Entanglement of Correlated electron states: Metal-Insulator Crossover scaling form

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Plan:

1. **Many electron/spin Correlations**

2. **How entangled is a Spin/Electron state**

3. **Entanglement hierarchy in Many-electron states:**
   Diagonal/off-diagonal correlations and Electron double occupancy
   Metallic, Strongly-correlated, Superconducting states

4. **Multi-species entanglement: Quantum phase transitions**

5. **Block entanglement entropy of Correlated state**
   Area law, logarithmic correction, entanglement spectrum
   Scaling form for entanglement for metal-insulator crossover Metal-insulator Transitions in nano-chains of Ni

Many-Qubit/ Many-Electron States: 4 states/site, $\langle n_{i\uparrow} n_{j\uparrow} \rangle$, $\langle n_{i\uparrow} n_{j\downarrow} \rangle$

A fixed number of sites, up spins, down spins

Distinct Labeled Sptial Part

Strongly-Correlated States: No Double Occupancy, 3 States/site, On-site Spin Correlations

Spin-Only States: No holes either, Two states/site, Qubits $\langle S_i^z \rangle, \langle S_i^z S_j^z \rangle, \langle S_i^+ S_j^- \rangle$

$$\Gamma_{ij} \approx m^2 + \frac{A}{r^p} + B e^{-\frac{r}{\xi}}$$

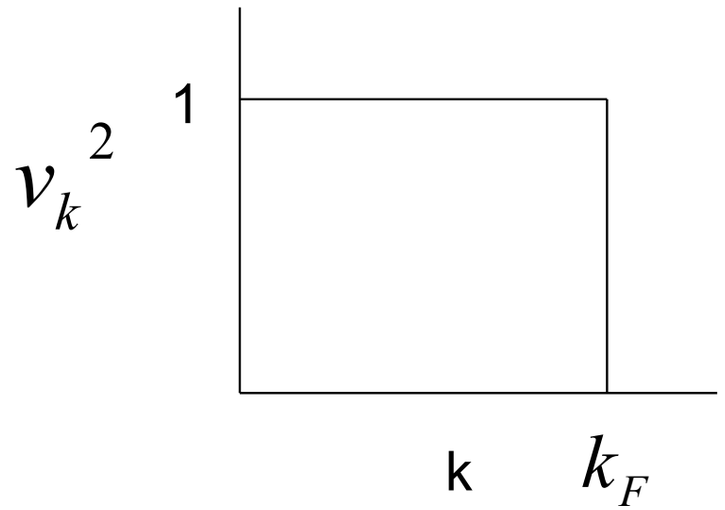
Diagonal LRO: Constant m nonzero, Similarly ODLRO

Long-ranged Correlations: A Nonzero

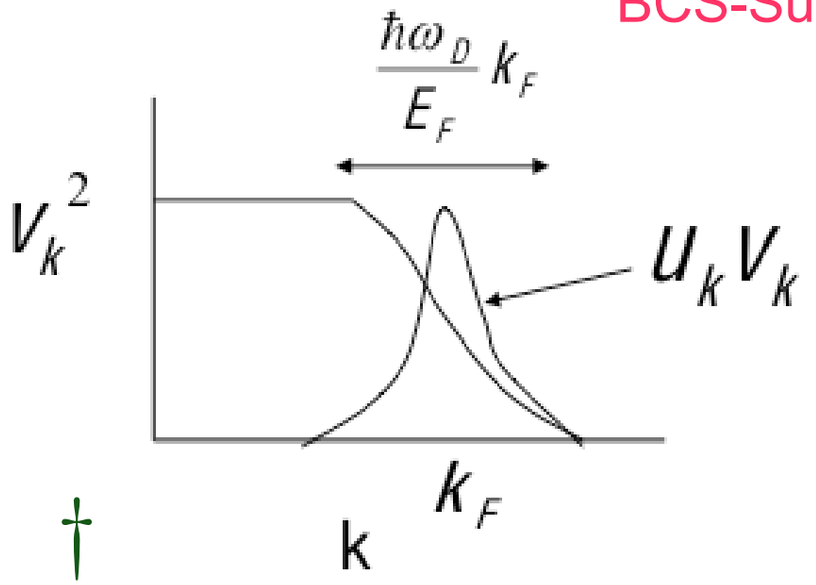
Question: Which type of states exhibit more Entanglement?

Many-eletcron State: $|\psi\rangle = \Pi_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|0\rangle$

Metallic/Uncorrelated



BCS-Superconductor



$$\nu_k^2 = \frac{1}{2}\left(1 - \frac{\epsilon_k - E_F}{\sqrt{(\epsilon_k - E_F)^2 + \Delta_k^2}}\right)$$

In the above range $\Delta_k = \Delta_0$

$$d = \frac{n^2}{4}(1+\zeta^2)$$

Double Occupancy

$$\frac{n}{2}\zeta \equiv |\langle c_{i\uparrow} c_{i\downarrow}\rangle| \approx \frac{3\Delta_0}{2E_F}\sinh^{-1}\frac{\hbar\omega_D}{\Delta_0}$$

Order Parameter

Strongly-Correlated electron state: Gutzwiller Projection, Inhibit double occupancy

Start from a metallic 'Uncorrelated' State

$$|\psi_g\rangle = \Pi_i \left(1-(1-g)n_{i\uparrow}n_{i\downarrow}\right)|F\rangle$$

$$d(g) \le \frac{n^2}{4}$$

Projection operator for the site Hilbert Space:

g=0 states with Doubly-occupied sites are projected out.

g=1 No Correlation, Metallic State, U=0: $d = n_\uparrow n_\downarrow$

g=0 Strong Correlation U=infinity : $d = 0$

1-D $$d(g) = \tfrac{1}{2}\frac{g^2}{(1-g^2)^2}(ng^2 - n - \ln[1-n-ng^2]) \qquad n \le 1$$

Metzner and Vollhardt (1988)

$$g \log g = -\frac{4t}{\pi U}$$

Fermi Liquid for nonzero g

$$Z(g) = \frac{4g}{(1+g)^2}$$

How Entangled Is a Spin State?

$|\psi(N, N_\uparrow, N_\downarrow)\rangle$

One-Qubit Reduced ρ_i

Ave. Site purity
Global Ent.

$$\varepsilon(\psi) = \frac{2}{N} \Sigma\, 1 - Tr\, \rho_i^2$$

Larger in a State implies better sharing of Ent.

Two-Qubit Reduced ρ_{ij}

$$E_{ij} = -Tr\, \rho_{ij} \ln \rho_{ij}$$

Entropy of the block
Ent. Between ij and rest

$$C_{ij}\ from\ [\rho_{ij}\ \rho_{ij}^T]$$

Concurrence of sites i and j
Bipartite entanglement

$$C_{ave} = \langle C_{ij} \rangle$$

$$\varepsilon = 1 - 4m^2$$

$$\frac{1}{2} C_{ij} = |\Gamma_{off-diag}| - \sqrt{\left(\frac{1}{4} + \Gamma_{diag}\right)^2 - m^2}$$

Diag. Correlations Decrease Ent.

* Off-diag correlations should dominate for a nonzero Concurrence!

* Ferromagnetic ordering (poor superposition) does not support much entanglement due to Dominant diag. correlations and a large magnetization

* Quantum Antiferromanetic ordering can support enanglement: Concurrence Nonzero only for two sites belonging to different sublattices!

Heisenberg Antiferromagnet GS: S=0 Spatially Uniform

$C_{ij}=0\,,\quad if\quad \Gamma_{diag}>0$ i,j belong to same sublattice

$=6(|\Gamma_{diag}|-\frac{1}{12})$ If Positive

$1-D\ \ Chain\quad C_{1,2}=0.398,\quad C_{1,l}=0\ \ l>2\quad C_{ave}=\frac{0.796}{N-1}$

$2-D\ \ Square\quad C_{1,2}=0.16,\quad C_{1,l}=0\ \ l>2\quad C_{ave}=\frac{0.64}{N-1}$

Kagome and Triangular: $C_{ij}=0$ No pair concurrences!

Dimer State:  $C_{ave}=\frac{1}{N-1}$

Average Site Mixedness $\varepsilon=1$ for all lattices!

