

The entanglement entropy in integrable quantum field theory

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Based on:

- J. Cardy, O.A. Castro Alvaredo, B.D., J. Stat. Phys. 130, 129 (2008)
- O.A. Castro Alvaredo, B.D., J. Phys. A 41 275203 (2008)
- B.D., Phys. Rev. Lett. 102 031602 (2009)
- O.A. Castro Alvaredo, B.D., J. Stat. Phys. 134, 105 (2009)

See the review:

O.A. Castro Alvaredo, B.D., *J. Phys. A* 42 504006 (2009) in special issue "Entanglement entropy in extended quantum systems", ed. by P. Calabrese, J. Cardy and B.D.

Entanglement in quantum mechanics

 Entanglement: the measurement of a quantum observable immediately affects future measurements of independent observables. Opposite-spin particles from pair production:

$$|\psi\rangle = \frac{1}{\sqrt{2}} \Big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\Big) , \quad \langle A\rangle = \langle\psi|A|\psi\rangle$$

- Entanglement is the most fundamental, non-classical phenomenon of quantum mechanics: neither pure-wave nor pure-particle. It is a useful "resource": at the basis of better performances of the (still theoretical) quantum computers.
- Mixed states may describe similar probabilities but without entanglement:

$$\rho = \sum_{\alpha} p_{\alpha} |\psi_{\alpha}\rangle \langle \psi_{\alpha}| , \quad \langle A \rangle = \operatorname{Tr}(\rho A)$$

(for pure states, $\rho = |\psi\rangle\langle\psi|$; for finite temperature, $\rho = e^{-H/kT}$). For instance,

$$\rho = \frac{1}{2} \Big(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |\downarrow\uparrow\rangle\langle\downarrow\uparrow| \Big)$$

How to measure (or quantify) quantum entanglement?

- There are various propositions for measures of quantum entanglement. Consider the **entanglement entropy**:
 - With the Hilbert space a tensor product $\mathcal{H} = s_1 \otimes s_2 \otimes \cdots \otimes s_N = A \otimes \overline{A}$, and a given state $|gs\rangle \in \mathcal{H}$, calculate the **reduced density matrix**:

$$\rho_A = \operatorname{Tr}_{\bar{A}}(|\mathrm{gs}\rangle\langle\mathrm{gs}|)$$

$$\cdots s_{i-1} \otimes \underbrace{s_i \otimes s_{i+1} \otimes \cdots \otimes s_{i+L-1} \otimes s_{i+L}}_{A} \cdots$$

- The entanglement entropy is the resulting **von Neumann entropy**:

$$S_A = -\operatorname{Tr}_A(\rho_A \log(\rho_A)) = -\sum_{\text{eigenvalues of } \rho_A} \lambda \log(\lambda)$$

 $\lambda \neq 0$

The entanglement entropy

- It is the entropy that is measured in a subsystem A, if its environement \overline{A} is "forgotten". It measures a "number of links" between the subsystem and its environment; the quantity of additional information in the subsystem about its environment.
- It was proposed as a way to understand black hole entropy [Bombelli, Koul, Lee, Sorkin 1986].
- Then it was proposed as a measure of entanglement [Bennet, Bernstein, Popescu, Schumacher 1996].
- Examples:

- Tensor product state:

$$|gs\rangle = |A\rangle \otimes |\bar{A}\rangle \Rightarrow \rho_{A} = |A\rangle\langle A| \Rightarrow S_{A} = -1\log(1) = 0.$$
- The state $|gs\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle\rangle + |\downarrow\uparrow\rangle\rangle):$

$$\rho_{1^{st} spin} = \frac{1}{2} (|\uparrow\rangle\rangle\langle\uparrow|+|\downarrow\rangle\langle\downarrow|) \Rightarrow S_{1^{st} spin} = -2 \times \left(\frac{1}{2}\log\left(\frac{1}{2}\right)\right) = \log(2)$$

One basic property of entanglement entropy

Entanglement entropy is not "directional": $S_A = S_{\bar{A}}$. Proof:

• Anti-linear maps:

 $f: A \to \overline{A}$ with $f|A\rangle = \langle A|gs\rangle$, $\overline{f}: \overline{A} \to A$ with $\overline{f}|\overline{A}\rangle = \langle \overline{A}|gs\rangle$.

