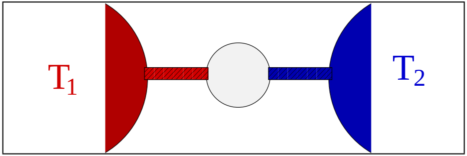
Entropy Density of Quasifree Fermionic States supported by Left/Right Movers



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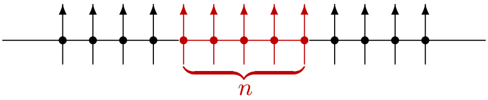
Contents

What are we physically interested in?

Question:

1. A sample is suitably coupled to thermal reservoirs s.t., for large times, the system approaches a nonequilibrium steady state (NESS).
2. We consider a class of quasifree fermionic NESS over the discrete line which are supported by so-called Left/Right movers.
3. *We ask:* What is the von Neumann entropy density $s_n = -\frac{1}{n}\mathrm{tr}(\varrho_n \log \varrho_n)$ of the reduced density matrix ϱ_n of such NESS restricted to a *finite string* of large length n?



4. The prominent XY chain will serve as illustration (in the fermionic picture).

Remark Several other correlators can be treated similarly (e.g. *spin-spin*, *EFP*).

What are we physically interested in?

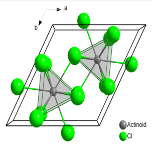
Specific model: XY chain [Lieb *et al.* 61, Araki 84]

- The Heisenberg Hamiltonian density reads

$$H_x = \sum_{n=1,2,3} J_n \sigma_n^{(x)} \sigma_n^{(x+1)} + \lambda \sigma_3^{(x)},$$

and the XY chain is the special case with $J_3 = 0$.

Experiments $SrCuO_2$, Sr_2CuO_3 [Sologubenko *et al.* 01] with $J_3 \neq 0$
$PrCl_3$ [D'Iorio *et al.* 83, Culvahouse *et al.* 69] with $J_1 = J_2$, $J_3 \approx 0$, *i.e.*, $J_3/J_1 \approx 10^{-2}$, and $\lambda = 0$



Formalism of quantum statistical mechanics

Rigorous foundation in the early 1930s:

1. An observable A is a selfadjoint operator on the Hilbert space of the system.
2. The dynamics of the system is determined by a distinguished selfadjoint operator H, called the Hamiltonian, through $A \mapsto A_t = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$.
3. A pure state is a vector ψ in the Hilbert space, and the expectation value of the measurement of A in the state ψ is $(\psi, A\psi)$.

Algebraic reformulation and generalization (von Neumann, Jordan, Wigner, ...):

Observables

C^* algebra $\mathfrak{A}$

Dynamics

(Strongly) continuous group τ^t of *-automorphisms on $\mathfrak{A}$

States

Normalized positive linear functionals ω on $\mathfrak{A}$, denoted by $\mathcal{E}(\mathfrak{A})$.

Example $\mathfrak{A} = \mathcal{L}(\mathfrak{h})$, $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$, and $\omega(A) = \mathrm{tr}(\varrho A)$ with density matrix ϱ

1.1 Quasifree setting

Observables

- The total observable algebra is:

CAR algebra

The *CAR algebra* $\mathfrak{A}$ over the *one-particle Hilbert space* $\mathfrak{h} = \ell^2(\mathbb{Z})$ is the C^* algebra generated by $\mathbb{1}$ and $a(f)$ with $f \in \mathfrak{h}$ satisfying:

- $a(f)$ is antilinear in f
- $\{a(f), a(g)\} = 0$
- $\{a(f), a^*(g)\} = (f, g)\,\mathbb{1}$

- The finite subalgebra of observables on the string is:

String subalgebra

Let $\mathfrak{h}_n = \ell^2(\mathbb{Z}_n)$ be the one-particle subspace over the *finite string* $\mathbb{Z}_n = \{1, 2, ..., n\}$. The *string algebra* $\mathfrak{A}_n$ is the C^* subalgebra of $\mathfrak{A}$ generated by $a(f)$ with $f \in \mathfrak{h}_n$.
By the Jordan-Wigner transformation, we have the isomorphism

$$\mathfrak{A}_n \simeq \mathbb{C}^{2^n \times 2^n}.$$

Quasifree setting

States

- For $F = [f_1, f_2] \in \mathfrak{h}^{\oplus 2}$, we define $JF = [cf_2, cf_1]$ with conjugation c, and

$$B(F) = a^*(f_1) + a(cf_2).$$

- The two-point function is characterized as follows:

