Title: Entanglement entropy of fermions and the Widom conjecture

Date: Apr 26, 2006 04:00 PM

URL: http://pirsa.org/06040025

Abstract: Entanglement entropy is currently of interest in several areas in physics, such as condensed matter, field theory, and quantum information. One of the most interesting properties of the entanglement entropy is its scaling behavior, especially close to phase transitions. It was believed that for dimensions higher than 1 the entropy scales like surface area of the subsystem. We will describe a recent result for free fermions at zero temperature, where the entropy in fact scales faster. The latter problem will be related to a mathematical conjecture due to H. Widom (1982). This is a joint work with I. Klich.

Perimeter Institute

April 26, 2006

Entanglement entropy of fermions and the Widom conjecture

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Univ. of Rochester

joint work with ISRAEL KLICH,
Phys. Dept., Caltech

① Definition of E.E.

② Known results

- 1D: spin chains
- D>1: ·· harmonic lattice
  ·· Kitaev model

③ New result

- $D \geq 1$ free fermions lattice/continuous setting
- connection with
  ·· Widom's conj.
  ·· Strong Szegö Limit Theorem
  ·· history: Onsager's work on 2D Ising model

where $\rho_A \equiv \mathrm{Tr}_{H_B}\, \rho = \sum_i c_i^2 \phi_{Ai} \phi_{Ai}^*$

and $\rho = \psi \psi^*$.

ψ below will be a ground state of some physical system

---

(2) <u>1D spin chain</u>

entanglement entropy of a block of L spins

Vidal, Latorre, Rico, Kitaev '03

Jin, Korepin '04

Its, Jin, Korepin '05

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$H_{XY} = \sum$

$$H_{XY} = \sum_{\ell} (1+\gamma)\,\sigma^x_\ell \sigma^x_{\ell+1} + (1-\gamma)\,\sigma^y_\ell \sigma^y_{\ell+1} + \lambda \sigma^z_\ell$$

$\gamma = 0$: XX model

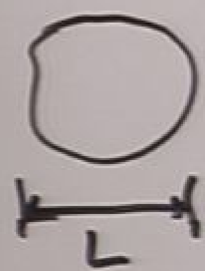
$\gamma = 1$: Ising chain

$-2 < \lambda < 2$ (for $|\lambda| > 2$ ferromagn. state, non critical)

$$\boxed{S_{XX}(L) \underset{L\to\infty}{\sim} \frac{1}{3} \log L}$$

Jin-Korepin using asympt. of Toeplitz det.
(a version of strong (2 term) Szegö limit theorem, Fisher-Hartwig proven by Basor)

$D>1$ Area law for entropy

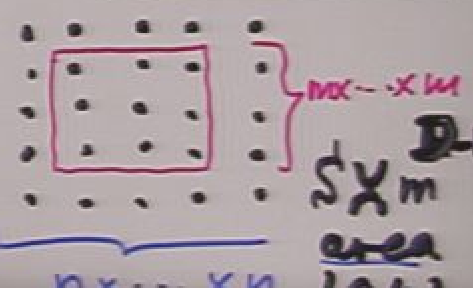


$$S(L) \sim L^{D-1}$$

- Bombelli, Koul, Lee, Sorkin '86
  e.e. of sc. field restr. to a s/syst. as a q. contrib. to Bekenstein-Hawking e.
- Srednicki '93 area law: $S \sim L^{D-1}$ sphere
  for a massless sc. field (e.g. acoustic modes of a lattice)
- Plenio, Eisert, Dreissig, Cramer '05 proved this for harm. lattice

$$H = \frac{\vec{p}\,\vec{p}^T}{2} + \frac{\vec{x}\,V\,\vec{x}^T}{2}$$

n.neighb. interact.