- Then $\rho_A = \bar{f}f : A \to A$ and $\rho_{\bar{A}} = f\bar{f} : \bar{A} \to \bar{A}$.
- If $\rho_A |A\rangle = \lambda |A\rangle$ then $\bar{f}f|A\rangle = \lambda |A\rangle$, hence $(f\bar{f})f|A\rangle = \lambda f|A\rangle$, whence $\rho_{\bar{A}}f|A\rangle = \lambda f|A\rangle$.
- Hence ρ_A and $\rho_{\bar{A}}$ have the same set of non-zero eigenvalues (with the same degeneracies).

Scaling limit

- Say $|gs\rangle$ is a ground state of some local spin-chain Hamiltonian, and that the chain is infinitely long.
- An important property of $|gs\rangle$ is the **correlation length** ξ :

 $\langle \mathrm{gs} | \sigma_i \sigma_j | \mathrm{gs} \rangle - \langle \mathrm{gs} | \sigma_i | \mathrm{gs} \rangle \langle \mathrm{gs} | \sigma_j | \mathrm{gs} \rangle \sim e^{-|i-j|/\xi} \text{ as } |i-j| \to \infty$

- Suppose there are parameters in the Hamiltonian such that for certain values, $\xi \to \infty$. This is a **quantum critical point**.
- We may adjust these parameters in such a way that the length L of A stays in proportion to ξ : $L/\xi = mr$. This is the scaling limit.
- The resulting entanglement entropy **diverges** in that limit: $S_A \propto \log(\xi) + f(mr)$. But the differences $f(mr_1) - f(mr_2)$ are **universal**, and are described by **quantum field theory**. r is the dimensionful length of A; m is the smallest mass of the spectrum.

First universal quantity: short- and large-distance entanglement entropy

Choosing appropriately $\varepsilon \propto 1/(m\xi)$, a non-universal cutoff with dimenions of length:

• Short distance: $0 \ll L \ll \xi$, logarithmic behavior [Holzhey, Larsen, Wilczek 1994; Calabrese, Cardy 2004]

$$S_A \sim \frac{c}{3} \log\left(\frac{r}{\varepsilon}\right) = \frac{c}{3} \log(L) + const.$$

• Large distance: $0 \ll \xi \ll L$, saturation

$$S_A \sim -\frac{c}{3}\log(m\varepsilon) + U = \frac{c}{3}\log(\xi) + U + const.$$

where c is the central charge of the corresponding critical point. In terms of lattice quantities:

$$U = \lim_{x \to \infty} \left(S_A |_{L=\infty, \xi=x} - S_A |_{\xi=\infty, L=x} \right)$$

Partition functions on multi-sheeted Riemann surfaces

[Callan, Wilczek 1994; Holzhey, Larsen, Wilczek 1994]

• We can use the "replica trick" for evaluating the entanglement entropy:

$$S_A = -\operatorname{Tr}_A(\rho_A \log(\rho_A)) = -\lim_{n \to 1} \frac{d}{dn} \operatorname{Tr}_A(\rho_A^n)$$

• For integer numbers *n* of replicas, in the scaling limit, this is a partition function on a Riemann surface:



Branch-point twist fields

[Cardy, Castro Alvaredo, Doyon 2007]

• Consider many copies of the QFT model on the usual \mathbb{R}^2 :

$$\mathcal{L}^{(n)}[\varphi_1,\ldots,\varphi_n](x) = \mathcal{L}[\varphi_1](x) + \ldots + \mathcal{L}[\varphi_n](x)$$

• There is an obvious symmetry under cyclic exchange of the copies:

 $\mathcal{L}^{(n)}[\sigma\varphi_1,\ldots,\sigma\varphi_n] = \mathcal{L}^{(n)}[\varphi_1,\ldots,\varphi_n], \quad \text{with} \quad \sigma\varphi_i = \varphi_{i+1 \mod n}$

