Entanglement in gapless systems with a quantum impurity

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Entanglement Entropy in Many-Body Quantum Systems
City University London, 3 June 2014

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XXZ chain with quantum impurity

$$H = J \sum_{i=-\infty}^{\infty} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z)$$

+ $(J' - J) (S_0^x S_1^x + S_0^y S_1^y + \Delta S_0^z S_1^z)$

- Bulk chain in gapless Luttinger liquid phase for $-1 < \Delta \le 1$
- ullet One modified link (J o J') in the middle of the chain
 - For J' > J existence of bound state
 - Consider henceforth weak-link case 0 < J' < J
- Dimension of perturbation is $h = 2 (1 + \pi^{-1} \arccos \Delta)$
 - Marginal for $\Delta = 0$: equivalent to Ising model with defect line [Oshikawa-Affleck 1996]
 - Relevant for $\Delta < 0$: healing RG-flow $(J' \to J)$, $\xi_X \sim (J')^{1/(h-1)}$

Continuum limit

- At low energy: Right (R) and Left (L) movers
- ullet Unfolding: Map formally $L \to R$ to get two chiral wires
- Form even/odd combinations: $\phi_{\rm R}^{\pm} = \frac{1}{\sqrt{2}} \left(\phi_{1\rm R}({\it x}) \pm \phi_{2\rm R}({\it x}) \right)$
- The odd one $\phi_{\mathbf{R}}^{-}$ decouples from impurity, so forget it.
- The even one $\phi := \phi_{\mathbf{R}}^+$ satisfies

$$H = v_{\rm F} \int_{-\infty}^{\infty} \mathrm{d}x \, (\partial_x \phi)^2 + \lambda \cos \left(\beta \phi(0)\right)$$

with $h = \beta^2/8\pi$.

Can fold back to obtain boundary sine-Gordon model

Two weak links: tunneling through a resonant level

$$H = J \sum_{i=-\infty}^{\infty} \left(S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \Delta S_{i}^{z} S_{i+1}^{z} \right)$$

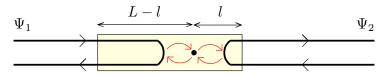
$$+ \left(J' - J \right) \sum_{i=-1}^{0} \left(S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + \Delta S_{i}^{z} S_{i+1}^{z} \right)$$

- Dimension of perturbation is now h/2 and is always relevant
- Healing length (Kondo temp.) $\xi_X := (T_B)^{-1} = (J')^{1/(h/2-1)}$
- Unfold and bosonise as before:

$$H = v_{\rm F} \int_{-\infty}^{\infty} \mathrm{d}x \, (\partial_x \phi)^2 + \lambda \left[\mathrm{e}^{i\frac{\beta}{\sqrt{2}}\phi} S^- + \mathrm{e}^{-i\frac{\beta}{\sqrt{2}}\phi} S^+ \right] (0)$$

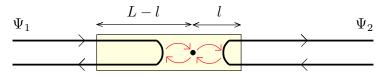
Can fold back to obtain anisotropic Kondo problem

Entanglement entropy



The problem (here for $\Delta = 0$ only)

- What is the entanglement entropy $S_A = -\text{Tr}_{\mathcal{H}_A} \left[\rho_A \log \rho_A \right]$ of an interval A of length L with the remainder of the system?
- Case $\alpha = \frac{1}{2}$ is easier [Saleur-Schmitteckert-Vasseur 2013]
 - 1st order IR perturbation [Sørensen-Chang-Laflorencie-Affleck 2006]
- Consider in general the asymmetric case with $\ell=\alpha L$ and $\alpha\neq\frac{1}{2}$



$\ell=\alpha L$: The case $\alpha=\frac{1}{2}$ versus $lpha eq \frac{1}{2}$

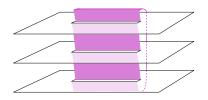
- Case $\alpha = \frac{1}{2}$ can be mapped to a boundary problem by folding
 - Applies in general to any massless integrable system
 - But physically contrived: we really want $\alpha = 0$ (i.e. A =one lead)!
- $\alpha \neq \frac{1}{2}$ requires defect scattering formalism (free systems only)

Limiting cases [Cardy-Calabrese 2004]