$S \propto m^{D-1}$ area law

D>1

Area law for entropy

6

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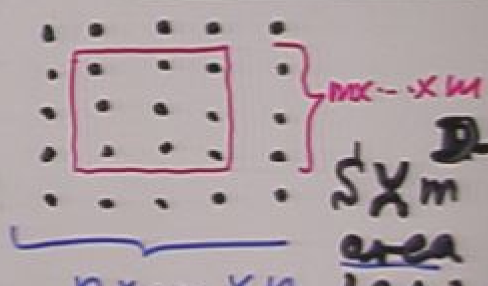

$S \propto m^{D-1}$ area law

- Hamma, Ionicioiu, Zanardi '05

area law for Kitaev model

lattice on a torus $\mathbb{T}^D$

star  $A_s = \prod_{j \in s} \sigma_j^x$

plaquette  $B_p = \prod_{j \in p} \sigma_j^z$

$$H = -\sum_s A_s - \sum_p B_p$$

③ our result G.-Klich
PRL '05
G. math.FA/02[illegible]12215
+ forthcoming
G.-Klich - Laptev

is the simplest example of <u>violation</u> of the <u>area law</u>

Free fermions in D dimensions on lattice or in continuum

$$H = \int d^D k \, \varepsilon(k) \, \psi_k^\dagger \psi_k$$

$T=0$, ground state is given by $\{k : \varepsilon(k) \le \varepsilon_F\}$

Study ent. entropy between region $L\Omega$ in real space and its complement as $L \to \infty$.

cont. Lattice 9

$\Gamma \subset \mathbb{R}^d$ or $\mathbb{T}^d$ compact set

$\Omega \subset \mathbb{R}^d$ or $\mathbb{Z}^d$ compact

Let $Q = \chi_{L\Omega}$ in $L^2(\mathbb{R}^d)$ or $\ell^2(\mathbb{Z}^d)$

$P = \mathcal{F} \chi_\Gamma \mathcal{F}^{-1}$ in $L^2(\mathbb{R}^d)$ or $\ell^2(\mathbb{Z}^d)$

$\mathcal{F}$ = F. transform or F. series.

Then [Klich, '05]

$$S_{\lambda\Omega,\Gamma} \equiv S(L) = -\operatorname{Tr} h(PQP),$$

$$h(t) = -t\log_2 t - (1-t)\log_2(1-t).$$

Other important quantities 10

avg. # of fermions $= \mathrm{Tr}\, PQP$

variance in ferm. # $= \mathrm{Tr}\, PQP(I - PQP)$

$$\equiv (\Delta N)^2$$

Results: $\Gamma = [-\frac{1}{2}, \frac{1}{2}]^D$

$\Omega = \prod_{j=1}^{D} [0, L_j]$ or $\prod_{j=1}^{D} \{0, \ldots, L_j\}$

CUBES

$$\frac{1}{2D} \sum_{j=1}^{D} S_1(L_j) \prod_{i \neq j} L_i \leq S(L_1, \ldots, L_D)$$

$$\leq \sum_{j=1}^{D} S_1(L_j) \prod_{i \neq j} L_i$$

In particular
for $L_1 = \cdots = L_D = L$

$$\frac{1}{2} L^{D-1} S_1(L) \leq S(L, \ldots, L)$$

$$\leq D L^{D-1} S_1(L)$$

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$$S(\cup C_i) \le \sum S(C_i) \le \frac{D}{3} \sum_k L_k^{D-1} \log_2 L_k$$
+ lower order.

Set with general bdaries:

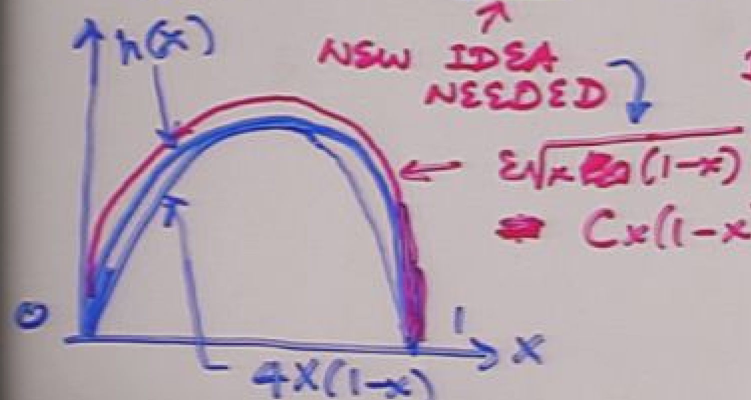
for Ω, Γ measurable (*)