How Entangled are Many-Electron States?

$$|\psi\rangle = \sum_{\{A_i, B_i\}} \varphi(A_1, B_1 .... A_N, B_N) | A_1, B_1 .... A_N, B_N \rangle$$

Occupancy of Up Spin at site 1

Now 4^N Numbers to Specify State

Metallic State: No spin correlations, Optimal Double Occupancy

Strong correlation: Double occupancy inhibited, Diagonal Correlations

Superconducting State: Double occupancy encouraged, Off-diagonal correlations

ρ_i : Global Entanglement

$$\varepsilon(\psi) = \frac{4}{3} \sum 1 - Tr \rho_i^2$$

$\rho_{i,j}$: 16-dim matrix, No Easy-to-calculate analog of Concurrence

A New possiblity: Single-site Concurrence! Nonzero in Superconductors!

Entanglement Hierarchy in Many-Electron States

Conserved densities

$$\rho = \begin{array}{c} \begin{array}{cccc} |0\rangle & |\uparrow\downarrow\rangle & |\uparrow\rangle & |\downarrow\rangle \end{array} \\ \begin{vmatrix} 1-n+d & 0 & 0 & 0 \\ 0 & d & 0 & 0 \\ 0 & 0 & n_\uparrow - d & 0 \\ 0 & 0 & 0 & n_\downarrow - d \end{vmatrix} \end{array}$$

Electron densities: $n_\uparrow, n_\downarrow$

Density of Doubly-occupied sites =d

Density of holes= 1-(n-2d) -d

$$n_{hole} = d = 1/4 \qquad n_\uparrow = n_\downarrow = 1/2$$

Maximize Entanglement
Each Eigenvalue=1/4 → $\varepsilon \equiv \frac{4}{3}(1 - Tr\rho^2)$ $\boxed{\varepsilon = 1}$

Strong Correlations U large d=0 Now only 3 states per site

Maximize Entanglement
Each Eigenvalue=1/3 → $n_{hole} = n_\uparrow = n_\downarrow = 1/3$ $\boxed{\varepsilon = \frac{8}{9}}$

Half-filled Case: No holes
Max. Ent. E.value=1/2 → $n_\downarrow = n_\downarrow = 1/2$ $\boxed{\varepsilon = \frac{2}{3}}$

Double Occupancy in Many-Electron States

$$d = \langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle$$

Uncorrelated 'Unentangled Spins'

Hubbard Model: $H = T + U \sum n_{i\uparrow} n_{i\downarrow}$

Ground State: Repulsive U makes double occupancy unfavorable

$$d(U) = d(0)(1 - \delta) \qquad 0 \le \delta(U, n_\uparrow, n_\downarrow, |\psi\rangle) \le 1$$

Particularly Simple Cases

$\delta = 0 \quad U = 0$

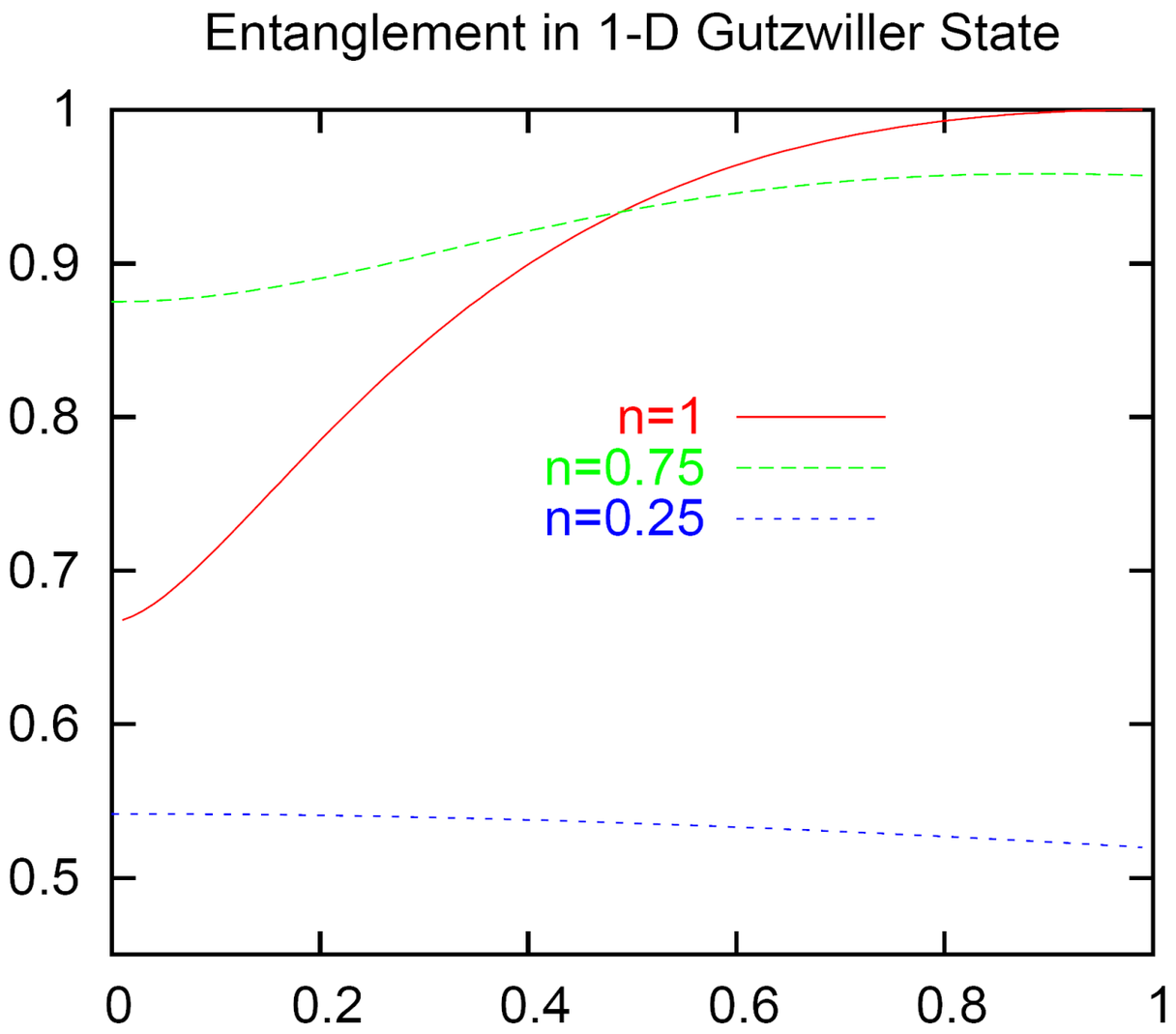
$\delta = 1 \quad U = \infty$

Independent of State and Energy

Exact result for 1-D through Gutzwiller Projection

$$|\psi_g\rangle = \Pi_i \left(1-(1-g)n_{i\uparrow}n_{i\downarrow}\right) |F\rangle$$

VS, Phys. Lett. A374, 3151 (2010



$$n_\uparrow = n_\downarrow = \frac{n}{2}$$

Dim. >1

Quite Complicated

Combinatorial

Strong Corr.
U=Infinity

Uncorrelated
No projection

Entanglement in the BCS Superconducting State

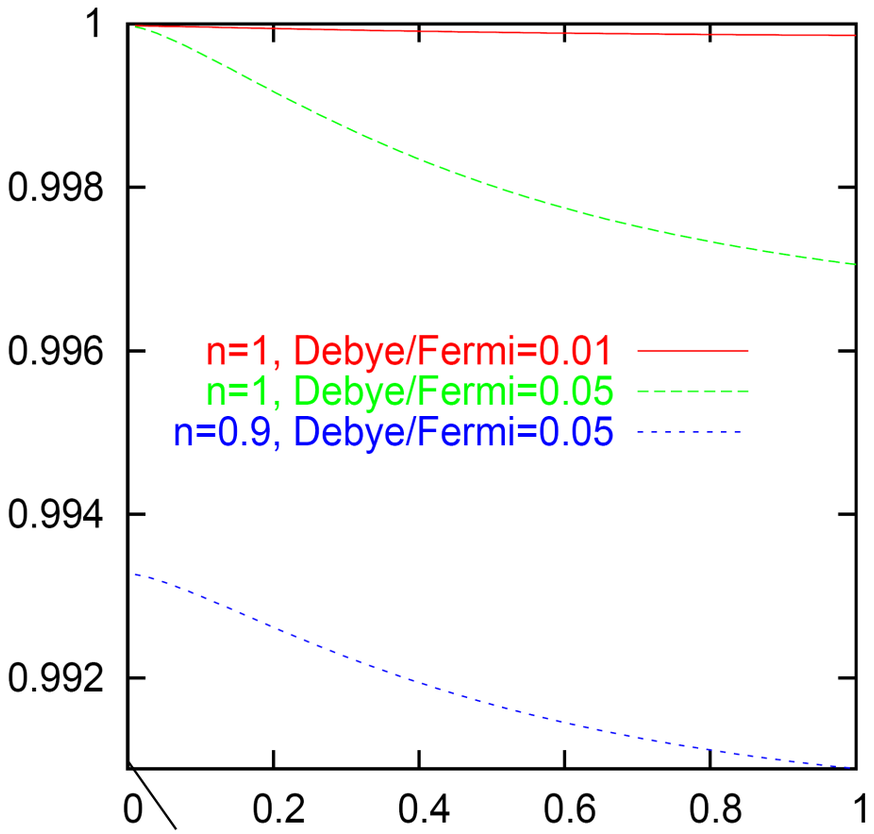
VS (2010)

