Shell-Filling Effect in the Entanglement Entropies of Spinful Fermions

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1. Ground state entanglement in 1+1 dim CFTs

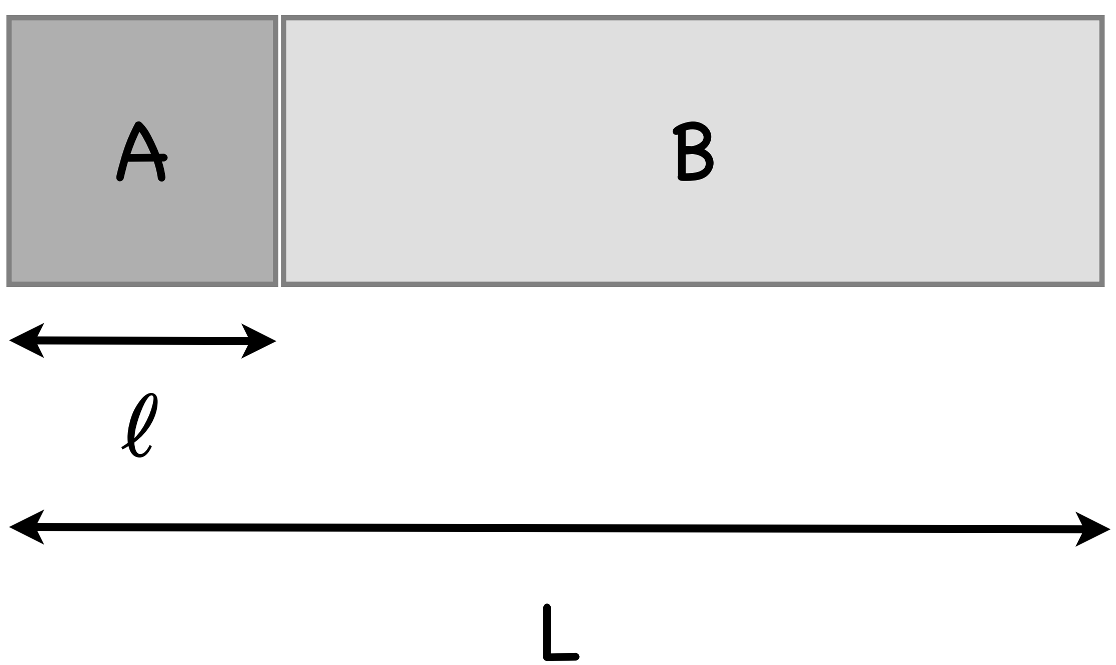
Calabrese&Cardy '04

Renyi:

$$S_n = \frac{c}{6}\left(1+\frac{1}{n}\right)\ln\left(\frac{L}{\pi}\sin\frac{\pi\ell}{L}\right) + c'_n + o(1)$$

von Neumann:

$$S_1 = \frac{c}{3}\ln\left(\frac{L}{\pi}\sin\frac{\pi\ell}{L}\right) + c'_1$$



$S_1 = -\mathrm{Tr}[\rho_A \ln(\rho_A)]$

$S_n = \ln(\mathrm{Tr}[(\rho_A)^n])/(1-n)$

OftP or ToS?

It's **useful** for finding QPTs!

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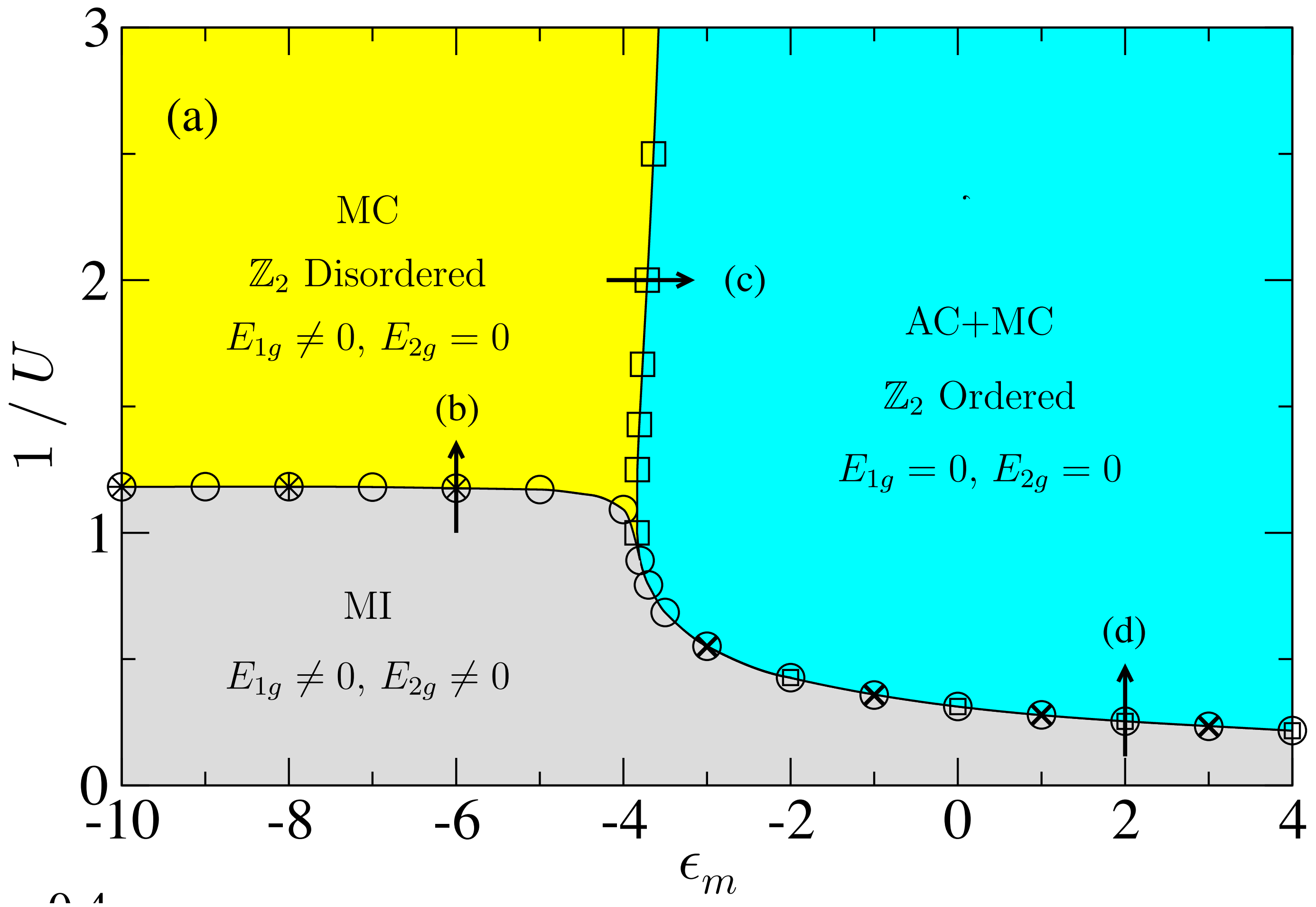
H_2O