$$4(\Delta N)^2 \le S_{\Omega,\Gamma}(L) \le (\Delta N)^2 \cdot O(\log_2 L)$$

both in cont. and lattice case

NEW IDEA NEEDED

$D=1$ Fannes–Haegeman–Mosonyi '03



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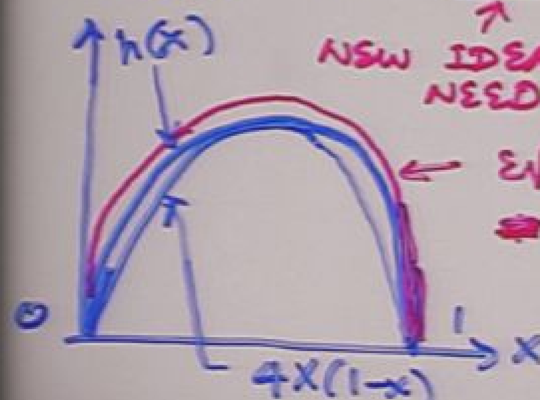

$\varepsilon\sqrt{x(1-x)}$

$Cx(1-x)\log\varepsilon$

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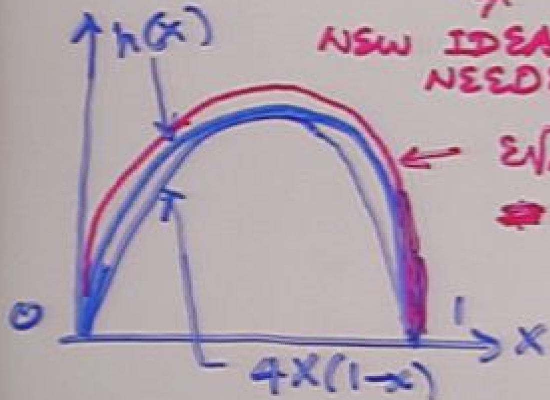

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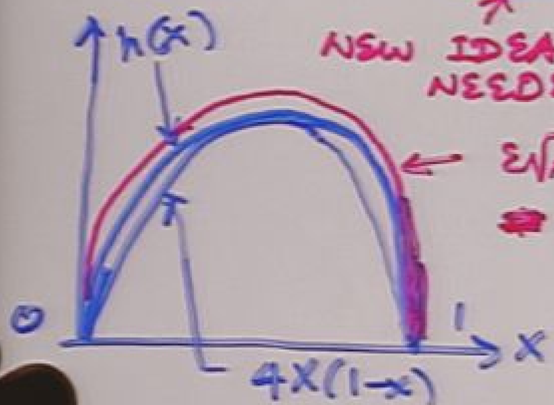

Rem (*) was indep. proven for cubes only in lattice case only by Wolf '05. 12

For cubes we have a correct order two-sided estimate.

Particle fluctuation asymptotics

Thm: If Ω, Γ are two compact

+lower order

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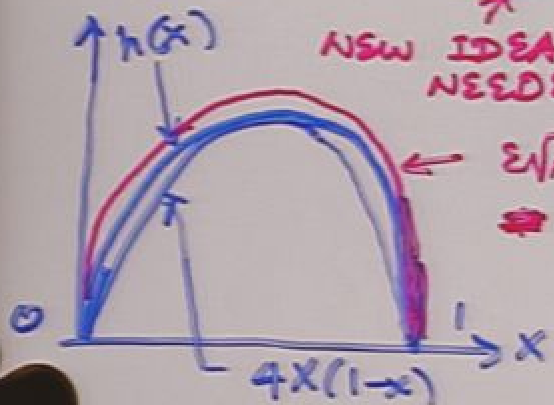

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Particle fluctuation asymptotics