$$\varepsilon = \frac{8}{3} d(2n - 2d - 1) + \frac{8}{3} n - \frac{1}{2} n^2$$

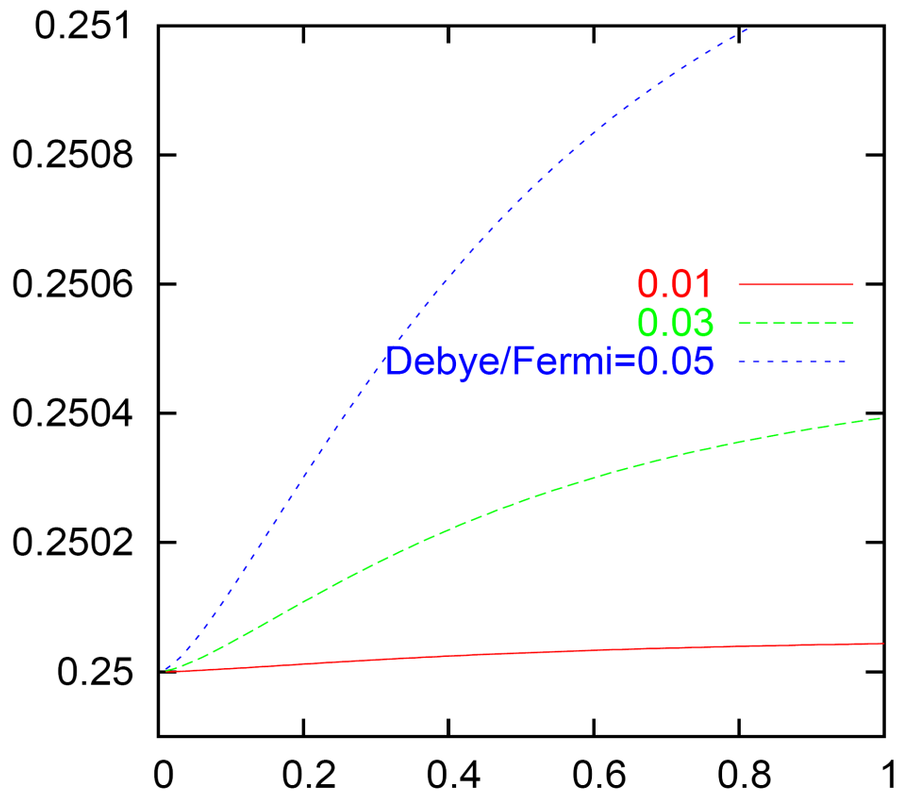
$$\zeta = \frac{3\Delta_0}{nE_F} \sinh^{-1} \frac{\hbar\omega_D}{\Delta_0}$$

$$d = \frac{n^2}{4}(1+\zeta^2)$$

ε



d



Uncorrelated
Matallic State

$\Delta_0/\hbar\omega_D$

Single-Site Concurrence

$$C_{\uparrow,\downarrow} = n\zeta - |n-2d|$$

Nonzero for n=1, if

$$\frac{3\Delta_0}{E_F} \sinh^{-1} \frac{n\omega_D}{\Delta_0} = \zeta > \sqrt{2}-1$$

Multi-Species Entanglement

VS, Quant. Inform. Comp. (2010)

Let u (v) denote the set of sites occupied by A (B) particles

$$|\psi\rangle = \sum_{u,v} \psi(u,v)\ |u\rangle_A\ |v\rangle_B$$

Strong exclusion: B occupies only sites unoccupied by A

Half filling: Total number of particles equals the number of sites

Now, v stands for the complement of the set u

$$|\psi\rangle = \sum_{u} \psi(u)\ |u\rangle_A\ |u\rangle_B$$

Many-particle wave function amplitudes are Schmidt numbers

$$S_A = -\sum_u |\psi(u)|^2 \log |\psi(u)|^2 \qquad \varepsilon_{A,B} = \lim_{N\to\infty} \frac{S_A}{N}$$

