\ell) = \Psi_{\mathrm{out}}(\ell)$$

$$\boxed{S_R = S_L^\dagger}$$

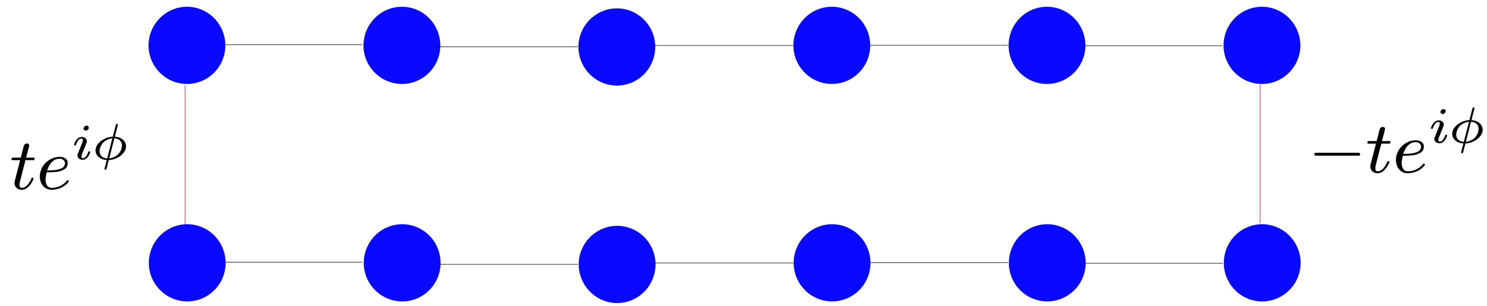
Lattice model implementation: a new method

At half-filling, the switched role of the left-movers and right-movers can be implemented by particle-hole and time reversal transformations.

$$T(i) = -i$$
$$C(c) = c^\dagger$$

$$H_R = T(C(H_L)) = T(C(H_{\text{boundary}})).$$

For example:



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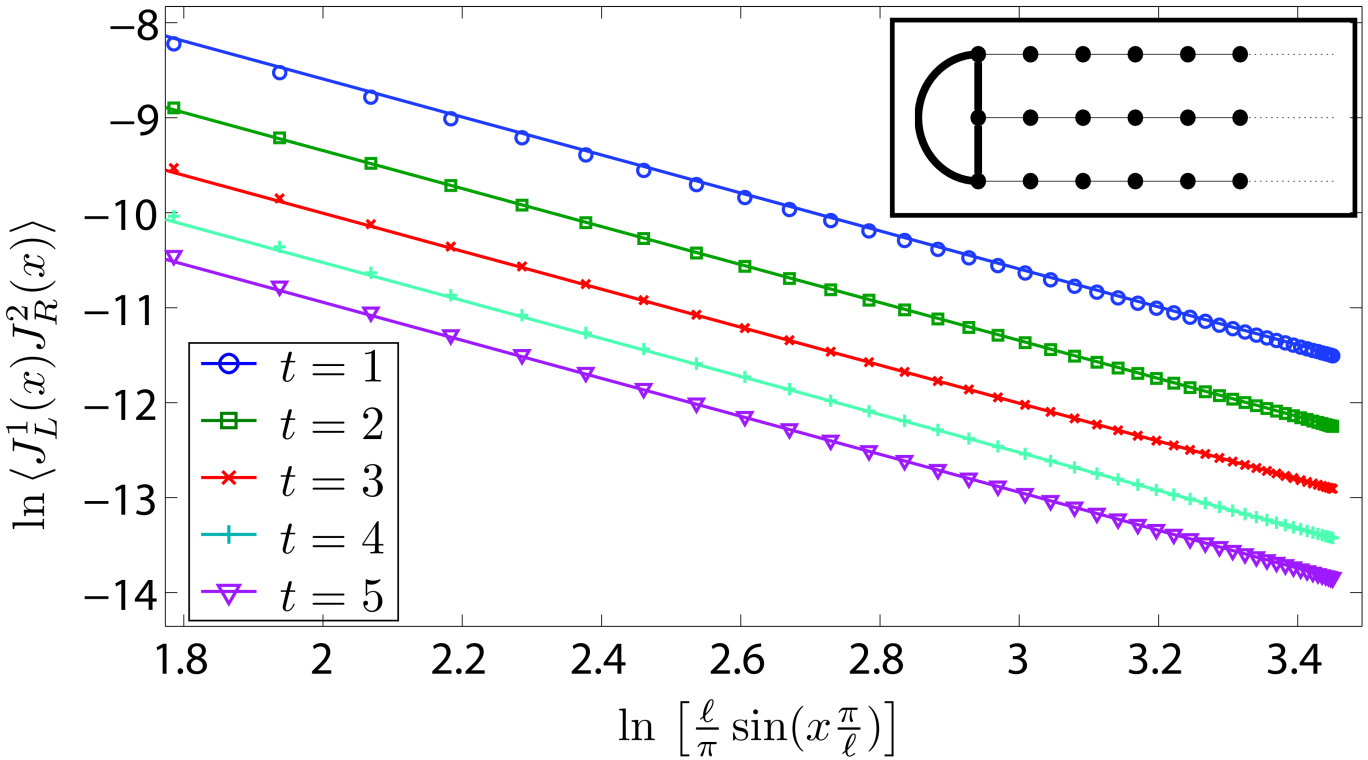
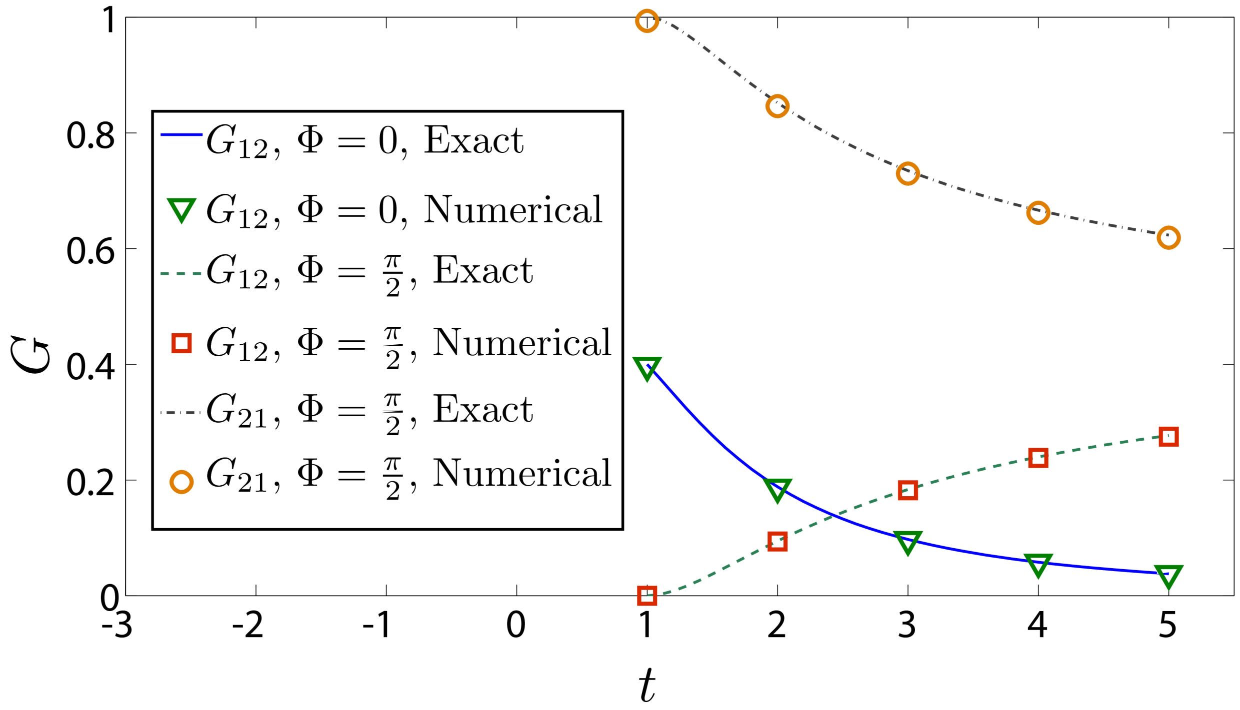
Numerical benchmarks

First, let us consider a non-interacting Y-junction. The exact conductance can be calculated from the scattering matrix.



Numerical benchmarks

$$G_{12,21} = \frac{4t^2(1 + t^2 \pm 2t \sin \Phi)}{1 + 6t^2 + 9t^4 + 4t^6 \cos^2 \Phi} \frac{e^2}{h}$$