Thm: If Ω, Γ are two compact sets in $\mathbb{R}^D$ (cont. case) with smooth bdaries then

$$(\Delta N)^2 = \frac{L^{D-1}\log_2 L}{(2\pi)^{D-1}} \frac{\ln 2}{4\pi^2} \iint_{\partial\Omega\,\partial\Gamma} |n_x \cdot n_\xi|\, dS_x\, dS_\xi + o(L^{D-1}\log_2 L).$$

Corollary

$$\Theta(L^{D-1}\log_2 L) \leq S_{\Omega,\Gamma}(L) \leq O(L^{D-1}\log_2^2 L)$$

Widom's Conjecture

f analytic on $\{z \mid |z| < R\}$, $R > 1$

$f(0) = 0$

$$\Rightarrow \mathrm{Tr}\, f(PQP) = \frac{L^D}{(2\pi)^D} f(1) \cdot \int_\Omega \int_\Gamma dx\, d\xi$$

$$+ \left(\frac{L}{2\pi}\right)^{D-1} \frac{\ln L}{4\pi^2} U(f) \cdot \int_{\partial\Omega} \int_{\partial\Gamma} |n_x \cdot n_\xi| \, dS_x \, dS_\xi$$

$$+ o(L^{D-1} \ln L), \quad L \to \infty,$$

where

$$U(f) = \int_0^1 \frac{f(t) - t f(1)}{t(1-t)} dt .$$

Landau

Widom '80 $D=1$

Widom '82, $-D=1$ '90 $- D \geq 2$, half space + compact

G. '02 math. FA/02■2215

$\llcorner D \geq 2$, one term w. sharp rem. + fractal bdaries

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Rem. h is not analyt.

BUT $h(1) = 0$

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$\therefore$ we conjectured:

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- consistent for $D=1$: $\frac{1}{12} \cdot 4 = \frac{1}{3}$
- checked numerically for lattice case $D = 2, 3$
  - .. Barthel, Chung, Schollwoeck cond-mat/0602077
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$+$ l.o.t.

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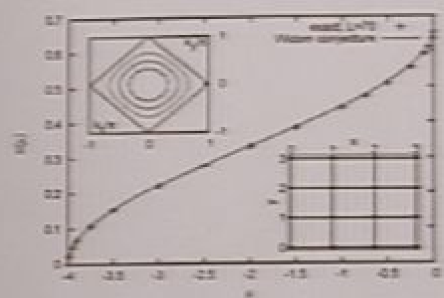

FIG. 1: The prefactor $c(\mu)$ in the entanglement scaling law as a function of the chemical potential μ for the ground state of the two-dimensional fermionic tight-binding model in comparison to the result of Gioev and Klich [16]. Insets show the hopping parameters and the Fermi surfaces for $\mu = -3, -2, -1, 0$.

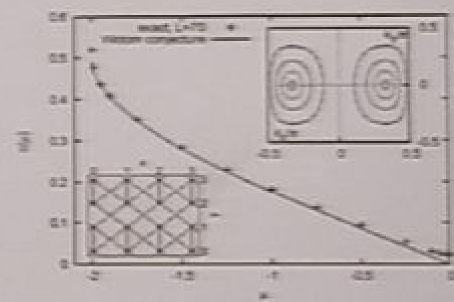

FIG. 2: The scaling prefactor $c(\mu)$ for the ground state of a two-dimensional fermionic tight-binding model with next-nearest neighbor hoppings in comparison to the result of [16]. Insets show the hopping parameters and the Fermi surfaces for $\mu \in [-0.25, -1.75]$ in the quartered Brillouin zone.