- UV limit $L \ll (T_B)^{-1}$:
 - Two half-chains and $S_A = \frac{c}{6} \left[\log(\ell) + \log(L \ell) \right]$
- IR limit $L \gg (T_B)^{-1}$:
 - One bulk chain and $S_A = \frac{c}{3} \log(L)$

Twist fields [Cardy-Calabrese 2004]

- Replica trick: $S_A = -\lim_{n \to 1} \frac{d}{dn} \operatorname{Tr}_{\mathcal{H}_A}(\rho_A)^n$
- Continue analytically from $n \in \mathbb{N}$
- Hence define theory on multi-sheeted Riemann surface



• Branch-point twist fields \mathcal{T} at $(x, y) = (a_1, 0)$ and $(a_2, 0)$

$$\text{Tr}_{\mathcal{H}_A}(\rho_A)^n \propto \left\langle \mathcal{T}(a_1,0) \tilde{\mathcal{T}}(a_2,0) \right\rangle_{\mathcal{L}^{(n)}}$$

• Map to $z \in \mathbb{R}^2$ via $z = \left(\frac{w-a_1}{w-a_2}\right)^{1/n}$, obtaining $h_n = \bar{h}_n = \frac{c}{24} \left(n - \frac{1}{n}\right)$

Form Factor approach

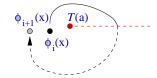
- We have a CFT in UV and IR, but in-between there is a flow
 - Hence we cannot directly use boundary CFT techniques
 - But we can use massless Form Factor (FF) approach [SSV 2013]

The problem can be attacked in several stages:

- FF approach to twist field in massive bulk theory [Cardy - Castro-Alvaredo - Doyon 2007]
- ② Map $\Delta = 0$ cases to Ising with boundary condition
- FF approach for massive boundary Ising problem [Castro-Alvaredo - Doyon 2008]
- For $\alpha = \frac{1}{2}$ take massless FF limit [SSV 2013]
- **5** For $\alpha \neq \frac{1}{2}$ use FF defect scattering formalism [Delfino-Mussardo-Simonetti 1994]

FF for branch-point twist fields [C-CA-D 2007]

- FF of local operator \mathcal{O} :
 - $F_k^{\mathcal{O}|\mu_1...\mu_k}(\theta_1,\ldots,\theta_k) := \langle 0|\mathcal{O}(0)|\theta_1,\ldots,\theta_k \rangle_{\mu_1,\ldots,\mu_k}^{\mathrm{in}}$
- k particles with quantum numbers μ_i and rapidities θ_i
- Assume integrable theory with single particle spectrum and no bound states (Ising, sinh-Gordon)
- For twist field \mathcal{T} , the replicated S-matrix is $S_{ij}(\theta) = (S(\theta))^{\delta_{ij}}$
- $\bullet \ F_k^{\mathcal{T}|\dots\mu_i\mu_{i+1}\dots}(\dots,\theta_i,\theta_{i+1},\dots) = \mathcal{S}_{\mu_i,\mu_{i+1}}(\theta_{i,i+1})F_k^{\mathcal{T}|\dots\mu_{i+1}\mu_i\dots}(\dots,\theta_{i+1},\theta_i,\dots)$
- $F_k^{\mathcal{T}|\mu_1\mu_2...\mu_k}(\theta_1 + 2\pi i, ..., \theta_k) = F_k^{\mathcal{T}|\mu_2,...,\mu_n,\mu_1+1}(\theta_2,...,\theta_k,\theta_1)$



Further axioms for kinematic residue equations

Two-particle approximation [C-CA-D 2007]

• Insert complete set in $\langle \mathcal{T}(r)\tilde{\mathcal{T}}(0)\rangle$ and truncate to two particles:

$$\langle \mathcal{T}(r)\tilde{\mathcal{T}}(0)\rangle \approx \langle \mathcal{T}\rangle^2 + \frac{1}{2!} \sum_{i,j=1}^n \int_{-\infty}^{\infty} \frac{\mathrm{d}\theta_1}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\theta_2}{2\pi} \left| F_2^{\mathcal{T}|ij}(\theta_{12},n) \right|^2 \mathrm{e}^{-rm(\cosh\theta_1 + \cosh\theta_2)}$$