2-component Bose-Hubbard-Feshbach problem

Ejima, Bhaseen, Essler et al '11

$$H = \sum_{i\alpha} \epsilon_\alpha n_{i\alpha} - \sum_i \sum_\alpha t_\alpha \left(b^\dagger_{i\alpha} b_{i+1\alpha} + \text{H.c.} \right) + \sum_{i\alpha\alpha'} \frac{U_{\alpha\alpha'}}{2} n_{i\alpha}(n_{i\alpha'} - \delta_{\alpha\alpha'}) + g \sum_i (m^\dagger_i a_i a_i + \text{H.c.}),$$

- bosonic atoms and molecules hopping on a 1D lattice
- repel when on the same site with U_{aa} ,U_{mm}, U_{am}
- Feshbach conversion term: 2 atoms ↔ 1 molecule



$$\epsilon_a = 0,\ U_{aa}/2 = U_{mm}/2 = U_{am} = g = U,$$

$$t_a = 1,\ t_m = 1/2,$$

2 particles per site

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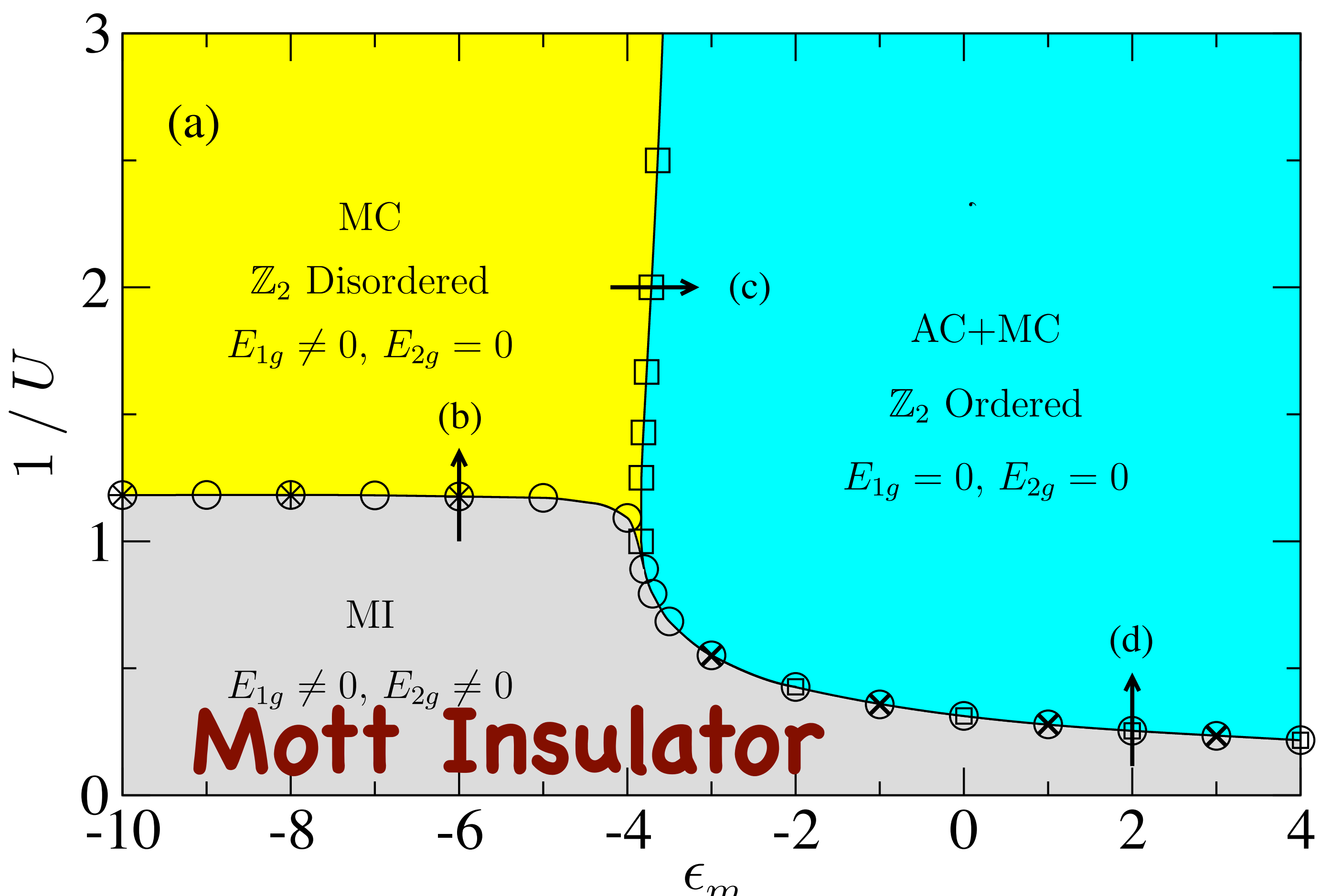

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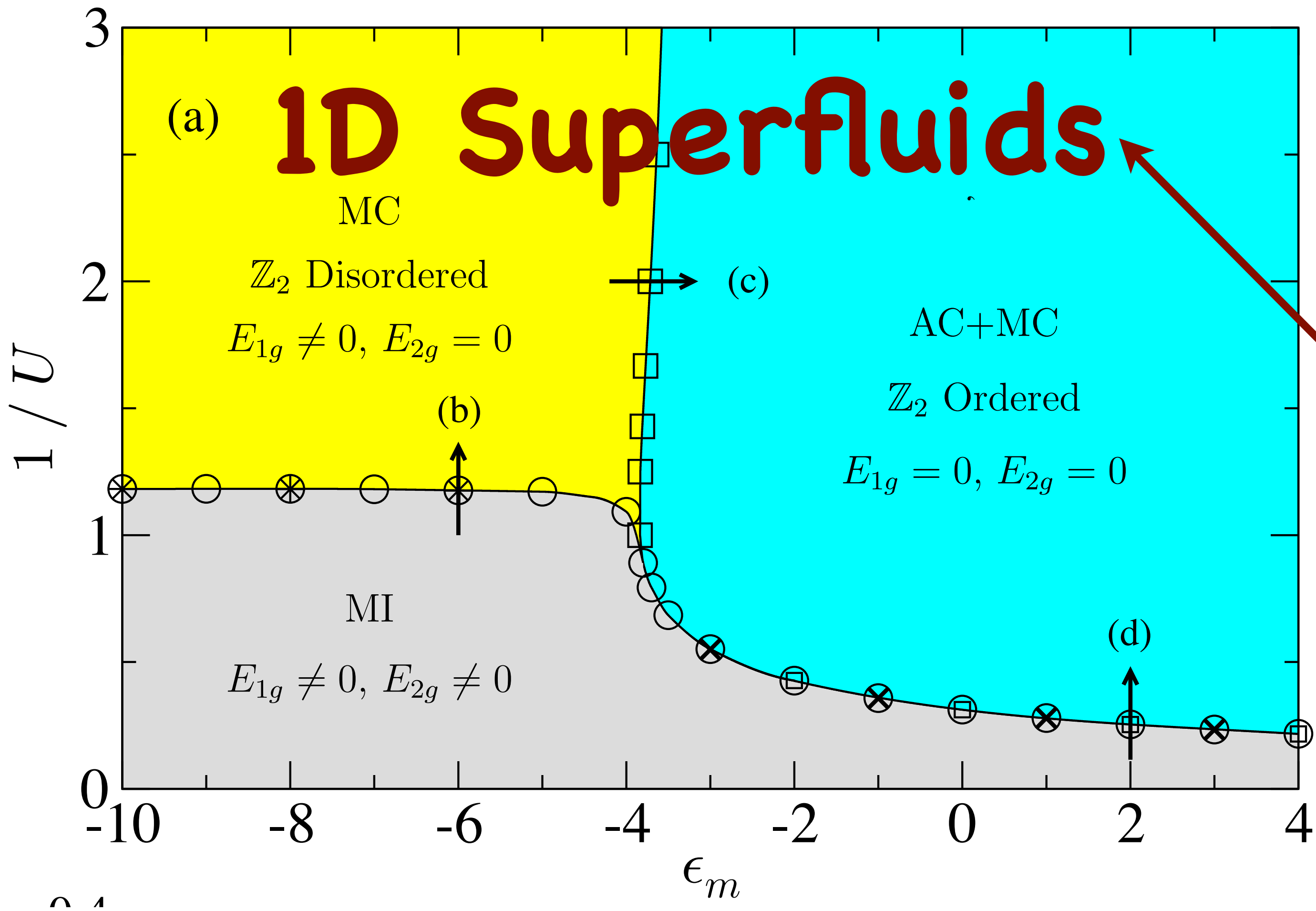