Density

The *density* of a state $\omega \in \mathcal{E}(\mathfrak{A})$ is the operator $R \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ satisfying $0 \leq R \leq 1$ and $JRJ = 1 - R$, and, for all $F, G \in \mathfrak{h}^{\oplus 2}$,

$$\omega(B^*(F)B(G)) = (F, RG).$$

- The class of states we are concerned with is:

Quasifree state

A state $\omega \in \mathcal{E}(\mathfrak{A})$ with density $R \in \mathcal{L}(\mathfrak{h}^{\oplus 2})$ is called *quasifree* if it vanishes on odd polynomials in the generators and if

$$\omega(B(F_1)...B(F_{2n})) = \mathrm{pf}\,[(JF_i, RF_j)]_{i,j=1}^{2n}.$$

1.2 Nonequilibrium steady states (NESS)

States

- For the nonequilibrium situation, we use:

NESS [Ruelle 01]

A *NESS* w.r.t the C^*-dynamical system $(\mathfrak{A}, \tau^t)$ with initial state $\omega_0 \in \mathcal{E}(\mathfrak{A})$ is a large time weak-$*$ limit point of $\omega_0 \circ \tau^t$ (suitably averaged).

- The nonequilibrium setting for the XY chain is:

Theorem: XY NESS [Dirren *et al.* 98, Araki-Ho 00, A-Pillet 03]

Let $h = \mathrm{Re}(u)\,[\oplus - \mathrm{Re}(u)]$ generate the *coupled* dynamics τ^t. Then, the *decoupled* quasifree initial state with density $R_0 = (1 + \mathrm{e}^{Q_0})^{-1}$ and $Q_0 = 0 \oplus \beta_L h_L \oplus \beta_R h_R$ converges under τ^t to the unique quasifree NESS with density $R = (1 + \mathrm{e}^{Qh})^{-1}$, where

$$Q = \beta_L P_L + \beta_R P_R, \quad P_\alpha = \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-ith} i_\alpha^* i_\alpha \mathrm{e}^{-ith}.$$

u right translation, $h_\alpha = i_\alpha h i_\alpha^*$ with the natural injection $i_\alpha : \ell^2(\mathbb{Z}_\alpha) \to \mathfrak{h} = \ell^2(\mathbb{Z})$

1.3 Left/Right movers

Left/Right mover state

An *L/R-state* $\omega_\varrho \in \mathcal{E}(\mathfrak{A})$ is a quasifree state whose density $R = (1-\varrho) \oplus c\varrho c$ is

$$\varrho = \rho(Qh) \quad \text{with} \quad Q = \beta_L P_L + \beta_R P_R,$$

where $\rho \in C(\mathbb{R}, [0,1])$, $0 < \beta_L \leq \beta_R < \infty$, and $h, P_\alpha \in \mathcal{L}(\mathfrak{h})$ satisfy:

Assumptions: Chiral charges

(A1)
- $h = h^*$, $P_\alpha = P_\alpha^*$
- $[P_\alpha, h] = 0$

(A2)
- $[h, u] = 0$, $[P_\alpha, u] = 0$

(A3)
- $[h, \theta] = 0$
- $\theta P_L = P_R \theta$

(A4)
- $\rho(x) = (1 + \mathrm{e}^{-x})^{-1}$

(A5)
- $P_\alpha^2 = P_\alpha$
- $P_L + P_R = 1$

$u, \theta \in \mathcal{L}(\mathfrak{h})$ are the right translation and the parity.