• Two-particle form factors $F_2^{\mathcal{T}|ij}(\theta_{12},n)$ given by

$$K(\theta) = \frac{F_2^{\mathcal{T}|11}}{\langle \mathcal{T} \rangle} = -i \frac{\cos\left(\frac{\pi}{2n}\right) \sinh\left(\frac{\theta}{2n}\right)}{n \sinh\left(\frac{i\pi + \theta}{2n}\right) \sinh\left(\frac{i\pi - \theta}{2n}\right)}$$

• Change to $\theta_1 \pm \theta_2$ variables and do one integral:

$$\begin{split} \langle \mathcal{T}(r)\tilde{\mathcal{T}}(0)\rangle &\approx &\langle \mathcal{T}\rangle^2 \left(1 + \frac{n}{4\pi^2} \int_{-\infty}^{\infty} \mathrm{d}\theta \, f(\theta, n) K_0(2rm \cosh(\theta/2))\right) \\ \langle \mathcal{T}\rangle^2 f(\theta, n) &= &\sum_{i=1}^n \left|F_2^{\mathcal{T}|1j}(\theta, n)\right|^2 \end{split}$$

• Analytic continuation $\tilde{f}(\theta, n)$ satisfies $\frac{\partial}{\partial n}\tilde{f}(\theta, n)\Big|_{n=1} = \pi^2 \tilde{f}(1)\delta(\theta)$

- For the Ising model, $\tilde{f}(n) = 1/2$ for all n
- So the sub-leading contribution to S_A for $rm \gg 1$ is $-\frac{1}{8}K_0(2rm)$. This is universal.
- Neglected four-particle contributions are $O(e^{-4rm})$

How to deal with the $m \rightarrow 0$ limit?

- Set $\frac{m}{2} = M e^{-\theta_0}$ with $\theta_0 \to \infty$. Finite-energy excitations have $\theta = \pm (\theta_0 + \beta)$ with β finite. They are LR movers with $\rho = \pm M e^{\beta}$ and $e = |\rho|$.
- Correction to S_A becomes: $-\frac{1}{8} \int_0^\infty \frac{d\omega}{\omega} e^{-2Mr\omega}$ (divergent at $\omega \ll 1$)
- **Γ-function regularisation:** $\int_0^\infty \mathrm{d}x \, x^{\eta-1} \mathrm{e}^{-2Mr\omega} = \frac{1}{(2Mr)^\eta} \Gamma(\eta) = \frac{1}{\eta} \log(2Mr) + \dots$
- Suppose we keep just the finite part: $S_A = \ldots + \frac{1}{8} \log(r) + \ldots$
- Higher-particle contributions will lead to $\frac{1}{6}\log(r) = \frac{c}{3}\log(r)$

Two weak links at $\Delta = 0$: Fermionic formulation

 Jordan-Wigner transformation of XX spin chain [Lieb-Schultz-Mattis 1961]

$$H = -J \sum_{i=-\infty}^{-2} c_{i+1}^{\dagger} c_i - J \sum_{i=1}^{\infty} c_{i+1}^{\dagger} c_i - J' (c_{-1}^{\dagger} c_0 + c_0^{\dagger} c_1) + \text{h.c.}$$

• Continuum limit: \longrightarrow

$$H = \int_{-\infty}^{0} i \left(\psi_{1L}^{\dagger} \partial_{x} \psi_{1L} - \psi_{1R}^{\dagger} \partial_{x} \psi_{1R} \right) dx + \int_{0}^{\infty} i \left(\psi_{2L}^{\dagger} \partial_{x} \psi_{2L} - \psi_{2R}^{\dagger} \partial_{x} \psi_{2R} \right) dx + \lambda \left[\left(\psi_{1}^{\dagger}(0) + \psi_{2}^{\dagger}(0) \right) d + \text{h.c.} \right]$$

• Unfold to get R movers only. Form $\Psi_R = \frac{1}{\sqrt{2}}(\psi_{1R} + \psi_{2R})$ (odd combination decouples). Refold (introducing Ψ_L):

$$H = -i \int_{-\infty}^{0} \left(\Psi_{R}^{\dagger} \partial_{x} \Psi_{R} - \Psi_{L}^{\dagger} \partial_{x} \Psi_{L} \right) dx + \lambda \sqrt{2} \left[\Psi^{\dagger}(0) d + \text{h.c.} \right]$$