• The associated twist fields \mathcal{T} , when inside correlation functions, gives

$$\langle \mathcal{T}(0)\cdots\rangle_{\mathcal{L}^{(n)}}\propto \int_{C_0} [d\varphi_1\cdots d\varphi_n]_{\mathbb{R}^2} \exp\left[-\int_{\mathbb{R}^2} d^2x \ \mathcal{L}^{(n)}[\varphi_1,\ldots,\varphi_n](x)\right]\cdots$$

with branching conditions on the line $x\in(0,\infty)$ given by

$$C_0 : \varphi_i(\mathbf{x}, 0^+) = \varphi_{i+1}(\mathbf{x}, 0^-) \quad (\mathbf{x} > 0)$$

• Graphically:



• In operator terms: equal-time exchange relations,

$$\varphi_i(\mathbf{x})\mathcal{T}(0) = \begin{cases} \mathcal{T}(0)\varphi_i(\mathbf{x}) & (\mathbf{x} < 0) \\ \mathcal{T}(0)\varphi_{i+1}(\mathbf{x}) & (\mathbf{x} > 0) \end{cases}$$

• Locality: commutation with Hamiltonian density $h(\mathbf{x})$,

$$[\mathcal{T}(0), h(\mathbf{x})] = 0 \quad (\mathbf{x} \neq 0)$$

• Another twist field $\tilde{\mathcal{T}}$ is associated to the inverse symmetry σ^{-1} , and we have

$$\langle \mathcal{T}(0)\tilde{\mathcal{T}}(r)\rangle_{\mathcal{L}^{(n)}} \propto \int_{C_{0,r}} [d\varphi_1 \cdots d\varphi_n]_{\mathbb{R}^2} \exp\left[-\int_{\mathbb{R}^2} d^2x \,\mathcal{L}^{(n)}[\varphi_1, \dots, \varphi_n](x)\right]$$

= Z_n



Short- and large-distance entanglement entropy revisited

Hence we have

$$Z_n/Z_1^n = D_n \varepsilon^{2d_n} \langle \mathcal{T}(0)\tilde{\mathcal{T}}(r) \rangle_{\mathcal{L}^{(n)}} , \quad S_A = -\lim_{n \to 1} \frac{d}{dn} Z_n$$

where D_n is a normalisation constant, and d_n is the scaling dimension of \mathcal{T} [Calabrese, Cardy 2004]:

$$d_n = \frac{c}{12} \left(n - \frac{1}{n} \right)$$

• Short distance: $0 \ll L \ll \xi$, logarithmic behavior

$$\langle \mathcal{T}(0)\tilde{\mathcal{T}}(r) \rangle_{\mathcal{L}^{(n)}} \sim r^{-2d_n} \Rightarrow S_A \sim \frac{c}{3} \log\left(\frac{r}{\varepsilon}\right)$$

Large distance:
$$0 \ll \xi \ll L$$
, saturation
 $\langle \mathcal{T}(0)\tilde{\mathcal{T}}(r) \rangle_{\mathcal{L}^{(n)}} \sim \langle \mathcal{T} \rangle_{\mathcal{L}^{(n)}}^2 \Rightarrow U = -\lim_{n \to 1} \frac{d}{dn} \left(m^{-2d_n} \langle \mathcal{T} \rangle_{\mathcal{L}^{(n)}}^2 \right)$

Evaluation of U

$$U = -\lim_{n \to 1} \frac{d}{dn} \left(m^{-2d_n} \langle \mathcal{T} \rangle_{\mathcal{L}^{(n)}}^2 \right)$$

• Idea of AI. Zamolodchikov (unpublished), for twist fields in general. In angular quantization, $x + iy = e^{\eta + i\theta}$, η the "space" and θ the "time":

twist fields = unitary operator \mathcal{U}_{σ} associated to transformation σ

$$\varphi_i(\eta)\mathcal{T} = \mathcal{T}\varphi_{i+1}(\eta) \quad \Rightarrow \quad \mathcal{T} \propto \mathcal{U}_{\sigma}$$

• \mathcal{U}_{σ} can be diagonalized simultaneously with angular-quantization hamiltonian $K^{(n)}$:

$$\langle \mathcal{T}(0) \cdots \rangle_{\mathcal{L}^{(n)}} = \operatorname{Tr}_{\operatorname{ang},\mathcal{L}^{(n)}} \left[e^{2\pi i K^{(n)}} \mathcal{U}_{\sigma} \cdots \right]$$