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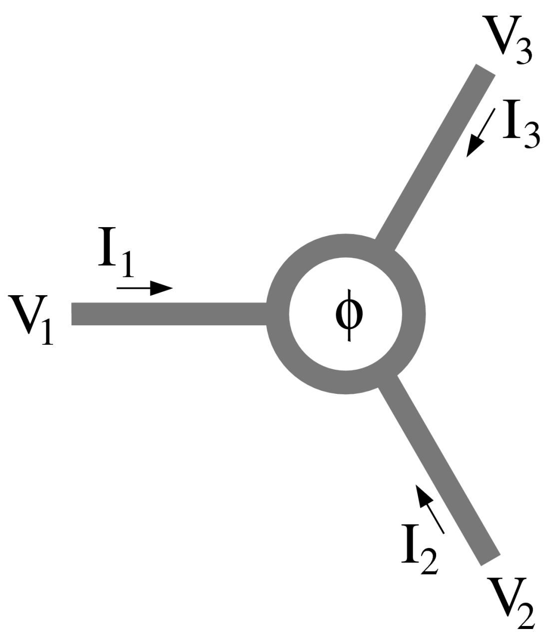
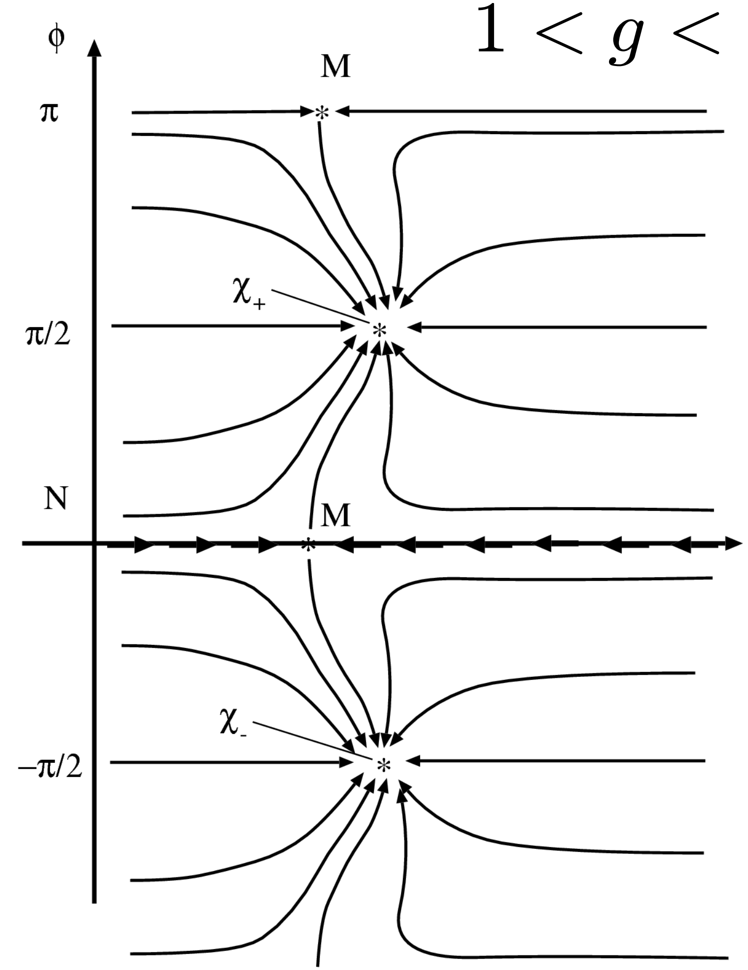
Application to an interacting Y-junction

Consider a Y-junction of interacting quantum wires threaded by a magnetic flux. Several fixed points were theoretically predicted for this system.



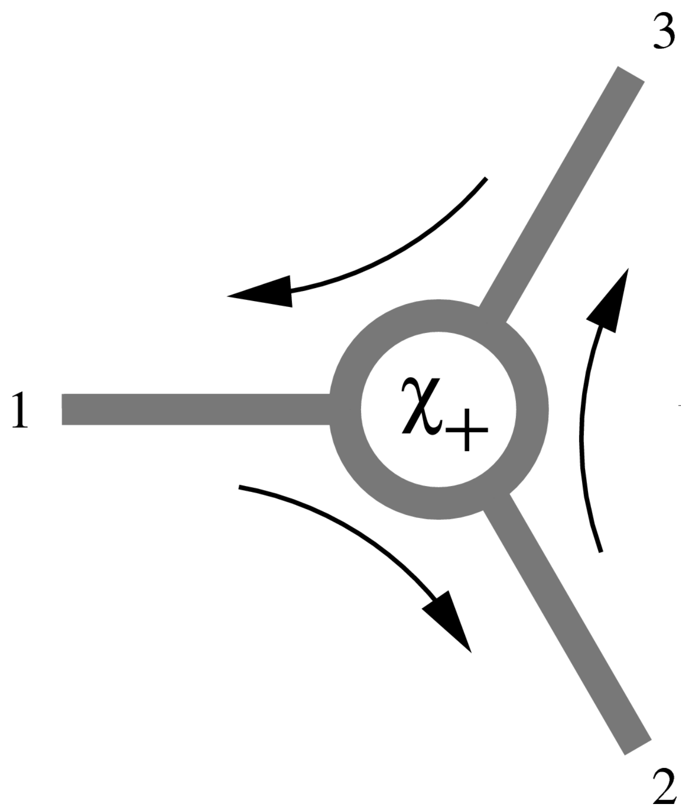
$1 < g < 3$



C. Chamon, M. Oshikawa and I. Affleck, Phys. Rev. Lett. 91 (2003) 206403;
M. Oshikawa, C. Chamon and I. Affleck, J.Stat.Mech. 0602 (2006) P008.