- Decompose into $\Psi_R = \frac{1}{\sqrt{2}}(\xi_{1R} + i\xi_{2R})$ and $d = \frac{1}{\sqrt{2}}(d_2 + id_1)$.
- We get $H = H_1 + H_2$ for real fermions (k = 1, 2) with

$$H_k = -\frac{i}{2} \int_{-\infty}^0 \left(\xi_{kR} \partial_x \xi_{kR} - \xi_{kL} \partial_x \xi_{kL} \right) \mathrm{d}x + (-1)^{k-1} \frac{i}{\sqrt{2}} \lambda \xi_k(0) d_k$$

- Two independent Majorana fermions with boundary field $\sim \pm \lambda$
- Suggests computing S_A for $\alpha = \frac{1}{2}$ in boundary Ising model
- This was done in [SSV 2013] by extensive use of:
 - the FF results of [Castro-Alvaredo Doyon 2008]
 - the boundary state of [Ghoshal-Zamolodchikov 1994]
- Does not work for $\alpha \neq \frac{1}{2}$, since folding is incompatible with the geometry of the interval A

FF computation: scattering on the defect

$$\langle \mathcal{T}(r)\tilde{\mathcal{T}}(0)\rangle \approx \langle \mathcal{T}\rangle^2 + \frac{1}{2!} \sum_{i,j=1}^n \int_{-\infty}^{\infty} \frac{\mathrm{d}\theta_1}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\theta_2}{2\pi} \left| F_2^{\mathcal{T}|ij}(\theta_{12}, \mathbf{n}) \right|^2 e^{-rm(\cosh\theta_1 + \cosh\theta_2)}$$

• Instead we can now have two particles (RR or LL) created by \mathcal{T} , transmitted by the defect, and absorbed on $\tilde{\mathcal{T}}$:

$$\frac{1}{2} \sum_{i,j=1}^n \int \frac{\mathrm{d}\theta_1}{2\pi} \frac{\mathrm{d}\theta_2}{2\pi} \hat{T}(\theta_1) \hat{T}(\theta_2) \left| F_2^{\mathcal{T}|ij}(\theta_{12},n) \right|^2 \mathrm{e}^{-Lm(\cosh\theta_1+\cosh\theta_2)}$$

• Or two LR pairs created by $\mathcal T$ (or $\tilde{\mathcal T}$: formally $\ell \to L - \ell$) and reflected on the impurity:

$$\langle \mathcal{T} \rangle \sum_{i,j=1}^{n} \int \frac{\mathrm{d}\theta_{1}}{4\pi} \frac{\mathrm{d}\theta_{2}}{4\pi} \hat{R}(\theta_{1}) \hat{R}(\theta_{2}) F_{4}^{\mathcal{T}|iij}(\theta_{1}, -\theta_{1}, \theta_{2}, -\theta_{2}, n) e^{-2\ell m(\cosh \theta_{1} + \cosh \theta_{2})}$$

• Other diagrams are forbidden by \mathbb{Z}_2 symmetry of the Ising model. It requires an even number of L and R. Note that indeed $F_2^{\mathcal{T}|ii}(\theta, -\theta) \to 0$ for $m \to 0$.

• After a calculation one finds, in the massless limit:

$$S_A(\ell,L) = -\frac{1}{4} \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \mathrm{e}^{-2L\omega} \, \hat{T}(\omega)^2 - \frac{1}{8} \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \left[\mathrm{e}^{-4\ell\omega} + \mathrm{e}^{-4(L-\ell)\omega} \right] \hat{R}(\omega)^2$$

- Needs Γ -function regularisation in the $\omega \ll$ 1 limit
- "Renormalise" by a factor $\frac{4}{3}$ to produce correct limiting values
- One weak link: $\hat{T}(\omega)^2 = \cos^2 \xi$ and $\hat{R}(\omega)^2 = \sin^2 \xi$
 - Here $\xi = \frac{\pi}{2} 2\arctan(J'/J)$ independent of ω (marginal case)
- Two weak links: $\hat{T}(\omega)^2 = \left(\frac{T_B}{T_B + \omega}\right)^2$ and $\hat{R}(\omega)^2 = \left(\frac{\omega}{T_B + \omega}\right)^2$
 - Scaling function of $x = LT_B$, where $T_B = \frac{(J'/J)^2}{\sqrt{1-2(J'/J)^2}}$
 - Note that $\hat{R}^2 + \hat{T}^2 \neq 1$; the relation to reflexion / transmission probabilities involves a subtlety having to do with the choice of quantisation scheme.