Transverse Ising Model: Quantum Phase Transition in the ground state

$$\mathcal{H} = -J \sum_i \sigma_i^x \sigma_{i+1}^x - h \sum_i \sigma_i^z$$

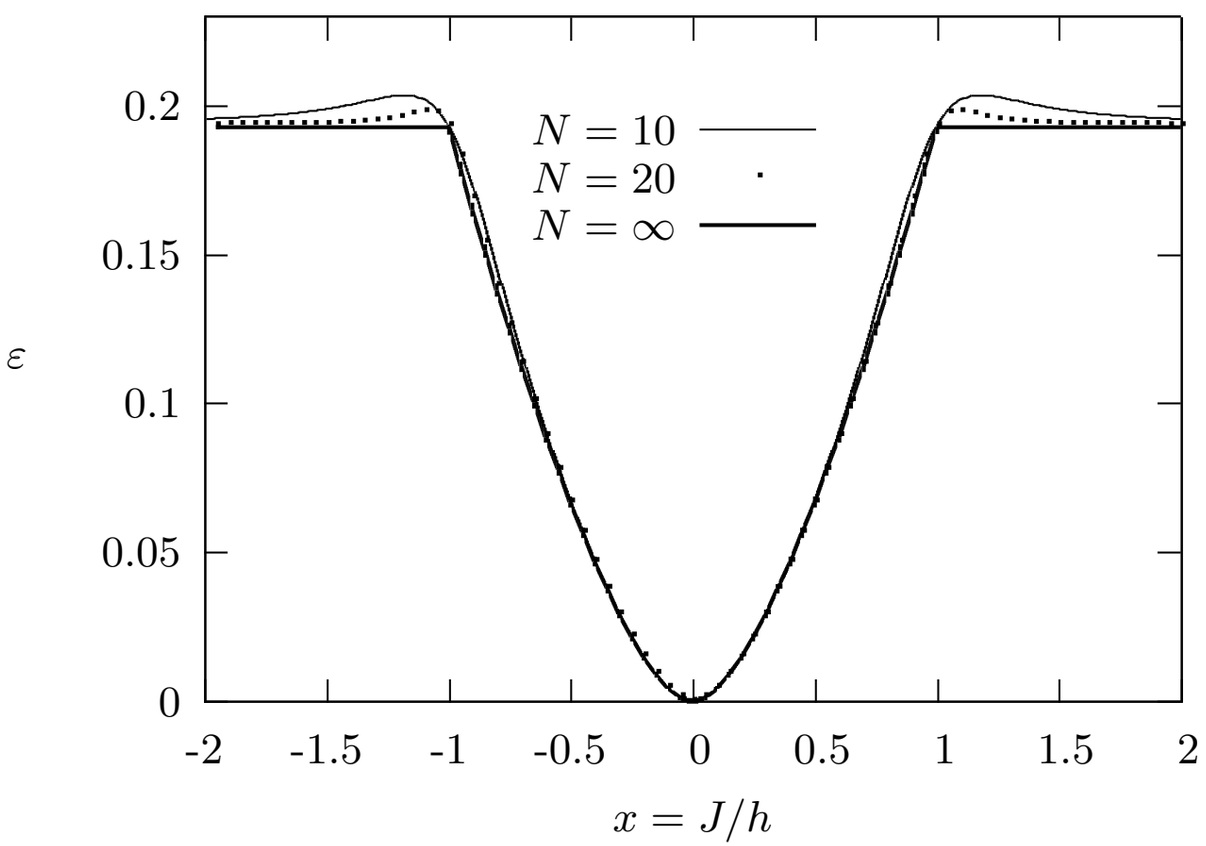
◄ Pauli operators

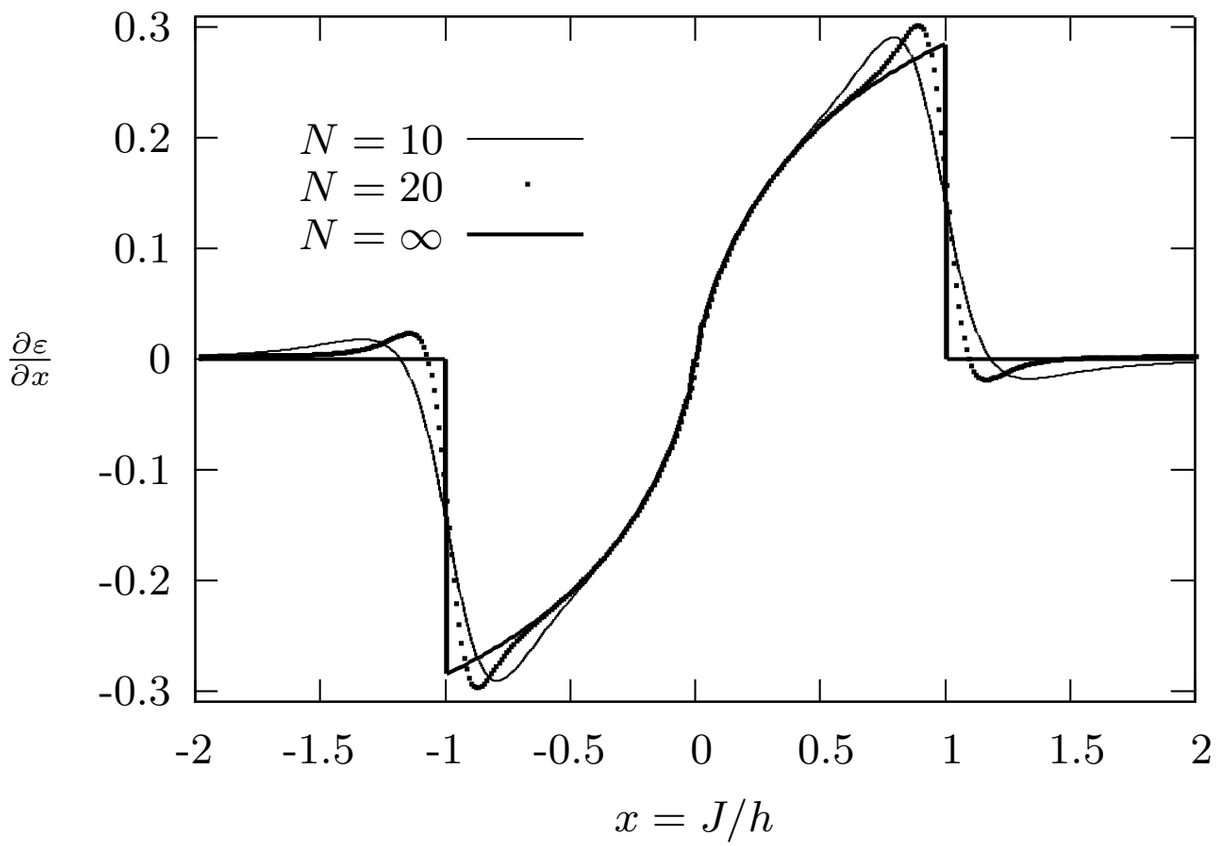
$$|G\rangle = \prod_{q>0} (a_q|0\rangle + b_q|\phi_q\rangle) \qquad |\phi_q\rangle \equiv c_q^\dagger c_{-q}^\dagger |0\rangle \qquad |a_q|^2 = \frac{1}{2}(1 - \frac{h + J\cos q}{\sqrt{h^2 + J^2 + 2Jh\cos q}})$$

Entanglement between ↑ and ↓ particles

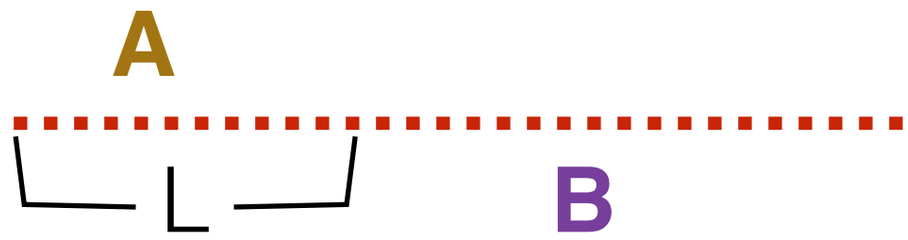
$$\varepsilon(x) = \frac{1}{N} \sum_{i=1}^{N/2} H(p_i) \qquad p_i = |a_{q_i}|^2$$

Shannon Binary Entropy





Block Entropy



$$S_L = -Tr\rho_A \; Log \; \rho_A$$

$$S_L \approx Area \sim O(1)$$

Area Law

System away from Critical point

System at criticality:
long-range correlations

$$S_L \approx \frac{c}{3} Log_2 L$$

$$\frac{c}{3} Log_2 (N\pi \sin \frac{\pi L}{N})$$ CFT Result For a finite system

Conformal Anomaly / Central Charge is independent of L

C=1 Noninteracting fermions

C=1 S=1/2 Heisenberg Antiferromagnet

C=1/2 Ising spins in a transverse field

* State is given

* Reduced density matrix is 2^{16} for N=16
As there are 4 states per site

* Most of the eigenvalues are nearly zero
Still, need to diagonalize large matrices

* Numerical estimate for finite N not very reliable

* Periodic boundary conditions and free boundary conditions give different central charge values!

* Even and odd effects for even/odd L

Block Entanglement of Gutzwiller State:

E(N,g,n)

Largest block L=N/2

Archak Purkaystha, VS (arXiv1307.1781)

$$|\psi_g\rangle = \Pi_i \left(1-(1-g)n_{i\uparrow}n_{i\downarrow}\right) |F\rangle$$