XY NESS $h = \mathrm{Re}(u)$ and $P_\alpha = \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-ith} i_\alpha i_\alpha^* \mathrm{e}^{ith}$

2. von Neumann entropy

Reduction to the subsystem

- The restriction of the L/R-state to the string subalgebra is:

Reduced density matrix

The *reduced density matrix* $\varrho_n \in \mathfrak{A}_n$ of the string associated to the L/R-state $\omega_\varrho \in \mathcal{E}(\mathfrak{A})$ is

$$\omega_\varrho(A) = \mathrm{tr}(\varrho_n A), \quad A \in \mathfrak{A}_n.$$

- The correlation of the string with the environment is measured by:

von Neumann entropy

The *von Neumann entropy* of the string in the L/R-state $\omega_\varrho \in \mathcal{E}(\mathfrak{A})$ is

$$S_n = -\mathrm{tr}(\varrho_n \log \varrho_n).$$

Remark S_n is a widely used measure of *entanglement* in the ground state ($T = 0$).

2.1 Toeplitz Majorana correlation

L/R-Majorana correlation matrix: $d_i^* = d_i$, $\{d_i, d_j\} = 2\delta_{ij}$

Let $F_i = [f_i^1, f_i^2] \in \mathfrak{h}_n^{\oplus 2}$, $f_i^1(x) = [\tau^{\oplus n}]_{i,2x}$, $f_i^2(x) = [\tau^{\oplus n}]_{i,2x-1}$, and $\tau = \begin{bmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{bmatrix}$. Then, $d_i = B(F_i)$ for $i = 1, \ldots, 2n$ are Majorana operators. The *L/R-Majorana correlation matrix* $\Omega_n \in \mathbb{C}^{2n \times 2n}$ is defined by

$$\Omega_n = [\omega_\varrho(d_i d_j)]_{i,j=1}^{2n}.$$

Proposition: Toeplitz structure

Let (A1) and (A2) hold. Then,

$$\Omega_n = 1 + \mathrm{i}\, T_n[a] \quad \text{with} \quad T_n[a] = -T_n[a]^{\mathrm{t}} \in \mathbb{R}^{2n \times 2n},$$

where the symbol $a = -a^* \in L^\infty_{2\times 2}(\mathbb{T})$ of the block Toeplitz operator $T[a] \in \mathcal{L}(\ell^2_2(\mathbb{N}))$ is given by

$$a = \begin{bmatrix} \mathrm{i}(\widehat{\varrho} - \widehat{\theta\varrho}) & \widehat{\varrho} + \widehat{\theta\varrho} - 1 \\ 1 - \widehat{\varrho} - \widehat{\theta\varrho} & \mathrm{i}(\widehat{\varrho} - \widehat{\theta\varrho}) \end{bmatrix}.$$

Toeplitz Majorana correlation

Toeplitz operators

- Let $\ell^2_N(\mathbb{N})$ be the square summable $\mathbb{C}^N$-valued sequences and $L^\infty_{N\times N}(\mathbb{T})$ the $\mathbb{C}^{N\times N}$-valued functions with components in $L^\infty(\mathbb{T})$.

Toeplitz theorem [Toeplitz 11]

Let $\{a_x\}_{x\in\mathbb{Z}} \subset \mathbb{C}^{N\times N}$ and let the operator T on $\ell^2_N(\mathbb{N})$ be defined on its maximal domain by the action

$$Tf = \left\{ \sum_{j=1}^{\infty} a_{i-j} f_j \right\}_{i=1}^{\infty}.$$

Then, $T \in \mathcal{L}(\ell^2_N(\mathbb{N}))$ iff there is an $a \in L^\infty_{N\times N}(\mathbb{T})$, called the *(scalar/block) symbol* (if $N = 1/N > 1$), s.t., for all $x \in \mathbb{Z}$,

$$a_x = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, a(k)\, \mathrm{e}^{-\mathrm{i}kx}.$$

In this case, we write $T = T[a]$ and $T_n[a] = P_n T[a] P_n$, where $P_n\{x_1, x_2, \ldots\} = \{x_1, \ldots, x_n, 0, 0, \ldots\}$.

2.2 Reduced density matrix

Proposition: Density matrix [Vidal *et al.* 03, Latorre *et al.* 04, A 07]

Let (A1) and (A2) hold. Then, there exists a set of fermions $\{c_i\}_{i=1}^n \subset \mathfrak{A}_n$ s.t.

$$\varrho_n = \prod_{i=1}^n \left(\frac{1+\lambda_i}{2}\, c_i^* c_i + \frac{1-\lambda_i}{2}\, c_i c_i^* \right),$$

where $\{\pm \mathrm{i}\lambda_i\}_{i=1}^n \subset \mathrm{i}\mathbb{R}$ are the eigenvalues of the Toeplitz matrix $T_n[a]$.