is $E(\mathbf{k}) = -2\,(\cos k_x + \cos k_y)$. The ground state Green's function matrix, from which we calculate the entanglement, reads in the thermodynamic limit

$$G_{\mathbf{r},\mathbf{r}'} = \int_{\Gamma(\mu)} \frac{d^2k}{(2\pi)^2}\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}, \tag{17}$$

with $\mathbf{r} = (x, y)$. Fig. 1 shows the scaling prefactor $c(\mu)$ as fitted from the exact entanglement of an $L \times L$ square with the rest of the universe, which was obtained from (9). It is in excellent agreement with (15) and supports thus the Widom conjecture for $d = 2$. The same agreement was found in the model

$$\begin{aligned} H = -\textstyle\sum_{x,y}\big((1+(-1)^x)c^\dagger_{x,y}c_{x,y+1} \\ + c^\dagger_{x,y}c_{x+1,y+1} + c^\dagger_{x,y}c_{x-1,y+1} + h.c.\big) \end{aligned} \tag{18}$$

which has a two-banded dispersion relation $E(\mathbf{k}) = \pm 2\sqrt{1 + 4\cos k_x \cos^2 k_y + 4\cos^2 k_x \cos^2 k_y}$ and a disconnected Fermi surface for $\mu \in [-2, 2]$, Fig. 2.

Especially for a comparison with bosonic systems, it is interesting to investigate models with a zero-dimensional Fermi surface. In particular we choose the two-dimensional model

$$\begin{aligned} H = -\textstyle\sum_{x,y}\big(h\cdot c^\dagger_{x,y}c_{x+1,y} \\ + (1+(-1)^{x+y})c^\dagger_{x,y}c_{x,y+1} + h.c.\big), \end{aligned} \tag{19}$$

which has for $0 \le h \le 1$ the two-band dispersion relation $E(\mathbf{k}) = \pm 2\sqrt{1 + h^2\cos^2 k_x + 2h\cos k_x \cos k_y}$, i.e. a gap of size $4(1-h)$ at $\mathbf{k} = (\pi, 0)$. Fig. 3 shows for $\mu = 0$ and $h \to 1$ how the entanglement converges to the area law with a *sublogarithmic* correction, $S_1(L) = L \cdot o(\log_2 L)$, meaning $\lim_{L\to\infty} S_1(L)/(L \log_2 L) = 0$. The curves $S_1(L)/L$ for finite gaps were extrapolated

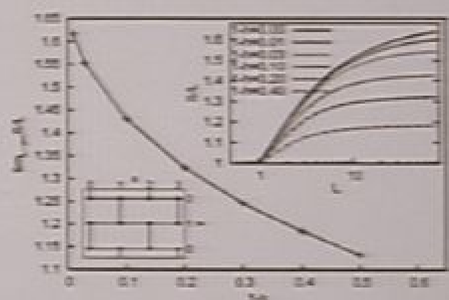

FIG. 3: The upper right inset shows the entanglement entropy per surface unit $S_1(L)/L$ (block of $n = L^2$ sites) for a two-dimensional fermionic tight-binding model with modulated vertical hopping (see the second inset) at $T = 0$. The energy gap $4(1-h)$ closes in the point $\mathbf{k} = (\pi, 0)$. The extrapolation $\lim_{L\to\infty} S_1(L)/L$ suggests a divergence for $h \to 1$.

to obtain $\lim_{L\to\infty} S_1(L)/L$. Those values indicate indeed a divergence for $h \to 1$. This result is consistent with Eq. (14), as the scaling coefficient $c(\mu)$, Eq. (15), vanishes for systems in $d > 1$ dimensions with a zero-dimensional Fermi surface. Further investigations have to determine the analytical form of the sublogarithmic correction and its universality.

Critical bosonic entanglement.— An important question is whether the logarithmic correction observed in the entanglement scaling law for critical one-dimensional bosonic systems is also present in higher dimensional systems. To investigate this, we examine a two-dimensional shows an expected power-law decay in the critical phases and an exponential decay in the non-critical one.