Half filling

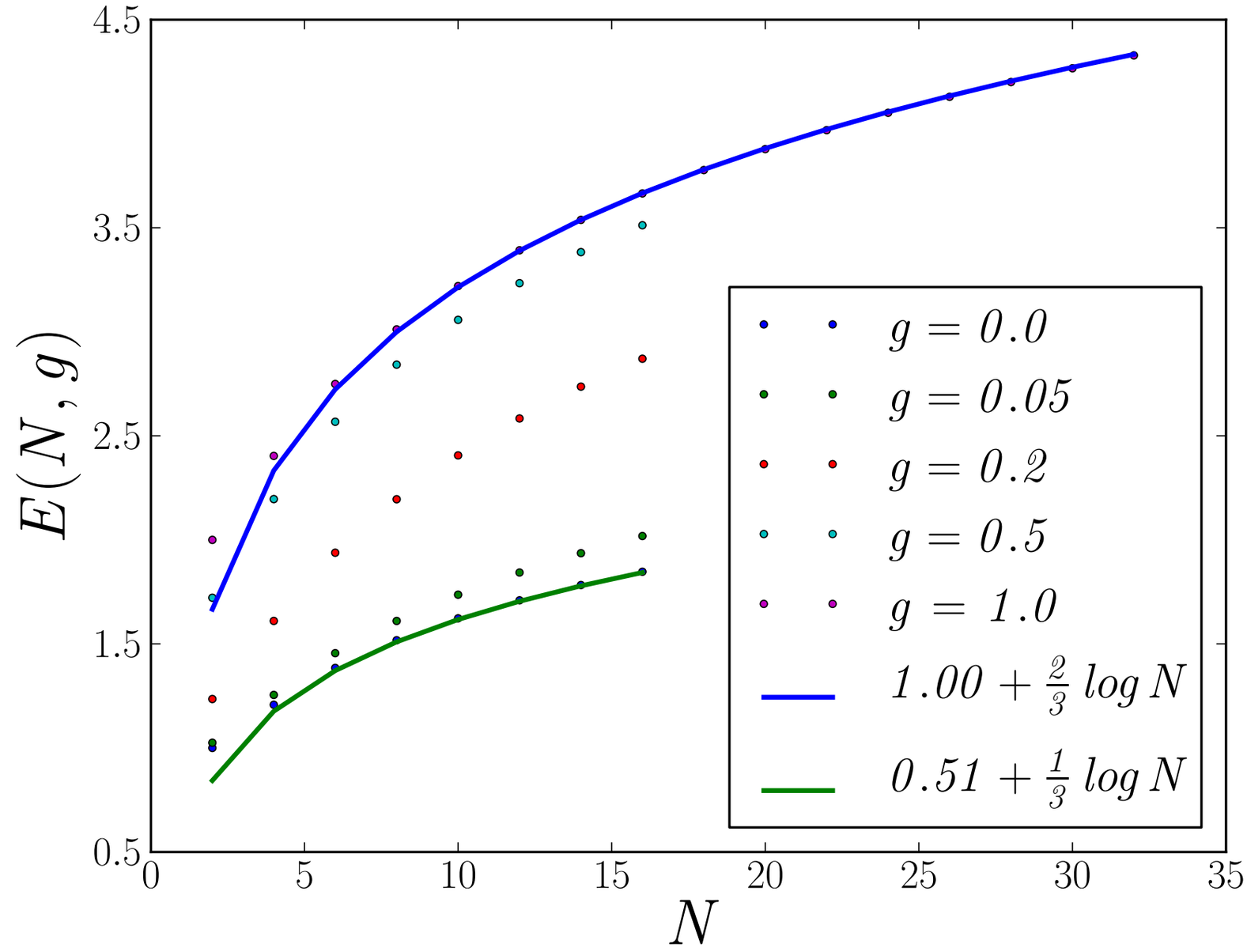
$$n = \frac{N_e}{N},\ N_\uparrow = N_\downarrow$$

$$E(N,0) \approx \frac{1}{3}\log_2 N$$

C=1 Only Spin degrees
No Charge degrees
Insulating State

$$E(N,1) \approx \frac{2}{3}\log_2 N$$

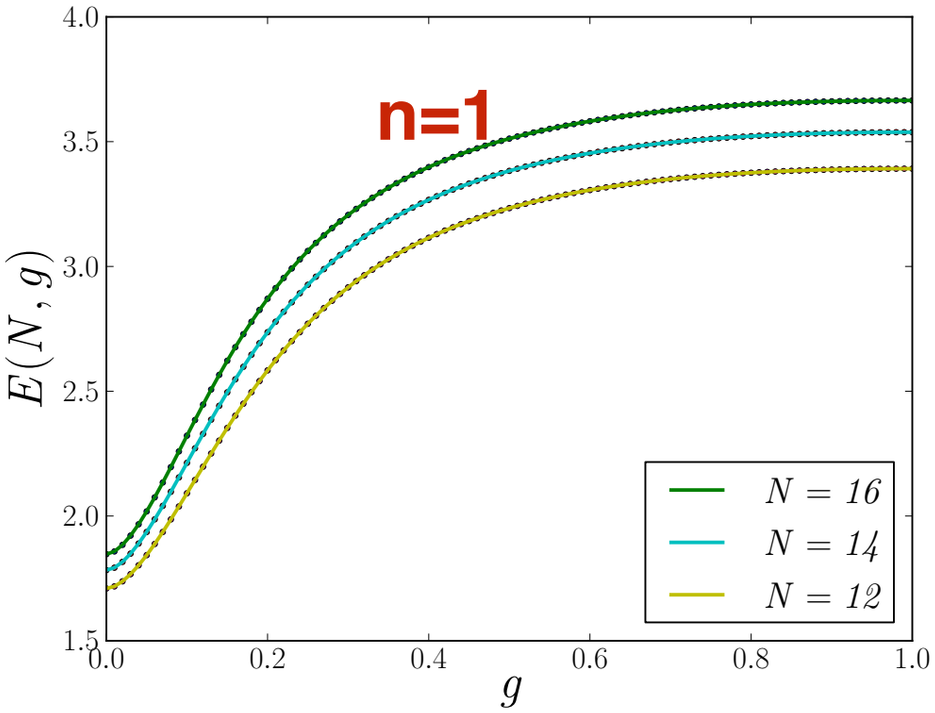
C=2, Charge and Spin degre
Metallic State