Proof.

1. [*Basis from fermions*] For any family of fermions $\{c_i\}_{i=1}^n \subset \mathfrak{A}_n$, we set $e_i^{11} = c_i^* c_i$, $e_i^{12} = c_i^*$, $e_i^{21} = c_i$, and $e_i^{22} = c_i c_i^*$.
   Then, $\{\prod_{i=1}^n e_i^{\alpha_i \beta_i}\}_{\alpha_1,\ldots,\beta_n = 1,2}$ is an ONB of $\mathfrak{A}_n$ w.r.t. $(A,B) \mapsto \mathrm{tr}(A^* B)$, and we can write

$$\varrho_n = \sum_{\alpha_1,\ldots,\beta_n=1,2} \omega_\rho \left(\left[\prod_{i=1}^n e_i^{\alpha_i \beta_i} \right]^* \right) \prod_{j=1}^n e_j^{\alpha_j \beta_j}.$$

Reduced density matrix

2. [*Special choice of fermions*] For any $V \in O(2n)$, set $G_i = [g_i^1, g_i^2] \in \mathfrak{h}_n^{\oplus 2}$ with $g_i^1(x) = \left[\tau^{-1\oplus n} V \tau^{\oplus n}\right]_{2i-1,2x}$ and $g_i^2(x) = \left[\tau^{-1\oplus n} V \tau^{\oplus n}\right]_{2i-1,2x-1}$. Then, $c_i = B(G_i)$ is a family of fermions,
$$\{c_i, c_j\} = \left[\tau^{-1\oplus n} V V^{\mathrm{t}} \bar{\tau}^{\oplus n}\right]_{2i-1,2j-1} = 0,$$
$$\{c_i^*, c_j\} = \left[\tau^{-1\oplus n} V V^{*} \tau^{\oplus n}\right]_{2i-1,2j-1} = \delta_{ij}.$$
3. [*Special choice of V*] Let $\{\pm \mathrm{i}\lambda_i\}_{i=1}^n \subset \mathrm{i}\mathbb{R}$ be the eigenvalues of $T_n[a]$. Since $T_n[a] = -T_n[a]^{\mathrm{t}} \in \mathbb{R}^{2n\times 2n}$, there exists a $V \in O(2n)$ s.t.
$$V T_n[a] V^{\mathrm{t}} = \oplus_{i=1}^n \lambda_i \mathrm{i}\sigma_2.$$
4. [*Factorization*] This block diagonalization leads to
$$\omega_\varrho(c_i c_j) = \frac{1}{4}\left[\tau^{*\oplus n} V \Omega_n V^{\mathrm{t}} \bar{\tau}^{\oplus n}\right]_{2i-1,2j-1} = 0,$$
$$\omega_\varrho(c_i^* c_j) = \frac{1}{4}\left[\tau^{\mathrm{t}\oplus n} V \Omega_n V^{\mathrm{t}} \bar{\tau}^{\oplus n}\right]_{2i-1,2j-1} = \delta_{ij}\frac{1+\lambda_i}{2}.$$

Hence, we can factorize as $\omega_\rho\left(\prod_{i=1}^n e_i^{\alpha_i\beta_i}\right) = \prod_{i=1}^n \delta_{\alpha_i\beta_i}\, \omega_\varrho\left(e_i^{\alpha_i\alpha_i}\right)$.

□

2.3 Asymptotics

Theorem: L/R entropy density [A 07]

Let (A1)-(A4) hold. Then, with Shannon's entropy H, the asymptotic von Neumann entropy density in the Left mover-Right mover state $\omega_\varrho \in \mathcal{E}(\mathfrak{A})$ is

$$\lim_{n\to\infty} \frac{S_n}{n} = \sum_{\varepsilon=0,1} \frac{1}{2} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, \mathrm{H}\big(\mathrm{th}\big[\tfrac{1}{2}\widehat{\theta}^{\varepsilon}\widehat{Qh}\widehat{\theta}^{\varepsilon}\big]\big).$$

Proof.