$$\epsilon_a = 0,\ U_{aa}/2 = U_{mm}/2 = U_{am} = g = U,$$

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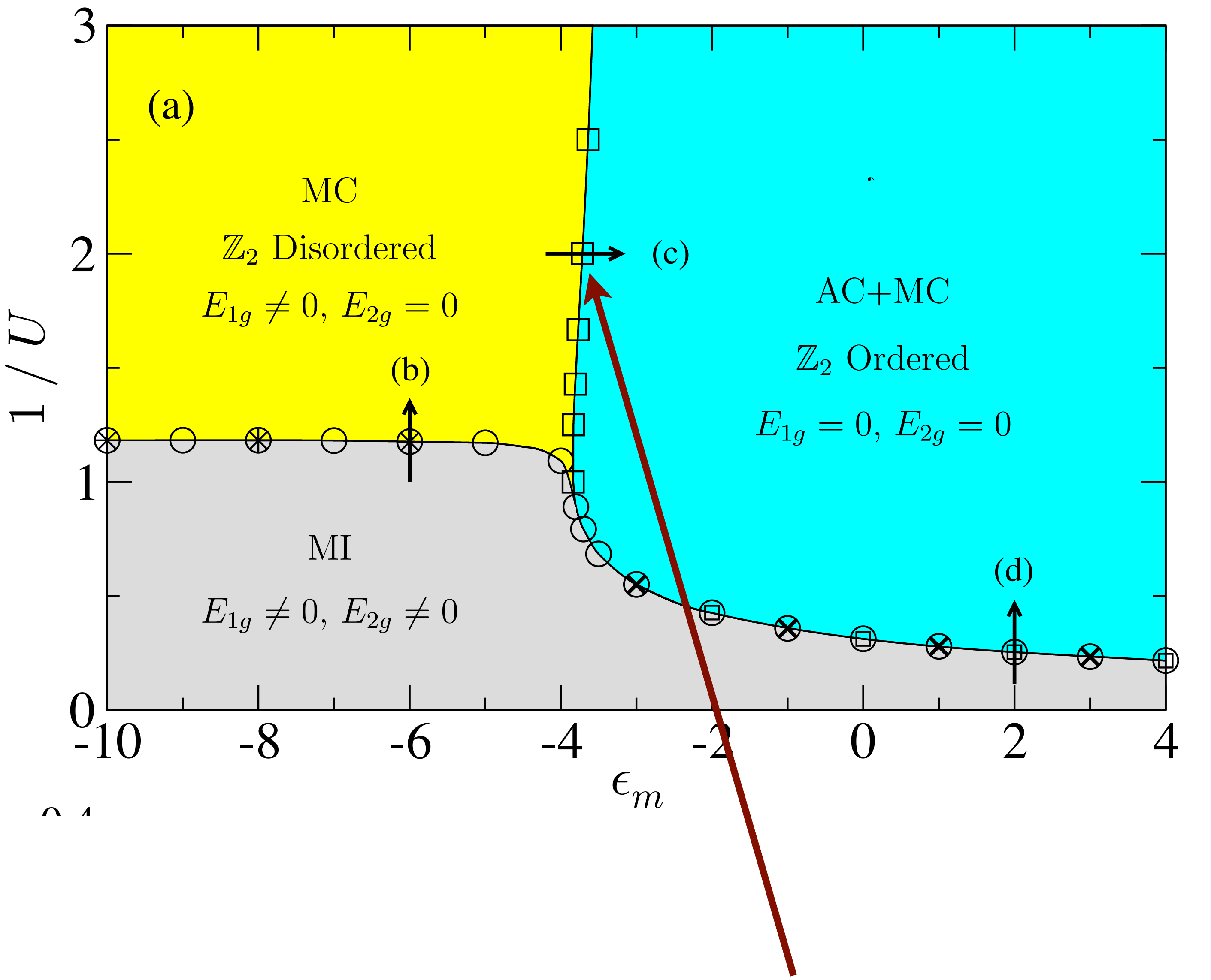
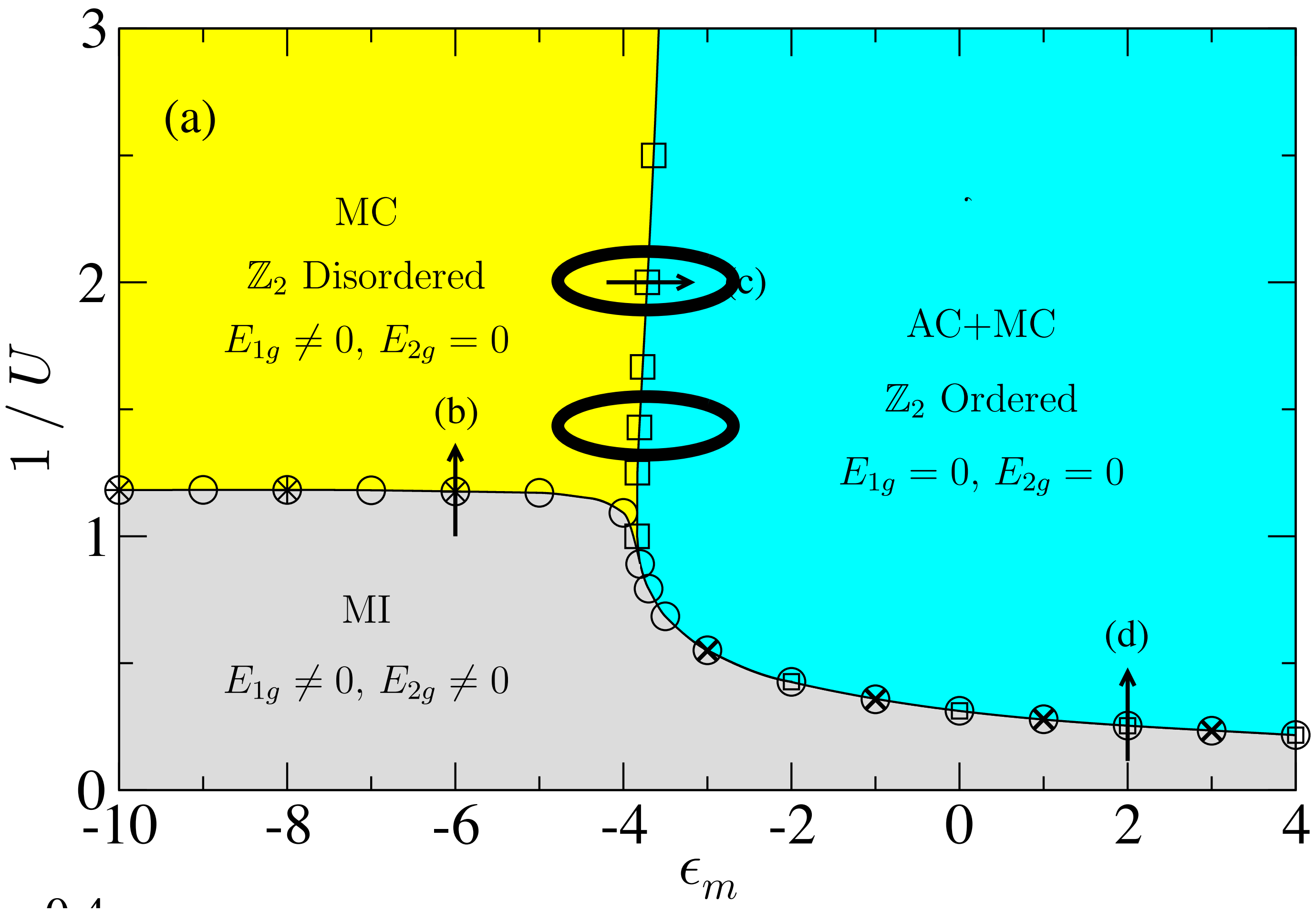
c=1 CFT
(attractive Luttinger Liquids)