• Regularization necessary, performed explicitly in free-fermion models; Ising model [Cardy, Castro Alvaredo, Doyon 2007], [A. Zamoloschikov, Lukyanov 1997]:

$$U_{\text{Ising}} = \frac{1}{6} \log 2 - \int_0^\infty \frac{dt}{2t} \left(\frac{t \cosh t}{\sinh^3 t} - \frac{1}{\sinh^2 t} - \frac{e^{-2t}}{3} \right) = -0.131984...$$

Second universal quantity: the next correction term

We found [Cardy, Castro Alvaredo, Doyon 2007], [Castro Alvaredo, Doyon 2008], [Doyon 2008]

$$S_A \sim -\frac{c}{3}\log(m_1\varepsilon) + U - \frac{1}{8}\sum_{\alpha=1}^{\ell} K_0(2rm_\alpha) + O\left(e^{-3rm_1}\right)$$

where ℓ is the number of particles in the spectrum of the QFT, and m_{α} are the masses of the particles, with $m_1 \leq m_{\alpha} \forall \alpha$.

- This next correction term depends only on the particle spectrum, but not on their interaction (i.e. not on the way they scatter off each other).
- In generic QFT, the largest mass is less than twice the smallest mass. Hence, the entanglement entropy provides "clean" information about "half" of the spectrum.

Form factors and two-point function

- In the *n*-replica model $\mathcal{L}^{(n)}$, there are *n* times as many particle types, which we will denote by $\mu = (\alpha, j)$ with $j = 1, \ldots, n$ the replica label.
- The two-point function of branch-point twist fields can be decomposed into the *in*-basis, giving a large-distance expansion:

$$\langle \mathcal{T}(0)\tilde{\mathcal{T}}(r) \rangle_{\mathcal{L}^{(n)}} = \langle \operatorname{vac} | \mathcal{T}(0)\tilde{\mathcal{T}}(r) | \operatorname{vac} \rangle =$$

$$\sum_{k=0}^{\infty} \sum_{\substack{\alpha_1,\dots,\alpha_k \\ j_1,\dots,j_k}} \int \frac{d\theta_1 \cdots d\theta_k}{(2\pi)^k} | F_{\mu_1,\dots,\mu_k}(\theta_1,\dots,\theta_k) |^2 e^{-r \sum_{i=1}^k m_{\alpha_i} \cosh \theta_i}$$

where the form factors are:

$$F_{\mu_1,\ldots,\mu_k}(\theta_1,\ldots,\theta_k) = \langle \operatorname{vac} | \mathcal{T}(0) | \theta_1,\ldots,\theta_k \rangle_{\mu_1,\ldots,\mu_k}^{in}$$

Analytic properties of two-particle form factors

Consider $F_{\mu_1,\mu_2}(\theta_1,\theta_2) = F_{\mu_1,\mu_2}(\theta_1 - \theta_2)$ (by relativistic invariance) as an analytic function of $\theta \equiv \theta_1 - \theta_2$.

• Such form factors for usual (non-twist) fields have a well-known analytic structure: using Mandelstam's *s*-variable $s = m_{\alpha_1}^2 + m_{\alpha_2}^2 + 2m_{\alpha_1}m_{\alpha_2}\cosh(\theta)$, there is a branch cut from $s = (m_{\alpha_1} + m_{\alpha_2})^2$ to ∞ , just above which we are describing the physical form factor with an *in*-state, and just below which it is the form factor with an *out*-state instead. Between 0 and $(m_{\alpha_1} + m_{\alpha_2})^2$, there may be poles due to bound states, and there are no other singularities on the physical sheet.



• Form factors for branch-point twist-fields have modified analytic properties.

Change of sign of θ (as usual)

For $\theta_1 < \theta_2$:

 $F_{\mu_1,\mu_2}(\theta_1 - \theta_2) = \langle \operatorname{vac} | \mathcal{T}(0) | \theta_1, \theta_2 \rangle_{\mu_1,\mu_2}^{out}$ $\stackrel{j_1 \neq j_2}{=} \langle \operatorname{vac} | \mathcal{T}(0) | \theta_2, \theta_1 \rangle_{\mu_2,\mu_1}^{in} = F_{\mu_2,\mu_1}(\theta_2 - \theta_1)$



Quasi-periodicity relation (different)

$$F_{\mu_1,\mu_2}(\theta + 2\pi i) = F_{\mu_2,\mu_1}(-\theta), \quad \mu = (\alpha, j + 1 \mod n)$$