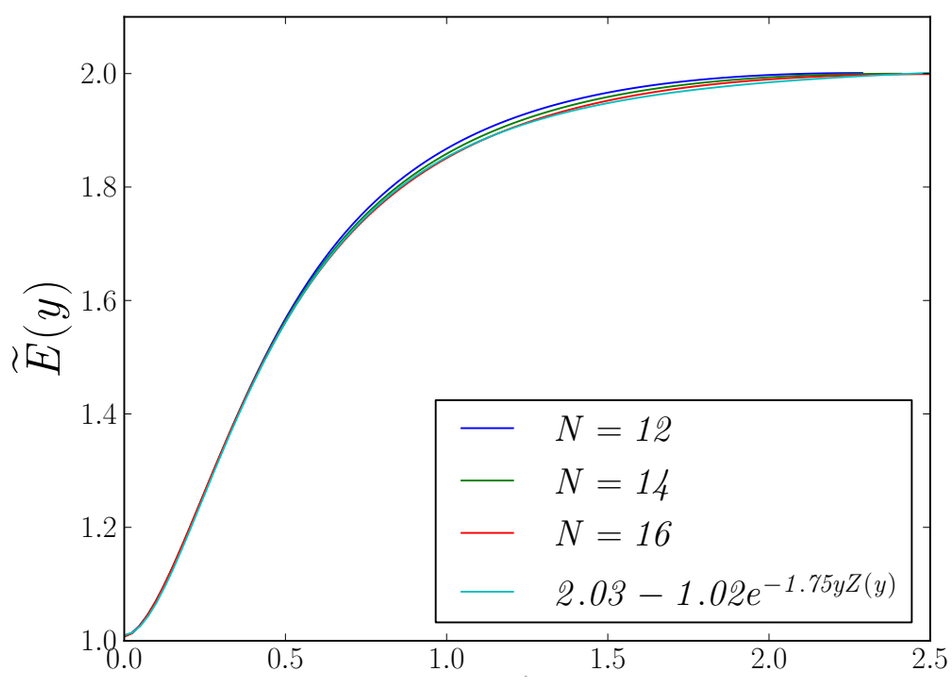


Metal-Insulator Transition: Crossover

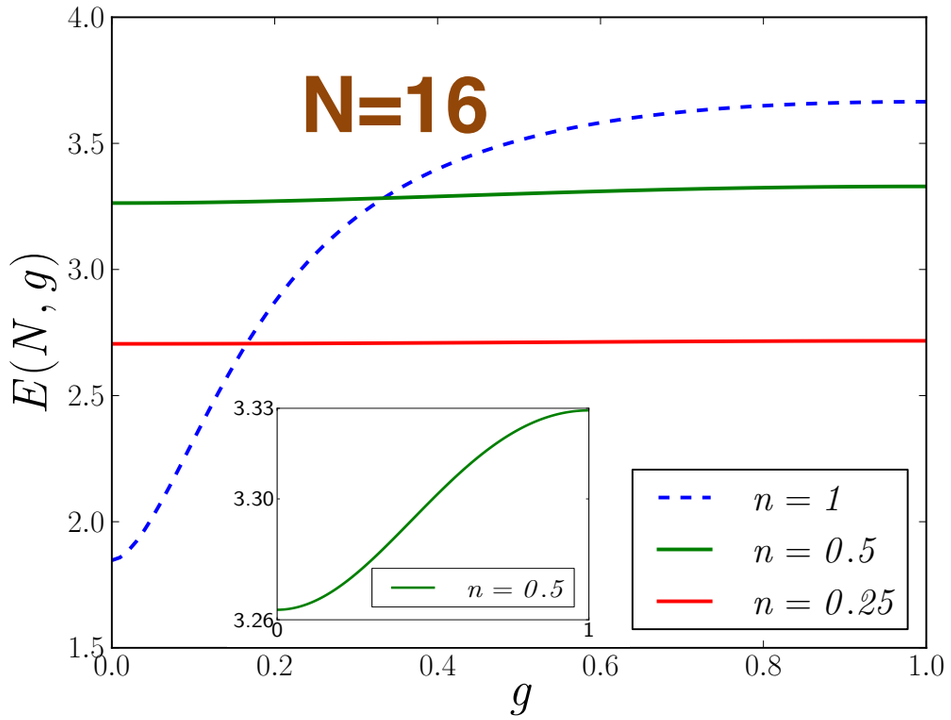
Scaling function

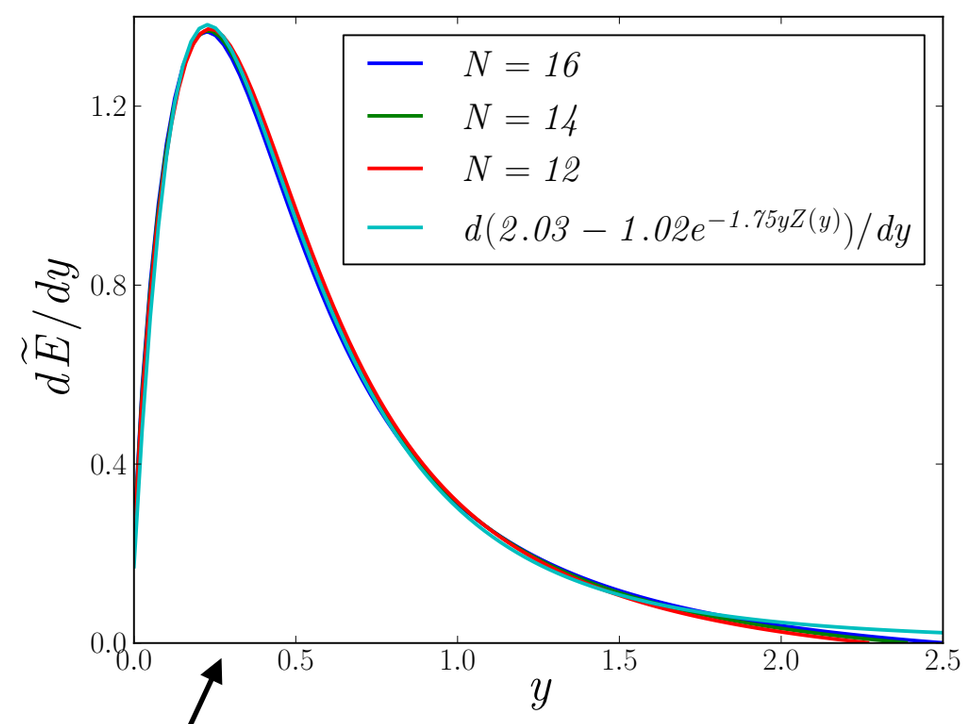
$$\widetilde{E}(y) = \frac{E(N,g)}{\frac{1}{2} + \frac{1}{3} log_2 N} \qquad y = N^{\frac{1}{3}} g$$