We then proceed to the evaluation of the block entropy of entanglement. The ground state of Eq.(2) is known to be a Gaussian state, whose density matrix can be expressed as the exponential of a quadratic fermion operator [20, 21]. To obtain the reduced density matrix of a L^d subsystem, Grassman algebra is needed [22]. Using a Bogoliubov transformation, the reduced density matrix ρ_L can then be written as

$$\rho_L = A \exp\left(-\sum_{l=1}^{L} \epsilon_l d_l^\dagger d_l\right), \tag{6}$$

where $d_l^\dagger, d_l$ are the new Fermi operators after the transformation, and A is a normalization constant to ensure $Tr(\rho) = 1$. The single-particle eigenvalues ϵ_l can be obtained from $\langle c_i^\dagger c_j\rangle$ and $\langle c_i^\dagger c_j^\dagger\rangle$ by the following formula[21]:

$$(C - F - \tfrac{1}{2})(C + F - \tfrac{1}{2}) = \tfrac{1}{4} P \operatorname{diag}\left\{\tanh^2\left(\tfrac{\epsilon_1}{2}\right), \tanh^2\left(\tfrac{\epsilon_2}{2}\right), \dots, \tanh^2\left(\tfrac{\epsilon_L}{2}\right)\right\} P^{-1} \tag{7}$$

where $C_{i,j} = \langle c_i^\dagger c_j\rangle$ and $F_{i,j} = \langle c_i^\dagger c_j^\dagger\rangle$;$P$ is the orthogonal matrix that diagonalizes the left side of the above equation. The Block entropy can then be calculated in terms of ϵ_l as:

$$S_L = \sum_{l=1}^{L}\left\{\ln[1 + \exp(-\epsilon_l)] + \frac{\epsilon_l}{\exp(\epsilon_l) + 1}\right\} \tag{8}$$

In $d = 1$ the above formulăe reproduce the scaling of the block entropy as observed in the XY model in a transverse field [5, 6]. In $d = 2$ the phase diagram is richer, and we need to consider the various phases one by one. We begin with the critical metallic phase (I), $\gamma = 0, 0 \le \lambda < d$. For this case a logarithmic correction to the area law, $S_L = (C(\lambda)/3)(\log_2 L)L^{d-1}$ is observed for all values of λ, as shown in Fig. 2. This is in full agreement with the results of Refs.[15, 16], which predict this behavior in presence of a finite Fermi surface. More specifically, Ref. 16 also supplies us with an explicit prediction for the λ dependence of $C(\lambda)$, based on the Widom's conjecture [23], in the form

$$C(\lambda) = \frac{1}{4(2\pi)^{d-1}} \int_{\partial\Omega} \int_{\partial\Gamma(\lambda)} |n_x \cdot n_p| dS_x dS_p \tag{9}$$

where Ω is the volume of the block normalized to one, $\Gamma(\lambda)$ is the volume enclosed by the Fermi surface, and the integration is carried over the surface of both domains. A numerical fit of the calculated asymptotic behavior of S_L through the formula $S_L = \frac{C}{3} L^{d-1}\log_2(L) + BL^{d-1} + AL^{d-2} + \dots$ provides us with the exact result for the $C(\lambda)$ prefactor. In Fig. 3 the prediction of Ref. 16, Eq.(9), for the case $(0 \le \lambda \le d, \gamma = 0)$ is compared to our

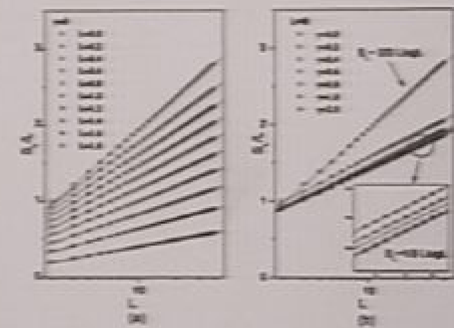

FIG. 2: Scaling of the block entropy S_L in $d = 2$ for $\gamma = 0$ (left panel) and $\lambda = 0$ (right panel). The solid lines correspond to fits according to the formula $S_L = \frac{C}{3} L \log_2(L) + BL + A$.