The structure of the two-particle form factors

Putting all that together, only $F_{(\alpha_1,1),(\alpha_2,1)}(\theta)$ matters, thanks to the relation $F_{(\alpha_1,j_1),(\alpha_2,j_2)}(\theta) = F_{(\alpha_1,1),(\alpha_2,1)}(\theta + 2\pi i(j_1 - j_2))$ for $0 \le j_1 - j_2 \le n - 1$. It has the following analytic structure:



Correction term to the entanglement entropy

• The two-particle contribution to the entanglement entropy is

$$\frac{d}{dn} \left(\langle \mathcal{T} \rangle \frac{n}{8\pi^2} \sum_{\alpha,\beta=1}^{\ell} \int_{-\infty}^{\infty} d\theta_1 d\theta_2 f_{\alpha,\beta}(\theta_1 - \theta_2, n) e^{-r(m_\alpha \cosh \theta_1 + m_\beta \cosh \theta_2)} \right)_{n=1} \\ \langle \mathcal{T} \rangle f_{\alpha,\beta}(\theta, n) = \sum_{j=0}^{n-1} |F_{(\alpha,1),(\beta,1)}(\theta + 2\pi i j)|^2$$

- The form factors themselves vanish like n-1 as $n \to 1$, because the branch-point twist field becomes the **identity field**.
- The only contribution to the entanglement entropy comes from the collision of kinematic poles at $\theta = 0$, giving $\left(\frac{d}{dn}f_{\alpha,\beta}(\theta,n)\right)_{n=1} = \frac{\pi^2}{2}\delta(\theta)\delta_{\alpha,\overline{\beta}}$:



Heuristic: entanglement density and pair creations

Entanglement entropy should "count" the connections between A and \overline{A} , for A of large enough extent:



- The entanglement density s(x x') should receive contributions whenever the quantum fluctuation at x is somehow correlated with that at x'.
- At large distances $x x' \gg m^{-1}$, the main contributions should be due to particles coming from a common virtual pair created far in the past.



(1)

• The particles have to survive a time t, and the probability for this is ruled by quantum uncertainty principles, $\propto e^{-Et}$, E the total energy, independently from the interaction.

General two-particle twist-fields form factors

Diagonal scattering without bound states, integral representation for scattering matrix:

$$S(\theta) = \exp\left[\int_0^\infty \frac{dt}{t}g(t)\sinh\left(\frac{t\theta}{i\pi}\right)\right]$$

The general "minimal" solution is

$$F_{j,k}^{\min}(\theta) = \exp\left[\int_0^\infty \frac{dt}{t\sinh(nt)}g(t)\sin^2\left(\frac{itn}{2}\left(1+\frac{i\theta-2\pi(j-k))}{\pi}\right)\right)\right]$$

and the full solution is

$$F_{j,k}(\theta) = \frac{\langle \mathcal{T} \rangle \sin\left(\frac{\pi}{n}\right)}{2n \sinh\left(\frac{i\pi(2(j-k)-1)+\theta}{2n}\right) \sinh\left(\frac{i\pi(2(k-j)-1)-\theta}{2n}\right)} \frac{F_{j,k}^{\min}(\theta, n)}{F_{j,k}^{\min}(i\pi, n)}$$

How to evaluate higher-particle twist-fields form factors

• In models of free fermionic particles, form factors are given by determinants / pfaffians:

$$\mathcal{T} = : \exp \int d\theta d\theta' \left[a^{\dagger}(\theta) a^{\dagger}(\theta') F(\theta, \theta') + a^{\dagger}(\theta) a(\theta') G(\theta, \theta') + a(\theta) a(\theta') H(\theta, \theta') \right] :$$