Results for one weak link

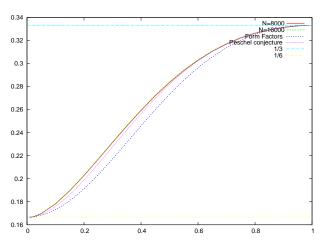
Γ-regularise and renormalise to find:

$$S_A(\ell, L) = \frac{\cos^2 \xi}{3} \log L + \frac{\sin^2 \xi}{6} \left[\log \ell + \log(L - \ell) \right]$$

- Symmetric case ($\ell = L/2$): $S_A = \frac{1}{3} \log L$, independent of ξ
 - Check of J'=J ($\xi=0$) case: $\frac{c}{3}=\frac{1}{3}$
 - Check of J'=0 ($\xi=\frac{\pi}{2}$) case: $2\times\frac{c}{6}=\frac{1}{3}$
- Totally asymmetric case: $\ell=0$ (or rather $\ell\sim$ lattice spacing)

$$S \sim \frac{1 + \cos^2 \xi}{6} \log L = \frac{1}{6} \left(1 + \frac{4(J'/J)^2}{\left(1 + (J'/J)^2\right)^2} \right) \log L$$

One weak link: comparison with numerics ($\alpha = 0$)



 Initial conjecture [Peschel 2005] slightly corrected by exact result [Peschel et al. 2008]

Results for two weak links

- Since there is a flow in $x = LT_B$, it is *not correct* to extract the apparent coefficient of log L.
- Instead set $\ell = \alpha L$ and compute the scaling function

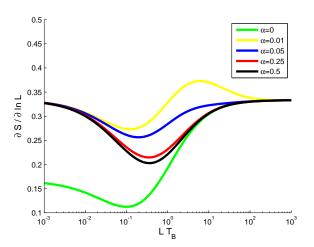
$$\frac{\partial \mathcal{S}_{A}(\alpha)}{\partial \log L} = F(LT_{B})$$

• After renormalisation we find:

$$F(x) = \frac{2}{3} \int_0^\infty \mathrm{d} v \, \mathrm{e}^{-2v} \left(\frac{x}{v+x}\right)^2 + \frac{2}{3} \int_0^\infty \mathrm{d} v \, \left(\alpha \mathrm{e}^{-4\alpha v} + (1-\alpha)\mathrm{e}^{-4(1-\alpha)v}\right) \left(\frac{v}{v+x}\right)^2$$

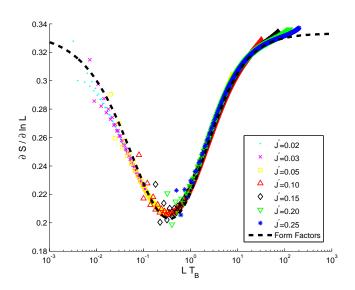
- No need to Γ-regularise (the derivative does the job)
- Case $\alpha = \frac{1}{2}$ coincides with [SSV 2013] which is quite non-trivial! "Bulk two-point function with defect scattering" versus "One-point function with boundary state"
- Several wrong results in the literature, due to considerations of the type $S_A \sim c_{\text{eff}} \log L$ and failure to introduce scaling function F(x)

$$F(x) = \frac{2}{3} \int_0^\infty dv \, e^{-2v} \left(\frac{x}{v+x}\right)^2 + \frac{2}{3} \int_0^\infty dv \, \left(\alpha e^{-4\alpha v} + (1-\alpha)e^{-4(1-\alpha)v}\right) \left(\frac{v}{v+x}\right)^2$$

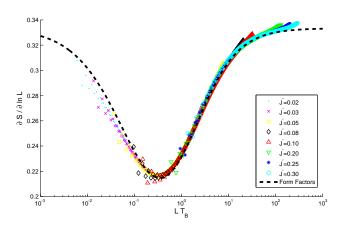


Note that
$$F(x)|_{\alpha\to 0} = \frac{1}{6} + F(x)|_{\alpha=0}$$
.