$$Z(g) = \frac{4g}{(1+g)^2}$$

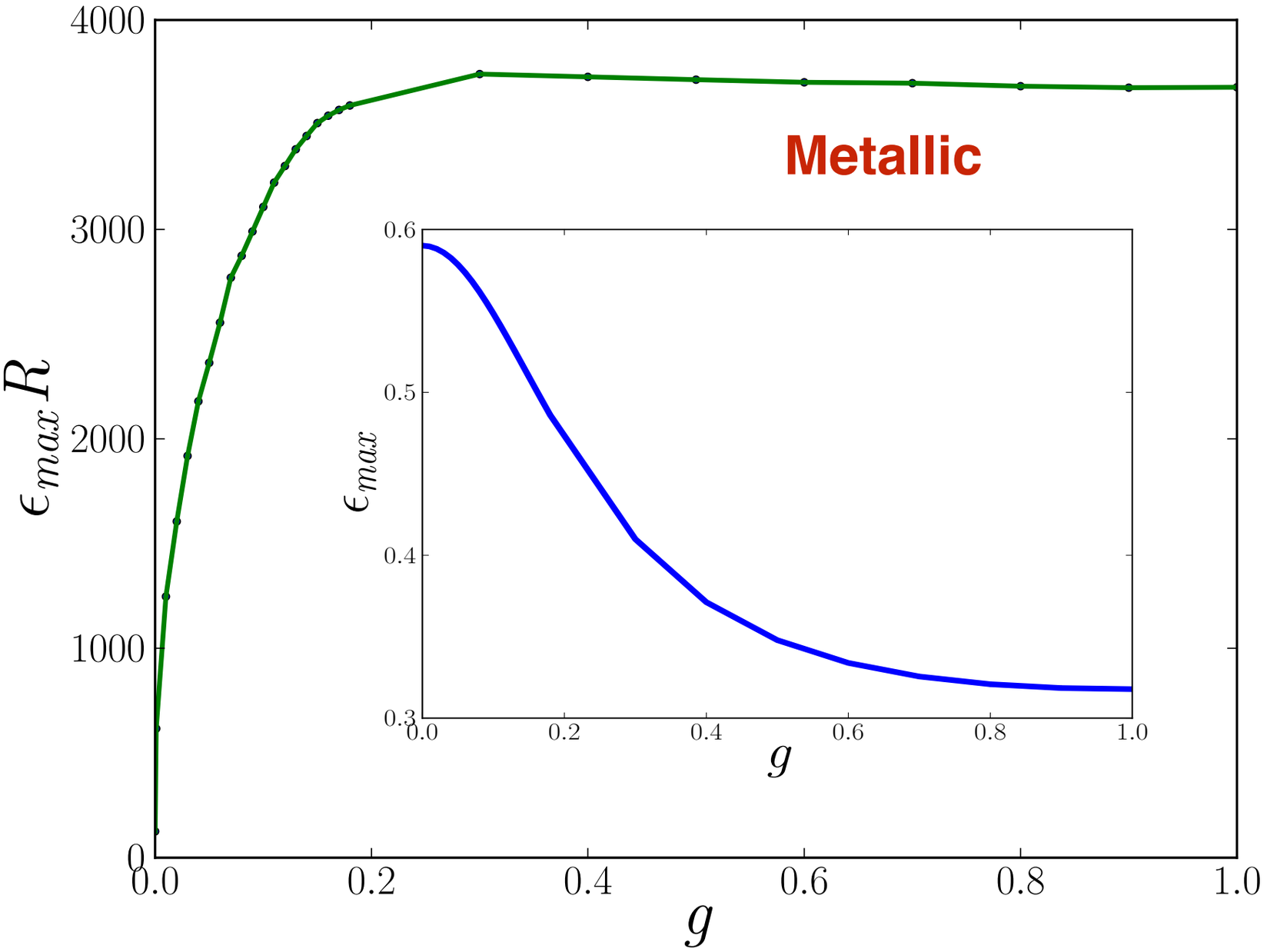




Fermi liquid
Jump in n(k)
at fermi surface

$$y_0 \simeq 0.24$$

ϵ_{max} *largest eigenvalue of* ρ_A R is the rank



N=16

Metallic

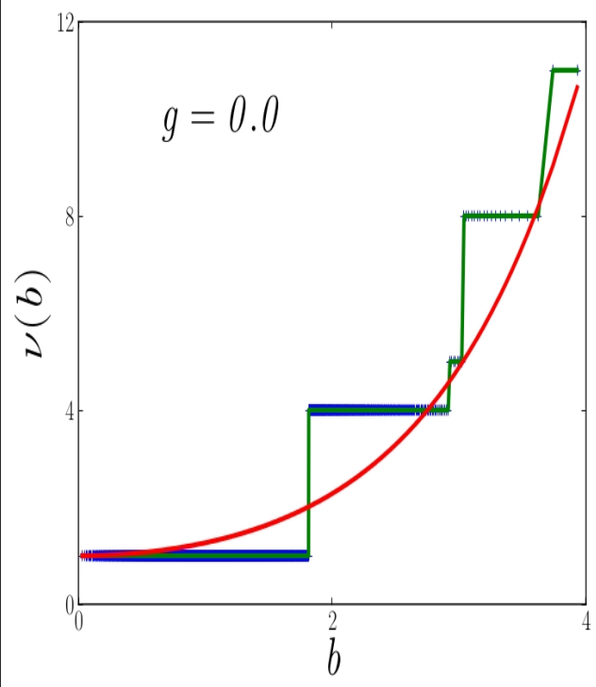
Insulating

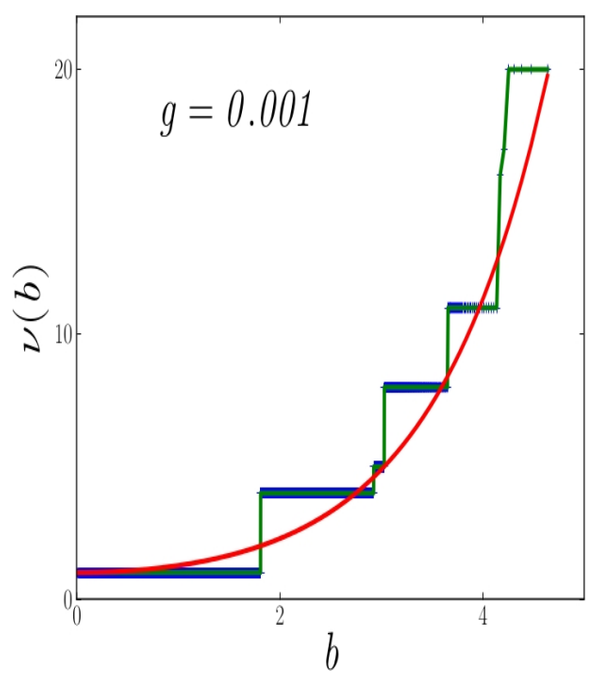
Entanglement Spectrum

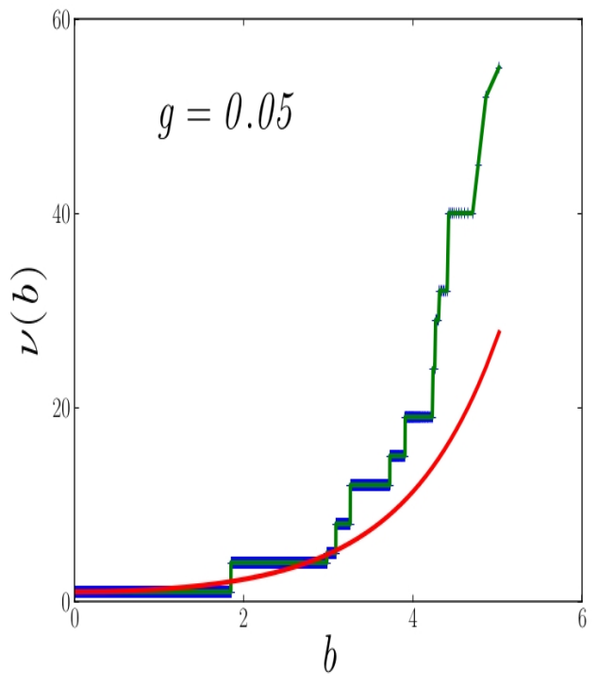
$$\nu(\epsilon) = \sum_i \Theta(\epsilon_i - \epsilon) = I_0(2\sqrt{-b_0 ln(\frac{\epsilon}{\epsilon_{max}})})$$

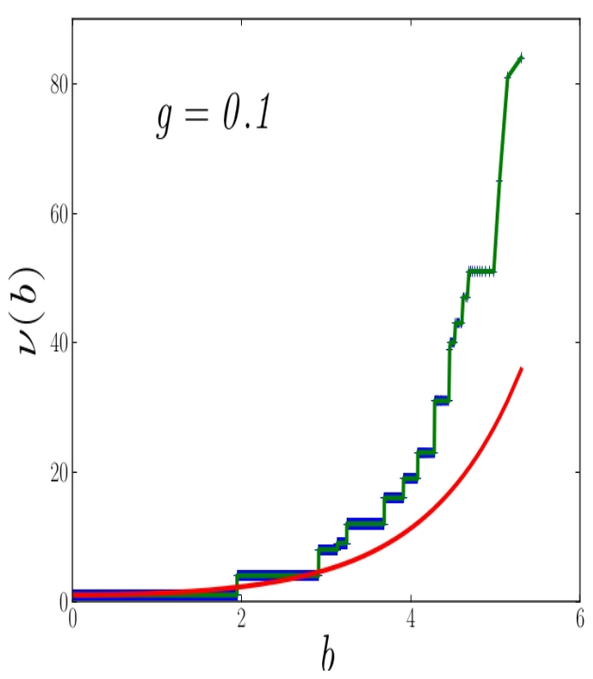
$$b = 2\sqrt{ln(\epsilon_{max}) ln(\frac{\epsilon}{\epsilon_{max}})}$$

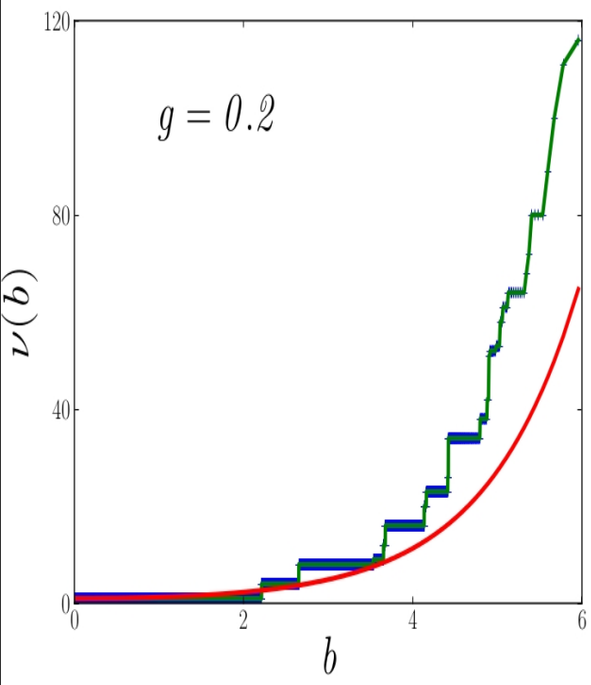
Calebrese, Lefevre, PRA (2008)