2-component Bose-Hubbard-Feshbach problem

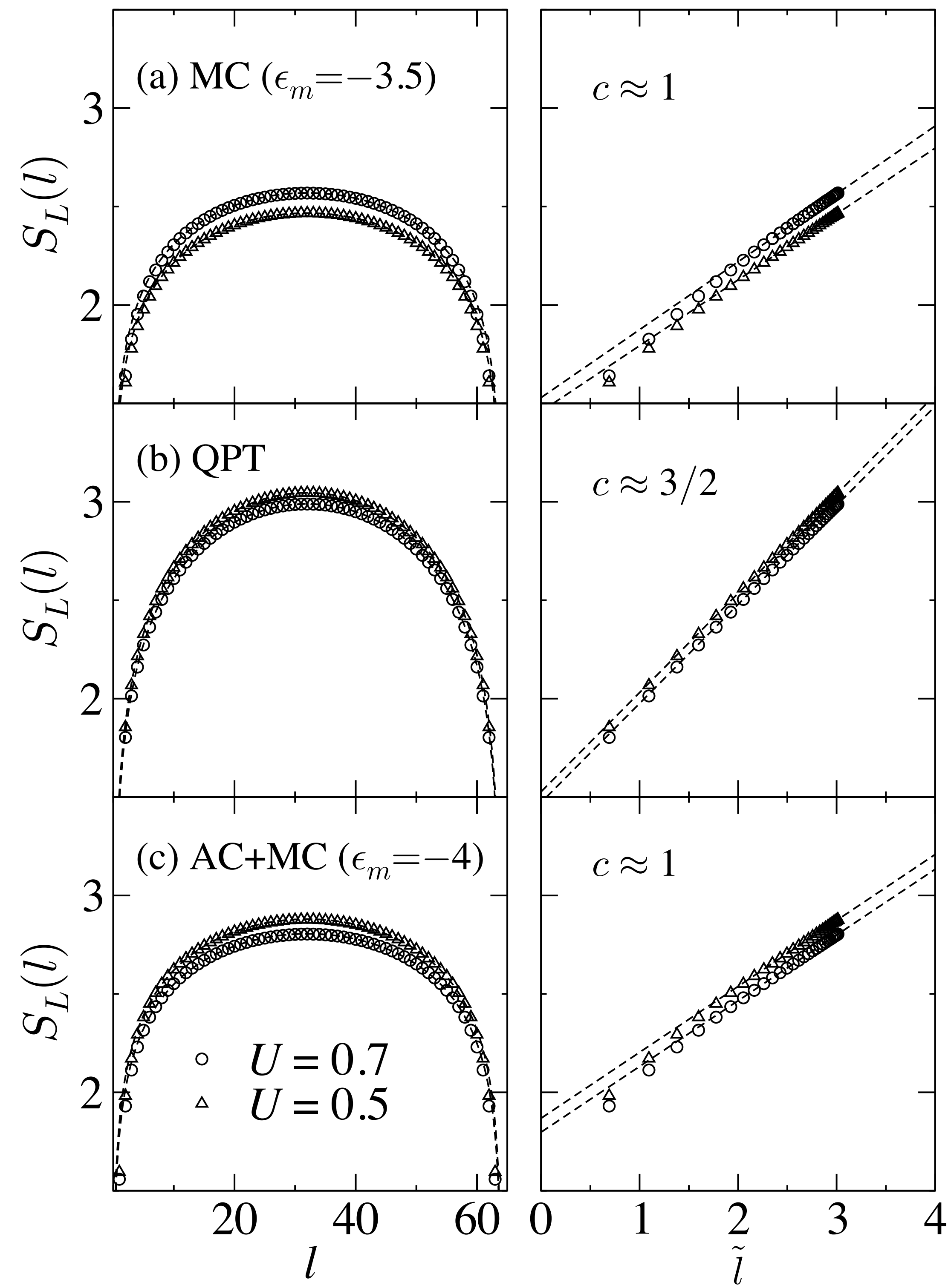


Transition between two c=1 CFTs!
What is the critical line ???

2-component Bose-Hubbard-Feshbach problem



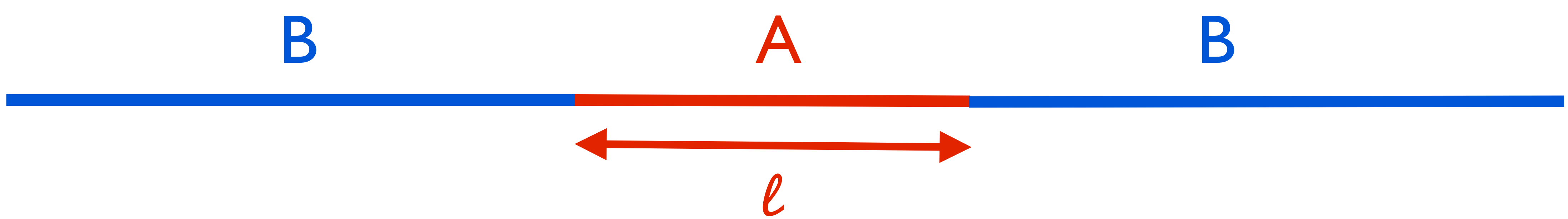
von Neumann entropies:



Ising transition **on top** of a Luttinger Liquid !