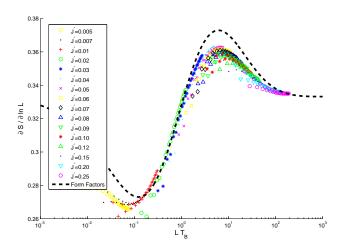
Two weak links: comparison with numerics $(\alpha = \frac{1}{2})$



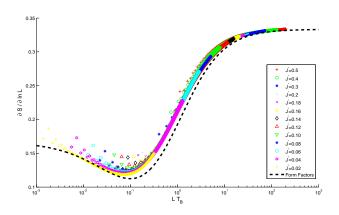
Two weak links: comparison with numerics ($\alpha = \frac{1}{4}$)



Two weak links: comparison with numerics ($\alpha = \frac{1}{100}$)



Two weak links: comparison with numerics ($\alpha = 0$)



UV and IR limits

- Consider e.g. $\alpha = 0$
- UV limit ($x \ll 1$):

$$F(x) = \frac{1}{6} + \frac{4}{3} (1 + \gamma + \log(4x)) x + \mathcal{O}(x^2)$$

- The logarithmic term shows that S_A is non perturbative
 - Already pointed out in [SSV 2013] for the case $\alpha = \frac{1}{2}$
- IR limit $(x \gg 1)$:

$$F(x) = \frac{1}{3} - \frac{1}{3x} + \mathcal{O}\left(\frac{1}{x^2}\right)$$

General scaling argument

 $S = -\frac{d}{dn}R_n\big|_{n=1}$ obtained from $R_n = \text{Tr } \rho^n$, where

$$R_n = c_n \left(\frac{L}{a}\right)^{-\frac{1}{6}(n-n^{-1})} \Omega(LT_B, n)$$

The non-universal c_n depends on aT_B . We find

$$S = h(LT_B) + k(aT_B)$$

with

$$h(LT_B) = -\frac{\mathrm{d}}{\mathrm{d}n}\Omega\bigg|_{n=1} + \frac{1}{3}\log(LT_B),$$

$$k(aT_B) = -\frac{\mathrm{d}}{\mathrm{d}n}c_n\bigg|_{n=1} - \frac{1}{3}\log(aT_B).$$

Deriving with respect to $\log L$ we get a function of LT_B as claimed.

Mutual information

- Mutual information of subsystems A and B: $I \equiv S_A + S_B S_{A \cup B}$
- $A = [-\ell_A, 0]$ and $B = [0, \ell_B]$
- *I* is upper bound on $S_{A,B}$ (negativity is better)
- Easy to express I in terms of $S_A(\ell, L)$ previously computed
- One weak link: $I = \frac{\cos^2 \xi}{3} \log \frac{\ell_A \ell_B}{\ell_A + \ell_B}$
 - Cf. negativity $\mathcal{E} \sim \frac{c}{4} \log \frac{\ell_A \ell_B}{\ell_A + \ell_B}$ [Calabrese-Cardy-Tonni 2012]
- Two weak links (e.g. with $\ell_A = \ell_B = L$):

$$\frac{\partial I}{\partial \ln L} := G(x) = \frac{4}{3} \int_0^\infty dv \left(e^{-2v} - e^{-4v} \right) \left(\frac{x}{v+x} \right)^2$$

• We have G(0) = 0 and $G(\infty) = \frac{1}{3}$

Conclusion and outlook

- Used massless Form Factor approach to compute correlation function of branch-cut twist operators, in the presence of scattering on a quantum impurity.
- Derived the universal scaling function F(x) of the entanglement entropy of a resonant level (quantum dot), with an asymmetrically placed sub-system.
- Validated F(x) against large-scale numerics ($N = 64\,000$ sites)

Perspectives

- Fidelity (talk by H. Saleur)
- Local quench
- Understand bound states for J' > J
- Take FF computation to higher order
- Two disjoint intervals, negativity,...