1. [*Planck Toeplitz symbol*] Using (A3) and (A4) in the previous form of the block symbol, we get, with $Q_\pm = \beta_\pm(P_R \pm P_L)$ and $\beta_\pm = (\beta_R \pm \beta_L)/2$,

$$\mathrm{i}\,a = \frac{1}{\mathrm{ch}\big[\widehat{Q}_+\widehat{h}\big] + \mathrm{ch}\big[\widehat{Q}_-\widehat{h}\big]} \begin{bmatrix} \mathrm{sh}\big[\widehat{Q}_-\widehat{h}\big] & -\mathrm{i}\,\mathrm{sh}\big[\widehat{Q}_+\widehat{h}\big] \\ \mathrm{i}\,\mathrm{sh}\big[\widehat{Q}_+\widehat{h}\big] & \mathrm{sh}\big[\widehat{Q}_-\widehat{h}\big] \end{bmatrix}.$$

2. [*Spectral radius*] Using $\|T[a]\| = \|a\|_\infty$, we have

$$\|T_n[a]\| \le \mathrm{ess\,sup}_{\mathbb{T}}\, \mathrm{th}\big[\tfrac{1}{2}\big(\big|\widehat{Q}_+\big| + \big|\widehat{Q}_-\big|\big)\big|\widehat{h}\big|\big] < 1.$$

Asymptotics

3. [*von Neumann entropy*] Let $\mathrm{H}(x) = -\sum_{\sigma=\pm} \log[(1+\sigma x)/2](1+\sigma x)/2$ for $x \in (-1,1)$ be the (symmetrized) Shannon entropy function. Then,

$$S_n = -\sum_{\varepsilon_1,\ldots,\varepsilon_n=0,1} \lambda_{\varepsilon_1,\ldots,\varepsilon_n} \log(\lambda_{\varepsilon_1,\ldots,\varepsilon_n}) = \sum_{i=1}^{n} \mathrm{H}(\lambda_i),$$

where $\lambda_{\varepsilon_1,\ldots,\varepsilon_n} = \prod_{i=1}^{n} \frac{1}{2}(1+(-1)^{\varepsilon_i}\lambda_i)$ are the 2^n eigenvalues of ϱ_n with $0 < \lambda_{\varepsilon_1,\ldots,\varepsilon_n} < 1$.

4. [*Asymptotics*] Since $\mathrm{i}a \in L^\infty_{2\times 2}(\mathbb{T})$ is selfadjoint, *Szegő's first limit theorem for block Toeplitz operators* yields the asymptotic first order trace formula

$$\lim_{n\to\infty} \frac{\operatorname{tr} \mathrm{H}(T_n[\mathrm{i}a])}{2n} = \frac{1}{2}\int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \operatorname{tr} \mathrm{H}(\mathrm{i}a(k)).$$

Using the evenness of the Shannon entropy, we arrive at

$$\operatorname{tr} \mathrm{H}(\mathrm{i}a) = \sum_{\varepsilon=0,1} \mathrm{H}\big(\mathrm{th}\big[\tfrac{1}{2}\widehat{\theta}^{\varepsilon}\widehat{Qh}\widehat{\theta}^{\varepsilon}\big]\big).$$

□

Asymptotics

Special cases.
We can rewrite the double of the integrand of the entropy density as

$$s = \sum_{\sigma=\pm} \mathrm{H}\big(\mathrm{th}\big[\tfrac{1}{2}\big(\beta_+\big|\widehat{P}_R + \widehat{P}_L\big| + \sigma\beta_-\big|\widehat{P}_R - \widehat{P}_L\big|\big)\big|\widehat{h}\big|\big]\big).$$

1. *Case* $\beta_- = 0$.
   We then have the two equal contributions
   $$s = 2\,\mathrm{H}\big(\mathrm{th}\big[\tfrac{1}{2}\beta_+\big|\widehat{P}_R + \widehat{P}_L\big|\big|\widehat{h}\big|\big]\big).$$
2. *Case with additional (A5), i.e.* $P_\alpha^2 = P_\alpha$ *and* $P_R + P_L = 1$.
   Since $(P_R - P_L)^2 = P_R + P_L$, we get
   $$s = \sum_{\sigma=\pm} \mathrm{H}\big(\mathrm{th}\big[\tfrac{1}{2}\big(\beta_+ + \sigma\beta_-\big)\big|\widehat{h}\big|\big]\big) = \mathrm{H}\big(\mathrm{th}\big[\tfrac{1}{2}\beta_R\big|\widehat{h}\big|\big]\big) + \mathrm{H}\big(\mathrm{th}\big[\tfrac{1}{2}\beta_L\big|\widehat{h}\big|\big]\big).$$