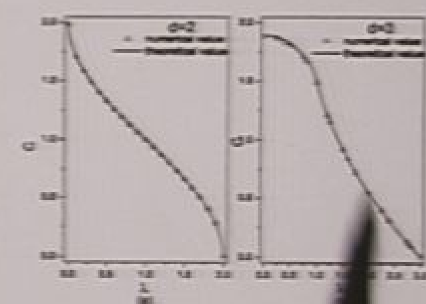

FIG. 3: λ-dependence of the C coefficient [illegible] (I) in $d = 2$ and $d = 3$. The values extracted from [illegible] numerical data are compared with the predictions [illegible] 16. In $d = 2$, the exact form of $C(\lambda)$ can be obtained [illegible] is equal to $\frac{4}{\pi}\cos^{-1}(\lambda - 1)$

numerical results both for $d = 2$ and [illegible]. The agreement is clearly striking. Moreover, [illegible] $= 0, \gamma > 0)$ in $d = 2$ the formula Eq.(9) predicts [illegible], which is also accurately verified by our data as [illegible] Fig. 2. This proves that the formula Eq.(9) is [illegible] providing a complete analytic form for the [illegible] behavior of the block-entropy scaling in arbitrary [illegible] for systems shows an expected power-law decay in the critical phases and an exponential decay in the non-critical one.

We then proceed to the evaluation of the block entropy of entanglement. The ground state of Eq.(2) is known to be a Gaussian state, whose density matrix can be expressed as the exponential of a quadratic fermion operator [20, 21]. To obtain the reduced density matrix of a L^d subsystem, Grassman algebra is needed [22]. Using a Bogoliubov transformation, the reduced density matrix ρ_L can then be written as

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In $d = 1$ the above formulãs reproduce the scaling of the block entropy as observed in the XY model in a transverse field [5, 6]. In $d = 2$ the phase diagram is richer, and we need to consider the various phases one by one. We begin with the critical metallic phase (I), $\gamma = 0, 0 \leq \lambda < d$. For this case a logarithmic correction to the area law, $S_L = (C(\lambda)/3)(\log_2 L)L^{d-1}$ is observed for all values of λ, as shown in Fig. 2. This is in full agreement with the results of Refs.[15, 16], which predict this behavior in presence of a finite Fermi surface. More specifically, Ref. 16 also supplies us with an explicit prediction for the λ dependence of $C(\lambda)$, based on the Widom's conjecture [23], in the form

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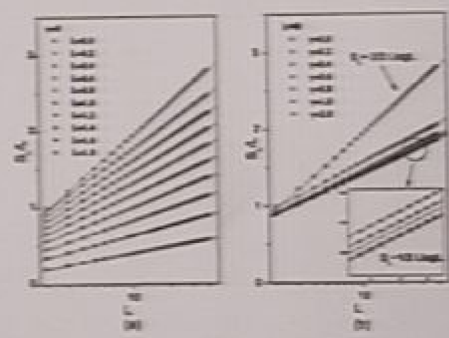

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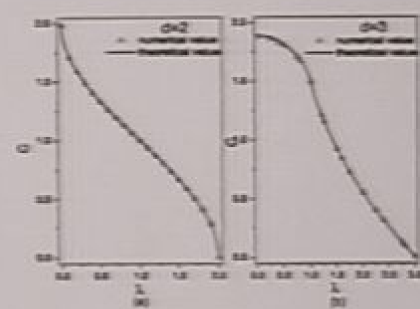

FIG. 3: λ-dependence of the C coefficient in Eq.(1) in $d = 2$ and $d = 3$. The values extracted from fits to our numerical data are compared with the predictions of Ref. 16. In $d = 2$, the exact form of $C(\lambda)$ can be obtained, which is equal to $\frac{2}{\pi}\cos^{-1}(\lambda - 1)$

numerical results both for $d = 2$ and $d = 3$. The agreement is clearly striking. Moreover, for $\{\lambda = 0, \gamma > 0\}$ in $d = 2$ the formula Eq.(9) predicts $C = 1$, which is also accurately verified by our data as shown in Fig. 2. This proves that the formula Eq.(9) is essentially providing a complete analytic form for the leading behavior of the block-entropy scaling in arbitrary dimensions for systems