2. Excited State Entanglement in 1+1 dim CFTs

Alcaraz, Berganza& Sierra '11



But now consider the system in an **excited state:** $\mathcal{O}(0,0)|0\rangle$

$\mathcal{O}(z,\bar{z})$ a primary field $\quad z = \exp\left(\frac{2\pi}{La_0}(vt - ix)\right)$

ground state

$$S_n = \frac{c}{6}\left(1+\frac{1}{n}\right)\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] + c'_n + \frac{1}{1-n}\ln\left[F_n(\ell/L)\right] + o(L),$$

$$F_n(x) = \frac{\langle \prod_{k=0}^{n-1} \mathcal{O}\left(\frac{\pi}{n}(x+2k)\right)\mathcal{O}^\dagger\left(\frac{\pi}{n}(-x+2k)\right)\rangle}{n^{2n(h+\bar{h})}\langle \mathcal{O}(\pi x)\mathcal{O}^\dagger(-\pi x)\rangle^n}\ .$$

evaluated on a cylinder

CFT results are **useful** for understanding critical properties of **lattice models** with quantum phase transitions.

But there are interesting caveats....

3. 1D Hubbard model (periodic bcs)

$$H_{\mathrm{Hubb}} = -t\sum_{j=1}^{L}\sum_{\sigma} c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + \mathrm{h.c.} + U\sum_{j} n_{j,\uparrow}\, n_{j,\downarrow},$$

1D Hubbard Model

Crucial Paradigm for Mott Metal-Insulator transition at half-filling

Low-energy theory below half-filling: two c=1 Luttinger liquids

$$H = \sum_{\mathrm{a}=c,s}\frac{v_{\mathrm{a}}}{2}\int dx\,\left[(\partial_x\Phi_{\mathrm{a}})^2 + (\partial_x\Theta_{\mathrm{a}})^2\right],$$

spin/charge velocities

Bose fields

dual fields

$$\left[\Phi_{\alpha}(x), \frac{\partial\Theta_{\beta}(y)}{\partial y}\right] = i\pi\delta_{\alpha\beta}\delta(x-y).$$

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$$H = \sum_{\mathrm{a}=c,s} \frac{v_{\mathrm{a}}}{2}\int dx\,\left[(\partial_x\Phi_{\mathrm{a}})^2 + (\partial_x\Theta_{\mathrm{a}})^2\right],$$

- Different velocities (not Lorentz invariant)
- Local operators particular combinations of spin/charge fields
- irrelevant perturbations (spin and charge coupled)

for **ground state:** $$S_1 = \frac{c}{3}\ln\left(\frac{L}{\pi}\sin\frac{\pi\ell}{L}\right) + c'_1$$ with c=2?

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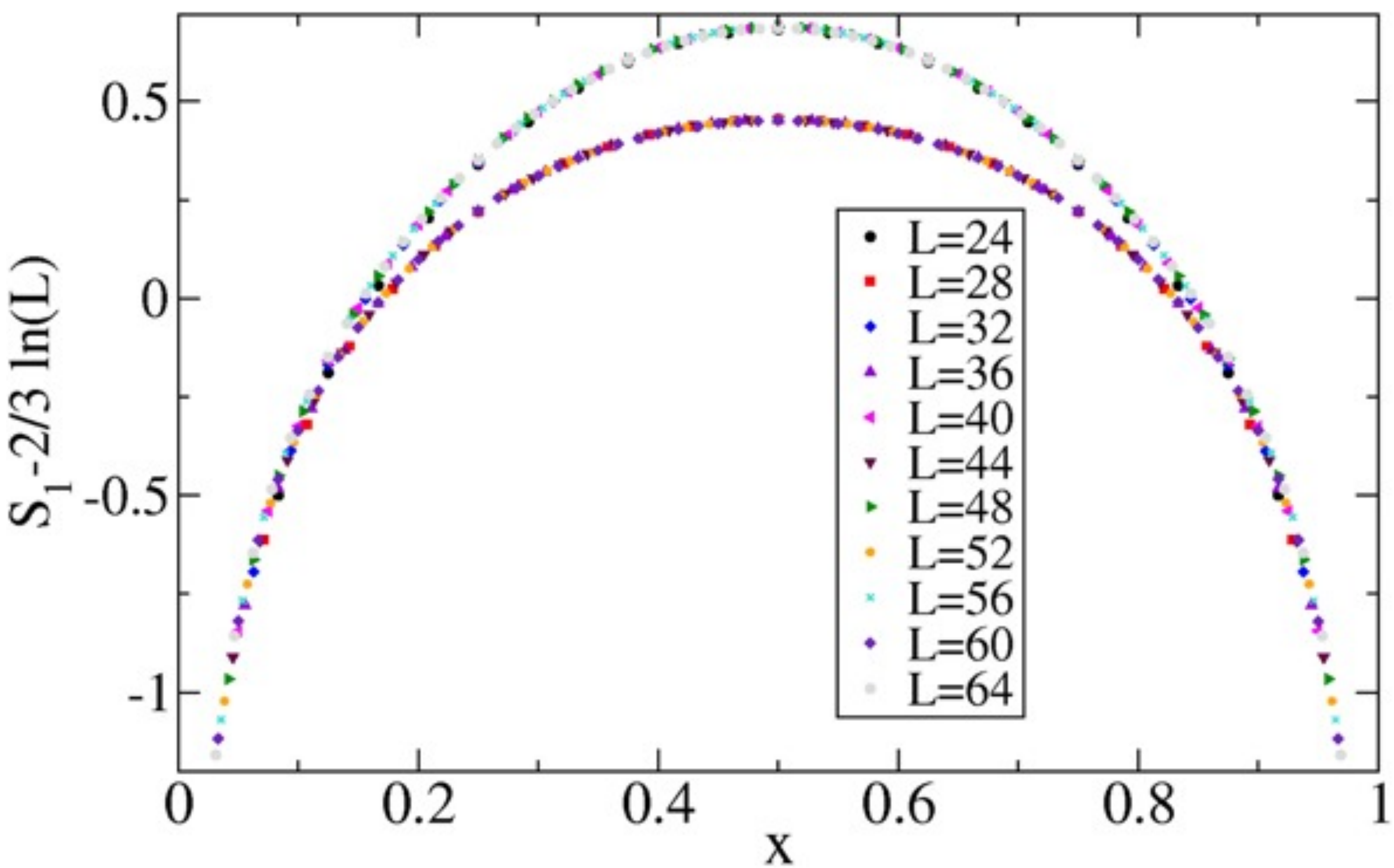


U=t

quarter filling

$x = \ell / L$

scaling collapse on **two curves:** L=0 mod 8 and L=4 mod 8

???

L=4 mod 8: Lieb&Wu '68 unique ground state from Bethe Ansatz

→ entropy agrees well with CFT prediction

L=0 mod 8: Essler, Korepin, Schoutens '91

ground state **degenerate** S=1 multiplet.