   XY NESS $P_\alpha = \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-ith} i_\alpha i_\alpha^* \mathrm{e}^{ith}$

Remarks

If (A1)-(A5) hold, then the block symbol $a \in L^\infty_{2\times 2}(\mathbb{T})$ of the Toeplitz operator is

$$\mathrm{i}\, a = \frac{1}{\mathrm{ch}\big[\beta_+\widehat{h}\big] + \mathrm{ch}\big[\beta_-\widehat{h}\big]} \begin{bmatrix} \mathrm{sign}\big(\widehat{P}_R - \widehat{P}_L\big)\mathrm{sh}\big[\beta_-\widehat{h}\big] & -\mathrm{i}\,\mathrm{sh}\big[\beta_+\widehat{h}\big] \\ \mathrm{i}\,\mathrm{sh}\big[\beta_+\widehat{h}\big] & \mathrm{sign}\big(\widehat{P}_R - \widehat{P}_L\big)\mathrm{sh}\big[\beta_-\widehat{h}\big] \end{bmatrix}.$$

Let P_R, P_L be nontrivial and $\widehat{h}$ sufficiently smooth.

Nonequilibrium ($\beta_- > 0$)

- **(Leading order)** The singular nature of the symbol does not affect the *leading* order of the entropy density asymptotics.
- **(Nonvanishing density)** Any strictly positive temperature in the system leads to a nonvanishing asymptotic entropy density. This is due to the fact, that, in such a case, the Toeplitz symbol $\mathrm{i}a$ has at least one eigenvalue with modulus strictly smaller than 1.
- **(Strong subadditivity)** The existence of a nonnegative entropy density for translation invariant spin systems can also be shown by using the strong subadditivity property of the entropy.

Remarks

Nonequilibrium ($\beta_- > 0$)

- **(Block symbols)** The effect of a true nonequilibrium on the Toeplitz determinant approach to quasifree fermionic correlators is twofold:
  (a) The symbol becomes nonscalar.
  (b) The symbol loses regularity.
  Since *Coburn's Lemma* [Coburn 66] does not hold in the block case, it is in general very difficult to establish invertibility. Moreover, *Szegő-Widom* [Widom 76] and *Fisher-Hartwig* [Widom, Basor, ... 73-...] are not applicable (higher order).

Equilibrium ($\beta_- = 0$)

- **(Symbol)** The entropy can be expressed using a scalar Toeplitz operator whose symbol is smooth.
- **(Subleading order)** Second order trace formulas then imply that the subleading term has the form $o(n) = C + o(1)$.

Remarks

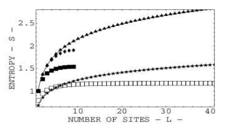
Ground state ($\beta_- = 0$, $\beta_+ = \infty$)

- **(Logarithmic growth)** For $\beta_+ \to \infty$, the entropy density vanishes. Using a proven case of the *Fisher-Hartwig conjecture* [Basor 79] and

$$S_n = \lim_{\varepsilon \to 0} \frac{1}{2\pi \mathrm{i}} \oint_{\gamma_\varepsilon} \mathrm{d}z \; \tilde{\mathrm{H}}(z) \, \frac{\mathrm{d}}{\mathrm{d}z} \log \det(T_n[a_{12}] - z)$$

  for suitable $\tilde{H}$ and γ_ε, one has $S_n = \frac{1}{3} \log n + C + o(1)$ [Jin-Korepin 03].

- **(Entanglement)** It plays an important role in:
  - *Strongly correlated quantum systems*
  - *Quantum information theory*
  - *Theory of quantum phase transitions*
    Long-range correlations, *e.g.*, critical entanglement in the XY/XXZ chains and CFT (logarithmic growth vs. saturation) [Vidal *et al.* 03, Calabrese-Cardy 04].



But quantum phase transitions can leave fingerprints at $T > 0$.