Strong Szegö limit theorem 17

$b(\theta) \geq \varepsilon > 0$ smooth on S^1

$$P_n = \sum_{|k| \leq n} e^{ik\theta} (\cdot, e^{ik\theta})$$

B = mpl. by b in $L^2(S^1)$

Then

$$\underbrace{\log \det P_n B P_n}_{= \mathrm{Tr} \log P_n B P_n} = (2n+1) \int_0^{2\pi} \overbrace{\log b(\theta) \frac{d\theta}{2\pi}}^{\mathrm{Tr}\, P_n \log B\, P_n}$$

$$+ \sum_{k=1}^{\infty} k \underbrace{\widehat{(\log b)}_k \widehat{(\log b)}_{-k}}_{\text{corr.}}$$

$$+ o(1), \quad n \to \infty$$

Widom's conj.:

$$\mathrm{Tr}\, f(PQP) = \mathrm{Tr}\, P f(Q) P$$

$$+ \text{corr.}, \quad \lambda \to \infty$$

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corr.

Widom's conj.:

$$\operatorname{Tr} f(PQP) = \operatorname{Tr} Pf(Q)P + \text{corr.}, \quad \lambda \to \infty$$

$B \sim (\; b_0 \; \hat{b}_0 \ldots$

17

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$f(P_nBP_n)$

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13

Widom's Conjecture

f analytic on $\{z \mid |z| < R\}$, $R > 1$

$f(0) = 0$

$$\Rightarrow \operatorname{Tr} f(PQP) = \frac{L^D}{(2\pi)^D} f(1) \cdot \iint_{\Omega\,\Gamma} dx\, d\xi$$

$$+ \left(\frac{L}{2\pi}\right)^{D-1} \frac{\ln L}{4\pi^2} U \quad \int |n_x \ldots$$

$f = t(1-t) \leftarrow$

$$+ o(L^{D-1} \ln L)$$

where

$$U(f) = \ldots$$

Landau

Widom '...

Widom '8...

G. '02

$D \geq 2$, ...

Widom's Conjecture

13

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$f = t(1-t)$

$$+ o(L^{D-1} \ln L), \quad L \to \infty,$$

where

$$U(f) = \int_0^1 \frac{f(t) - t f(1)}{t(1-t)} dt .$$

Landau

Widom '80 $D=1$

Widom '82, $-D=1$ '90 $- D \geq 2$, half space + compact

G. '02 math. FA/0212215

$D \geq 2$, one term w. sharp rem. + fractal bdaries

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$$f(P_n B P_n) \quad + o(1), \quad n \to \infty$$

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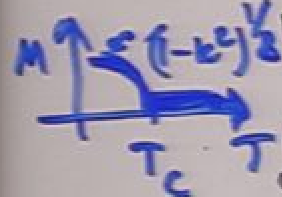
Onsager's comput. of spont. magnetiz. in 2D Ising model

$$Z = \sum_{\sigma=\pm 1} \prod_{n.n.} e^{K_1 \sigma_{\alpha,\beta}\sigma_{\alpha,\beta+1} + K_2 \sigma_{\alpha,\beta}\sigma_{\alpha+1,\beta}}$$

$$k = \left(\sinh \frac{2}{k K_1 T} \sinh \frac{2}{k K_2 T}\right)^{-1}$$

$$M^2 = \lim_{m \to \infty} \langle \sigma_{1,1}, \sigma_{1,1+m} \rangle$$



↑ Toepl. det. !

$\int \log b \, d\theta = 0!$

need subl. term exactly as in our case

$h(1) = 0$

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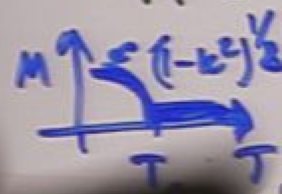

$$\int \log b \, d\theta = 0!$$

~~need suff. term~~ 17

~~strong Szegö limit theorem~~

~~exactly as in our case~~

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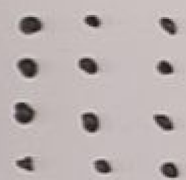

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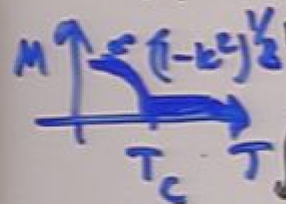

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