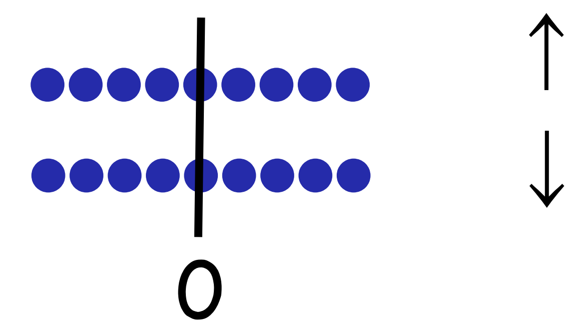
→ entropy disagrees with CFT prediction

To see what is going on, consider U→0 limit:

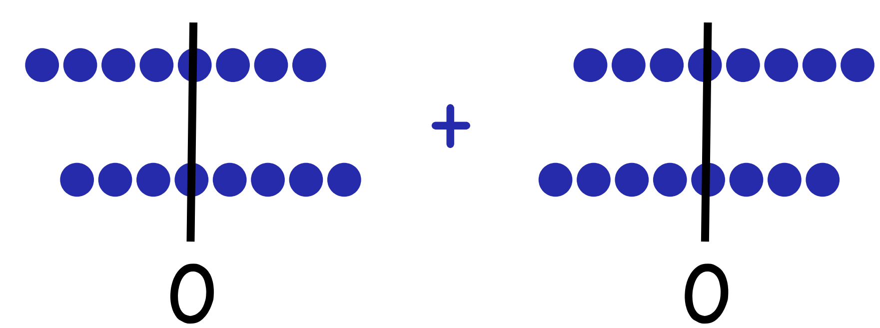
L=4 mod 8: $N_\uparrow = N_\downarrow =$ odd$=2n+1$

$p_m = 2\pi m/L$ GS is a symmetrically filled Fermi sea

$$|2n+1\rangle_{\rm FS} = \prod_{m=-n}^{n} c_\uparrow^\dagger(p_m) c_\downarrow^\dagger(p_m)|0\rangle$$



L=0 mod 8: $N_\uparrow = N_\downarrow =$ even$=2n$ U→0 GS is a superposition of asymmetrically filled Fermi seas

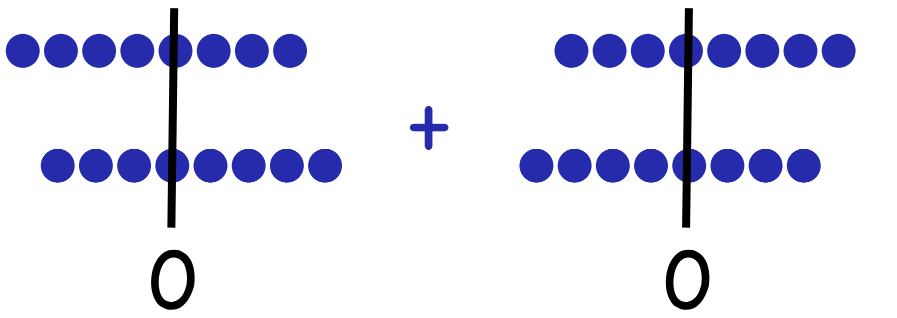


$$\frac{c_\uparrow^\dagger(k_F)c_\downarrow^\dagger(-k_F) + c_\downarrow^\dagger(k_F)c_\uparrow^\dagger(-k_F)}{\sqrt{2}}|2n-1\rangle_{\rm FS}$$

L=0 mod 8:

$N_\uparrow = N_\downarrow =$ even

$U \rightarrow 0$ GS is a superposition of asymmetrically filled Fermi seas



Intuitively higher entropy, because $P_\uparrow - P_\downarrow$ not fixed, but can take 2 values.

4. CFT Approach to Shell-Filling Effects

Bethe Ansatz & Bosonization:

$$H = \sum_{a=c,s} \frac{v_a}{2} \int dx \left[(\partial_x \Phi_a)^2 + (\partial_x \Theta_a)^2 \right]$$

Chiral Fields:

$$\Theta_a = \varphi_a - \bar{\varphi}_a$$

$$\Phi_a = \varphi_a + \bar{\varphi}_a$$

Mode expansions:

$$\bar{\varphi}_a(x,t) = \bar{P}_a + \frac{x_+}{La_0}\bar{Q}_a + \sum_{n=1}^{\infty} \frac{e^{-i\frac{2\pi n}{La_0}x_+}\bar{a}_{a,n} + \text{h.c.}}{\sqrt{4\pi n}}$$

$$\varphi_a(x,t) = P_a + \frac{x_-}{La_0}Q_a + \sum_{n=1}^{\infty} \frac{e^{i\frac{2\pi n}{La_0}x_-}a_{a,n} + \text{h.c.}}{\sqrt{4\pi n}},$$

$x_\pm = x \pm v_a t$

Zero modes: $[P_a, Q_a] = -\frac{i}{2} = -[\bar{P}_a, \bar{Q}_a]$

$$H = \sum_{a=c,s} \frac{v_a}{La_0} \left[Q_a^2 + \bar{Q}_a^2 + \sum_{n=1}^{\infty} 2\pi n (a^\dagger_{a,n} a_{a,n} + \bar{a}^\dagger_{a,n} \bar{a}_{a,n}) \right]$$

Difference between L=4 mod 8 and L=0 mod 8 is in quantization conditions for Q_a, $\overline{Q}_a$

L=4 mod 8:

eigenvalues of Q_a

$$q_c = \sum_{\sigma=\uparrow,\downarrow} \frac{K+1}{\sqrt{8K}} m_\sigma + \frac{K-1}{\sqrt{8K}} \bar{m}_\sigma$$

$$\bar{q}_c = \sum_{\sigma=\uparrow,\downarrow} \frac{K-1}{\sqrt{8K}} m_\sigma + \frac{K+1}{\sqrt{8K}} \bar{m}_\sigma$$

$$q_s = \frac{m_\uparrow - m_\downarrow}{\sqrt{2}} \qquad \bar{q}_s = \frac{\bar{m}_\uparrow - \bar{m}_\downarrow}{\sqrt{2}}$$

m_σ, $\bar{m}_\sigma$ integers

K_c Luttinger parameter (compactification radius)

Ground state: $|0,0,0,0\rangle$ (CFT vacuum)

notations: $|m_\uparrow, m_\downarrow; \bar{m}_\uparrow, \bar{m}_\downarrow\rangle$ annihilated by $a_{a,n}$, $\bar{a}_{a,n}$

zero-mode eigenvalues $q_a(m_\sigma, \bar{m}_\sigma)$ and $\bar{q}_a(m_\sigma, \bar{m}_\sigma)$

L=0 mod 8:

$m_\sigma \to m_\sigma + 1/2$

$\bar{m}_\sigma \to \bar{m}_\sigma + 1/2$

S^z=0 ground states:

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left[|1,0;0,1\rangle \pm |0,1;1,0\rangle\right]$$

N.B. Degeneracy between spin singlet and triplet is an artifact of CFT limit: broken by marginally irrelevant perturbation in the Hubbard model.

Can write our state of interest as $$|+\rangle \propto \lim_{z,\bar{z}\to 0} \cos\left(\sqrt{2\pi}\Phi_s(z,\bar{z})\right)|0\rangle$$

Not an excited state in our compact boson theory.

Nonetheless can apply method of Alcaraz, Berganza & Sierra (PRL '11) to determine **Renyi** entropies.