 In interacting integrable models, one way is to use Lukyanov's angular-quantization method [Lukyanov, 1995],

$$\langle \operatorname{vac} | \mathcal{T}(0) | \theta_1, \dots, \theta_k \rangle_{1,\dots,1}^{in} = \frac{\operatorname{Tr}_{\operatorname{ang},\mathcal{L}^{(n)}} \left[e^{2\pi i K^{(n)}} \mathcal{U}_{\sigma} Z_1(\theta_1) \cdots Z_1(\theta_n) \right]}{\operatorname{Tr}_{\operatorname{ang},\mathcal{L}^{(n)}} \left[e^{2\pi i n K} T_1(\theta_1) \cdots T_1(\theta_n) \right]}$$
$$= \frac{\operatorname{Tr}_{\operatorname{ang},\mathcal{L}} \left[e^{2\pi i n K} Z(\theta_1) \cdots Z(\theta_n) \right]}{\operatorname{Tr}_{\operatorname{ang},\mathcal{L}} \left[e^{2\pi i n K} \right]}$$

Lukyanov observed that:

$$\begin{split} K &= \int d\nu k(\nu) b_{\nu} b_{-\nu} \text{ (bilinear in free bosons),} \\ Z(\theta) &= \sum_{j} : e^{\int d\nu z_{\nu,j}(\theta) b_{\nu}} : \text{(linear combination of vertex operators).} \\ \text{Calculations: } \langle Z(\theta) Z(\theta') \rangle_{\text{Tr}} &= \exp\left[\int d\nu d\nu' z_{\nu}(\theta) z_{\nu'}(\theta') \langle b_{\nu} b_{\nu'} \rangle_{\text{Tr}}\right], \text{ etc.} \end{split}$$

Large-n behaviour of form factors?

[Castro Alvaredo, Doyon 2008]

$\propto n$	for renormalizable models
$\propto n \log n$	for marginally renormalizable models

$$V = s - \log \sqrt{f}$$

where s is the **boundary entropy** of Affleck and Ludwig (1991) and f is the fraction of the massive ground state degeneracy that is broken by the boundary condition.

1. $V = S^{\text{boundary}}(r)_{\text{critical}} - \frac{1}{2}S^{\text{bulk}}(2r)_{\text{critical}} - \log\sqrt{f}$ from looking at $S^{\text{boundary}}(r_1, r_2)$ 2. $S^{\text{boundary}}(r)_{\text{critical}} - \frac{1}{2}S^{\text{bulk}}(2r)_{\text{critical}} = s$ [Calabrese, Cardy 2004].

• Consequence:

$$\lim_{x \to \infty} \left(S_A |_{L=\infty,\xi=x} - S_A |_{\xi=\infty,L=x/2} \right) = U/2 + \log \sqrt{f} - s.$$

Ising model checks

- Consider Ising quantum chain in transverse magnetic field near to its critical point in the longitudinally-ordered phase, with boundary magnetic field h coupled longitudinally. Use $\kappa = 1 h^2/(2m)$. Integrable boundary state [Goshal, Zamolodchikov 1994].
- Exact form-factor expression for $V(\kappa)$; 500 terms re-summation of form factors agrees with $1/6\log(rm)+V(\kappa)$ where

$$V(\kappa) = \begin{cases} \sqrt{2} & \kappa > -\infty \quad \text{(free)} \\ 0 & \kappa = -\infty \quad \text{(fixed)} \end{cases}$$

This is $V(\kappa) = s - \log \sqrt{f}$ with f = 1/2.

- As $n \to 1$, only fully connected terms remain. Analytic continuation from region $n \gg 1$.
- $mr \to 0$ and $\kappa \to -\infty$ simultan.: critical bulk and non-critical boundary condition.
- For $\kappa > -1$ ("critical" value [Goshal, Zamolodchikov 1994]), entropy **not monotonic in** rm: approaches asymptotic value from above. Breaks "subadditivity".



Conclusions

- We have shown how three universal quantities associated to the entanglement entropy of one-dimensional quantum chains can be accessed using the methods of massive integrable QFT:
 - the difference between $L \gg \xi \gg 0$ and $\xi \gg L \gg 0$ (the universal constant U),
 - the first correction to saturation at $L\gg\xi\gg 0$ (in terms of the mass spectrum),
 - the difference between $L \gg \xi \gg 0$ and $\xi \gg L \gg 0$ in boundary case (in terms of Affleck and Ludwig's boundary entropy).

All these relations are valid beyond integrability, in any near-critical quantum chain (i.e. two-dimensional QFT).

• Open problems in massive integrable QFT: other universal corrections to saturation from higher-particle form factors; the entanglement entropy for *A* a disconnected region from multi-point correlation functions; the entanglement entropy for excited states; etc...