Application to an interacting Y-junction

Chiral fixed point:



M fixed point:

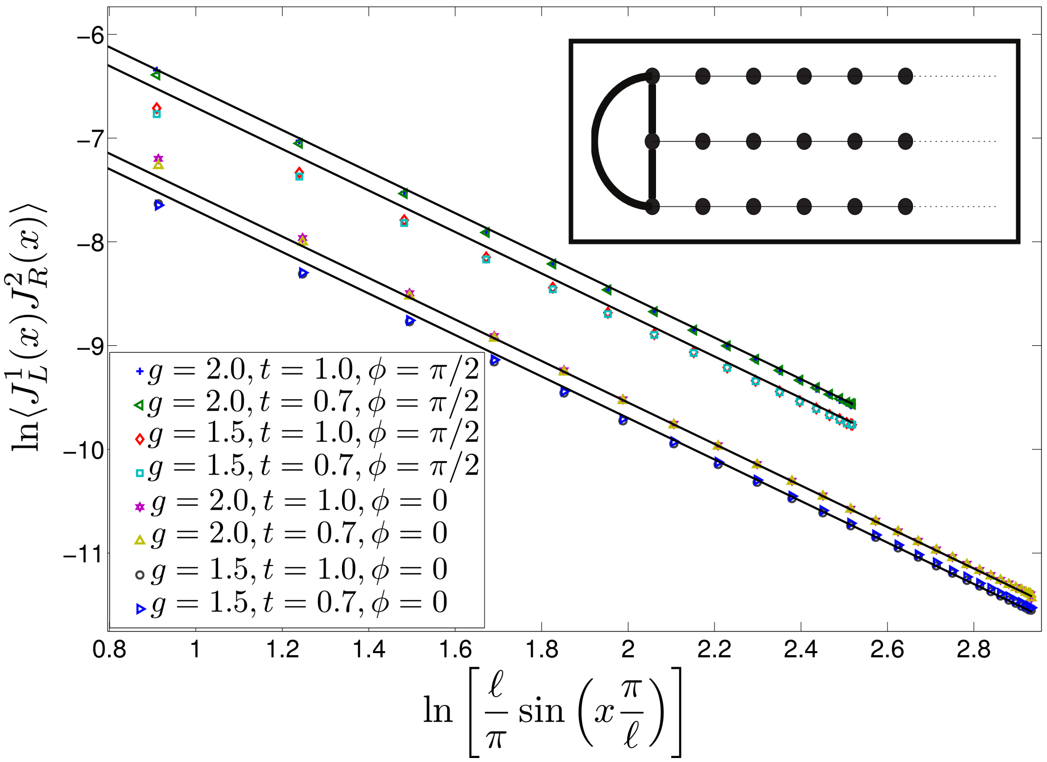
M stands for:

Mystery

$$G_{21} = -2\,\frac{g}{3+g^2}(g+1)\frac{e^2}{h}$$

Application to an interacting Y-junction

We used our method to verify the prediction for the conductance of the chiral fixed point and calculate the conductance of the M fixed point.



Application to an interacting Y-junction

What do we learn about the M fixed point? It has a different conductance than the chiral fixed point and a non-trivial dependence on the Luttinger parameter.

Let us connect the junction to Fermi liquid leads.

$$\bar{G} = (I + G_c^{-1} G)^{-1} G \qquad G_c^{-1} = (1 - g^{-1})/2$$

$$\bar{G}(g=1.5) = \begin{pmatrix} 0.8371 & -0.4185 & -0.4185 \\ -0.4185 & 0.8371 & -0.4185 \\ -0.4185 & -0.4185 & 0.8371 \end{pmatrix}, \qquad \bar{G}(g=2.0) = \begin{pmatrix} 0.8414 & -0.4207 & -0.4207 \\ -0.4207 & 0.8414 & -0.4207 \\ -0.4207 & -0.4207 & 0.8414 \end{pmatrix}$$

Conjecture: the g-dependence is such that the renormalized conductance is independent of g, we then have the entire g-dependence.

$$\bar{G}_{12} \stackrel{?}{=} 4/9$$

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Summary and conclusions

- We proposed method that allows us to calculate the universal conductance of junctions of quantum wires under very generic conditions.
- The method related the conductance to coefficients in certain static correlation functions in a finite system constructed with the junction and an appropriate mirror image.
- Using time-independent DMRG, we successfully verified the conductance of a theoretical prediction for a non-trivial chiral fixed point and calculated the conductance of the M fixed point, a previously unsolved quantum impurity problem.