5. Results

1. Renyi Entropies

$$S_n = \frac{c}{6}(1+\frac{1}{n}) \ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] + c'_n + \frac{1}{1-n}\ln\left[F_n(\ell/L)\right] + o(1)$$

c=2

$$[F_n(x)]^2 = \prod_{p=1}^{n}\left[1 - \frac{(n-2p+1)^2}{n^2}\sin^2(\pi x)\right] = \left[\left[\frac{2\sin(\pi x)}{n}\right]^n \frac{\Gamma\left(\frac{1+n+n\csc(\pi x)}{2}\right)}{\Gamma\left(\frac{1-n+n\csc(\pi x)}{2}\right)}\right]^2$$

2. von Neumann Entropy

by "analytic continuation" n→1

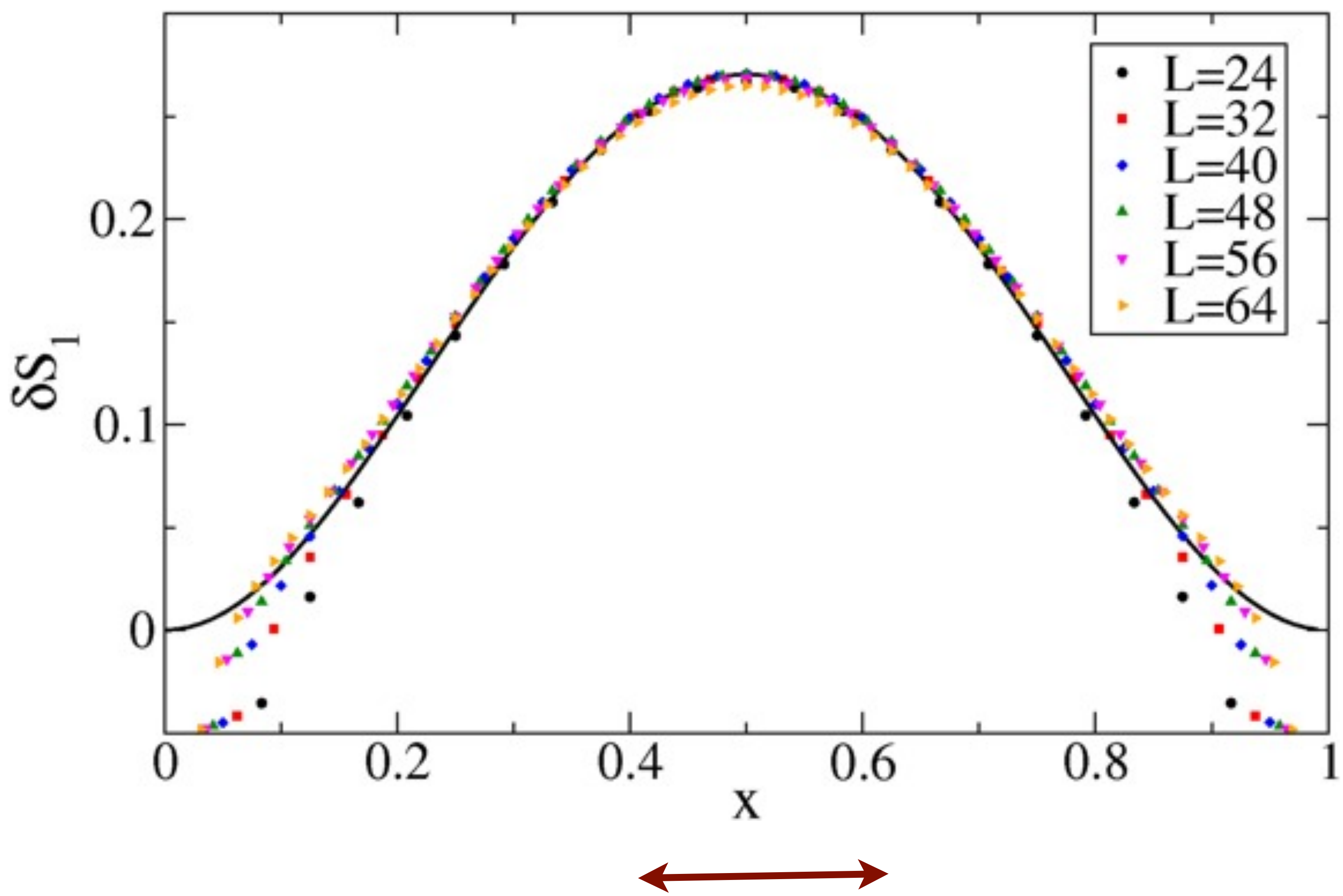
$$S_1 = \frac{c}{3}\ln\left[\frac{L}{\pi}\sin\frac{\pi\ell}{L}\right] + c'_1 - F'_1(\ell/L) + o(1)$$

$$F'_1(x) = \ln|2\sin(\pi x)| + \psi\left(\frac{1}{2\sin(\pi x)}\right) + \sin(\pi x).$$

Comparison with numerics (DMRG)

$$\delta S_1 \equiv S_1 - \frac{2}{3}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] - c_1'$$

for U=0.3t



good!

regime where CFT is expected to hold

Comparison with numerics (DMRG)

But agreement gets **worse** for **larger** U!

???

Hubbard model is perturbed CFT and
leading operator is only marginally irrelevant.

$$H = \sum_{a=c,s} \frac{v_a}{2} \int dx \left[(\partial_x \Phi_a)^2 + (\partial_x \Theta_a)^2 \right] + g \int dx \left[\frac{2}{\pi a_0} \cos\left(\sqrt{8\pi}\Phi_s\right) + \left(\partial_x \Theta_s\right)^2 - \left(\partial_x \Phi_s\right)^2 \right]$$

CFT | Perturbation

g flows to zero for $\ell \to \infty$, but DMRG data only for "small" ℓ

Difficult problem (RG improved PT on multi-sheeted Riemann surface).

cf Cardy&Calabrese '10 (ground state)

$$H = \sum_{a=c,s} \frac{v_a}{2} \int dx \left[(\partial_x \Phi_a)^2 + (\partial_x \Theta_a)^2\right] + g \int dx \left[\frac{2}{\pi a_0} \cos\left(\sqrt{8\pi}\Phi_s\right) + \left(\partial_x \Theta_s\right)^2 - \left(\partial_x \Phi_s\right)^2\right]$$

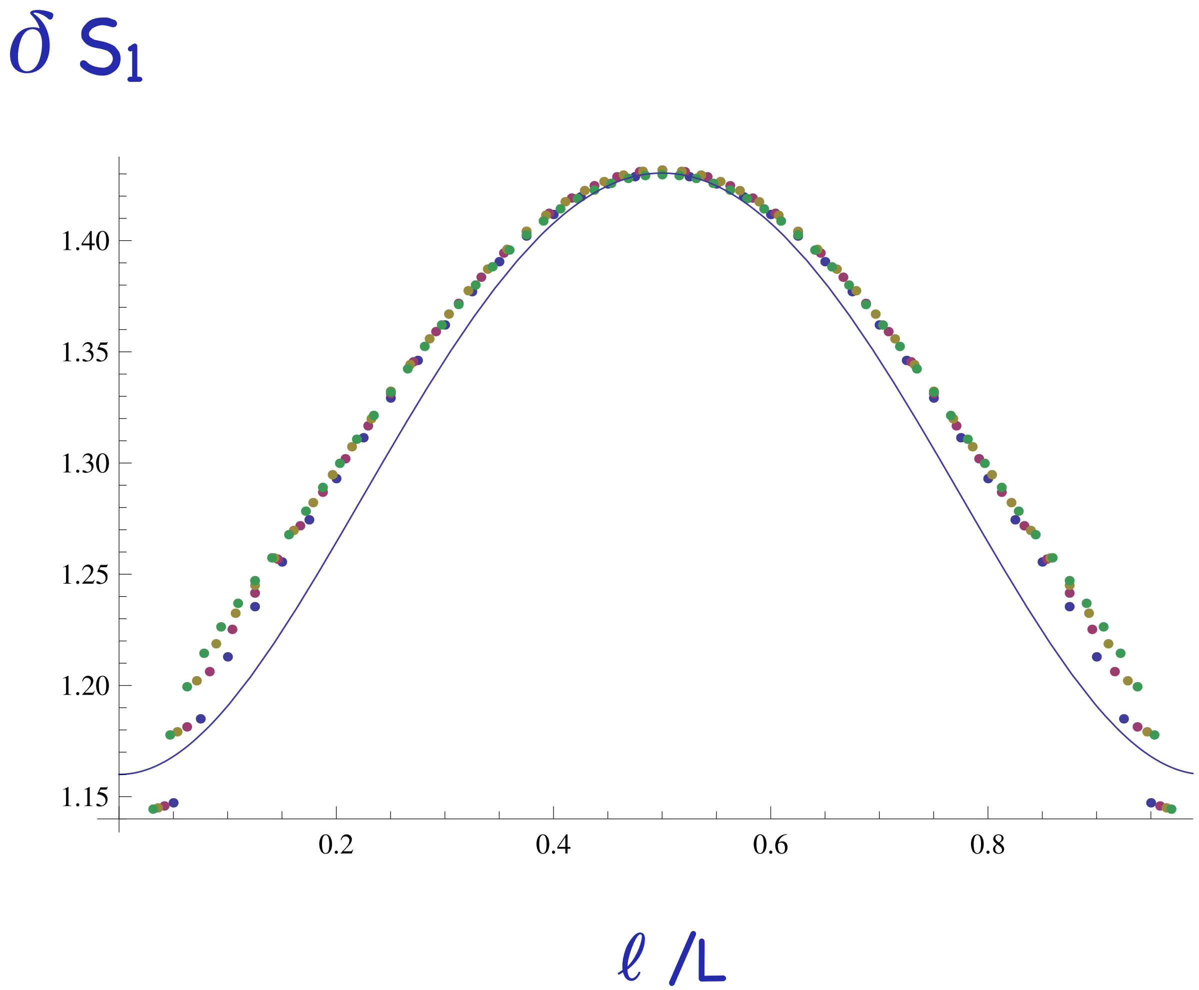
CFT

Perturbation

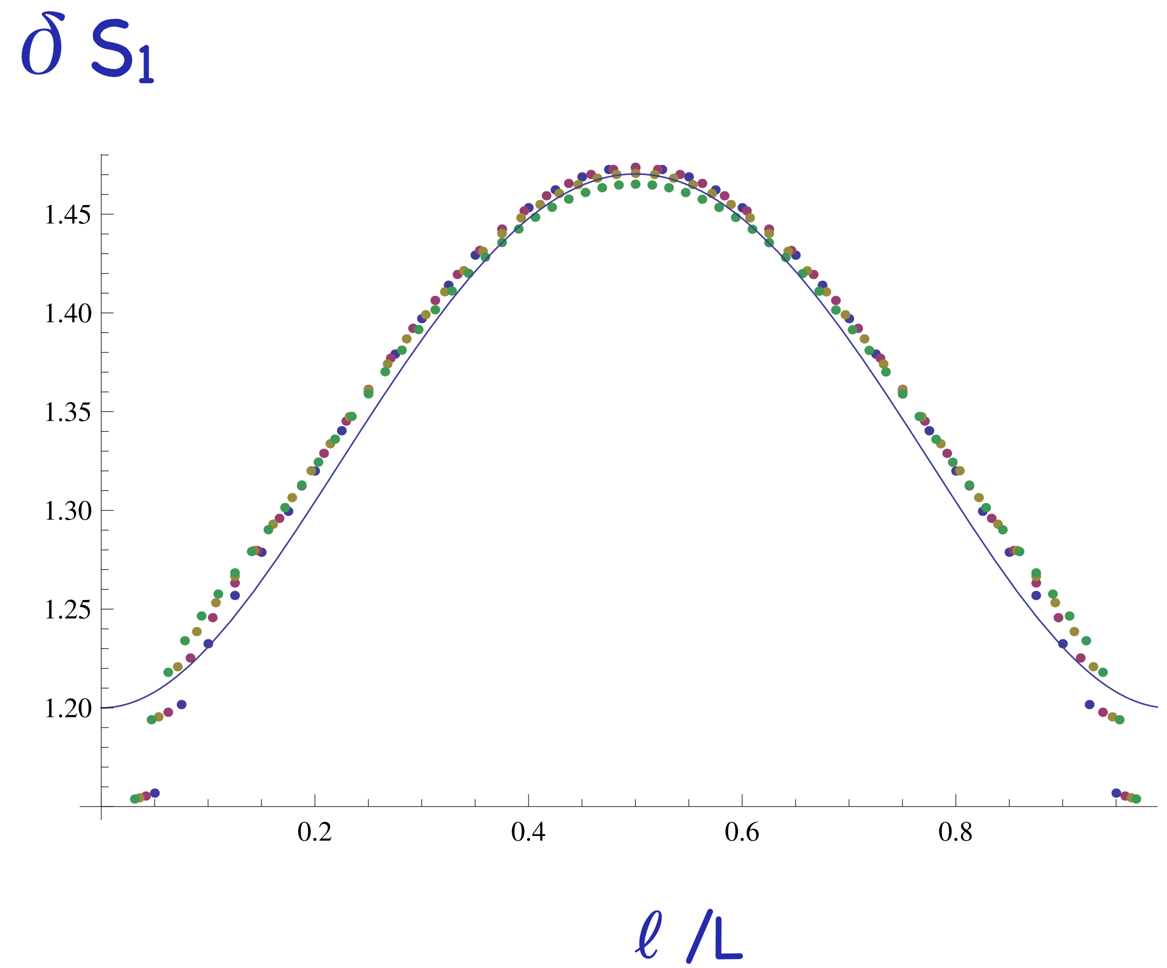
Idea: change lattice Hamiltonian to make **bare** coupling g small

$$H_{\text{ext}} = H_{\text{Hubb}} + V_2 \sum_{j,\sigma,\sigma'} n_{j,\sigma} n_{j+2,\sigma'}.$$

increasing V_2 decreases g (difficult to make g=0 because of **KT transition** when g changes sign)



$U=2t,\ V_2=0$



$U=2t,\ V_2=0.5$

Agreement improves !!!

6. Conclusions

- Have found a new O(1) effect for ground state entanglement entropies.
- Effect is actually rather general. Will occur in multi-species theories in any dimension etc.
- **Important for interpreting numerical studies.**
- For 1+1 dim quantum critical models we have developed a CFT approach.
- Using results of Alcaraz et al obtained **exact scaling functions**.
- Observed **very strong effects** of marginally irrelevant perturbation. (cf corrections to excited state **energies**)