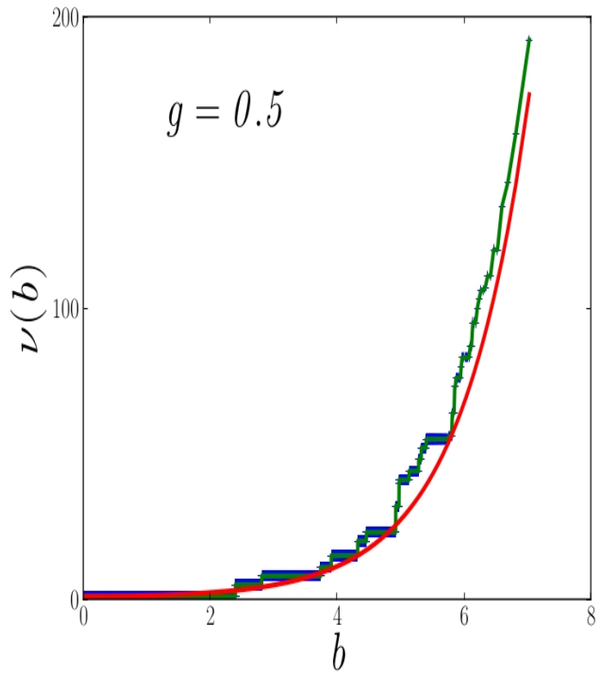


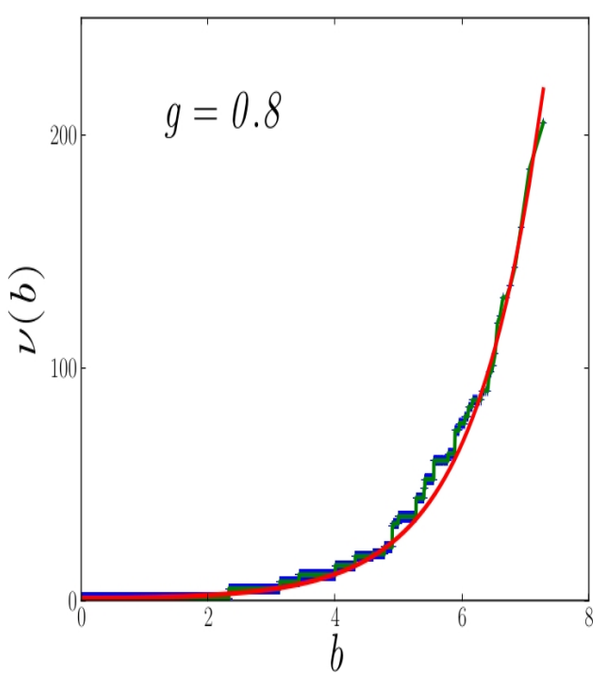


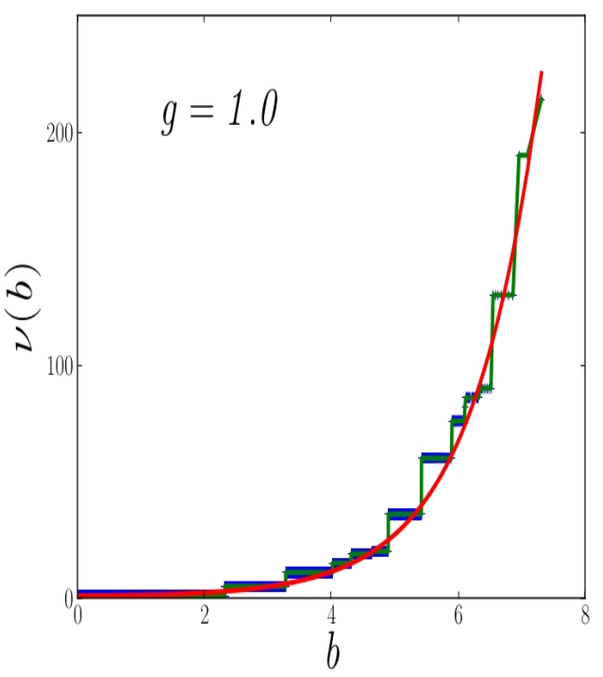












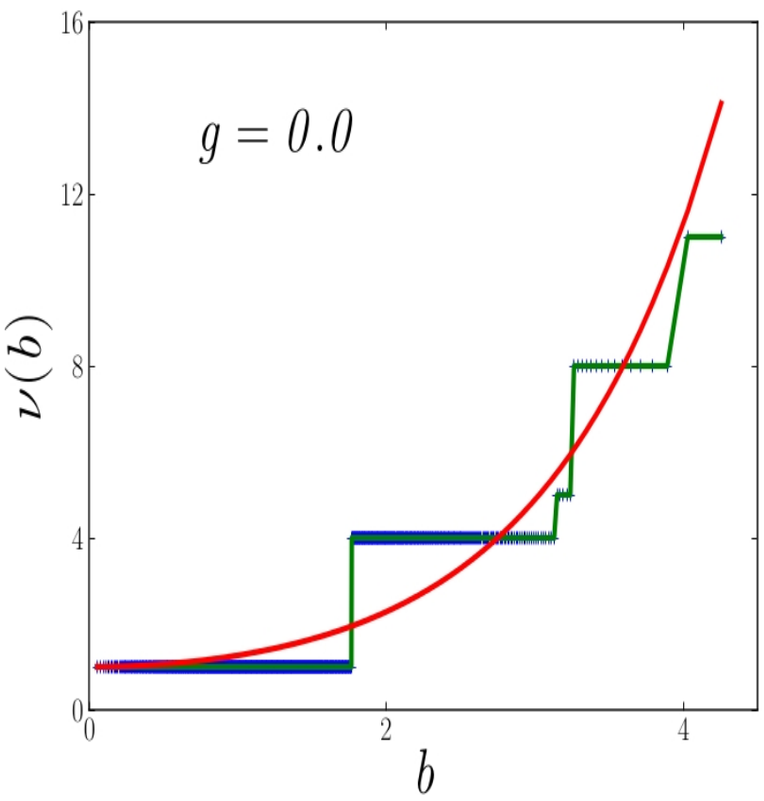
Entanglement Spectrum follows CFT result both in metal and insulator regimes

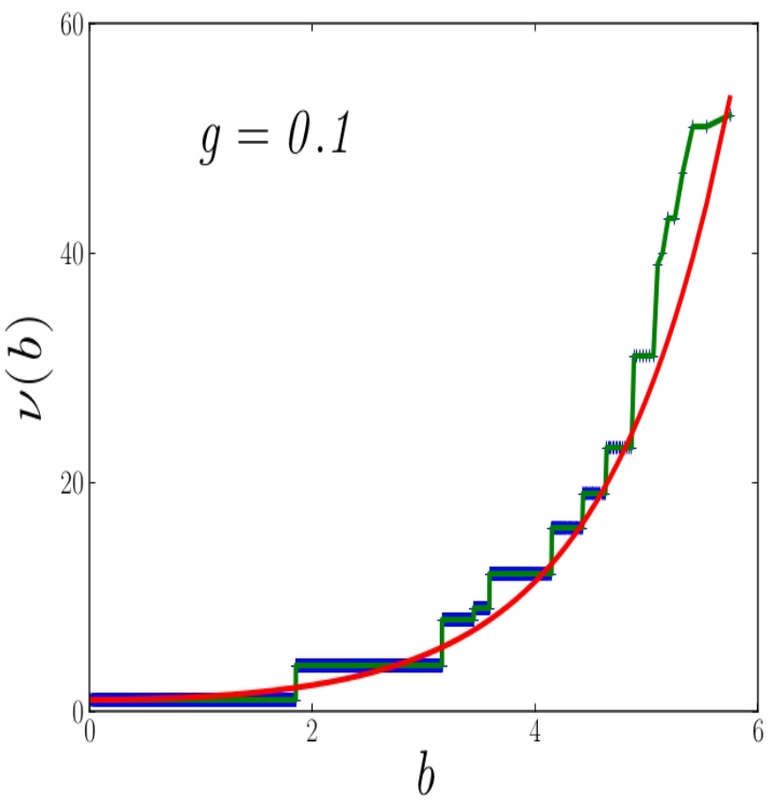
Deviation from CFT prediction: Metal-insulator crossover

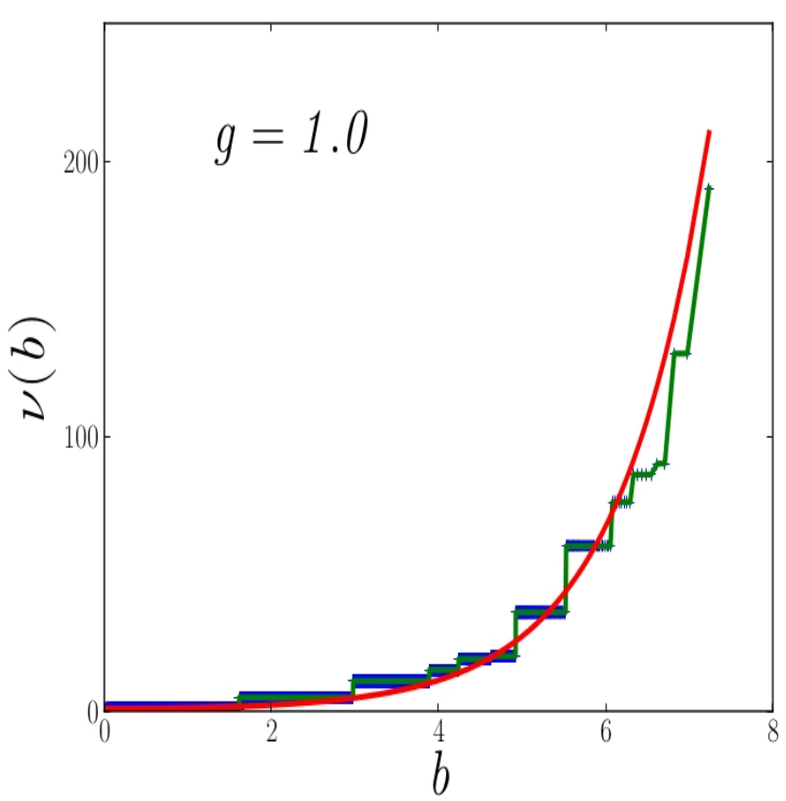
$$b_0 = \frac{\widetilde{E}(y)}{6} log_2\, N_s$$

Modification for crossover regime AP, VS (2013)

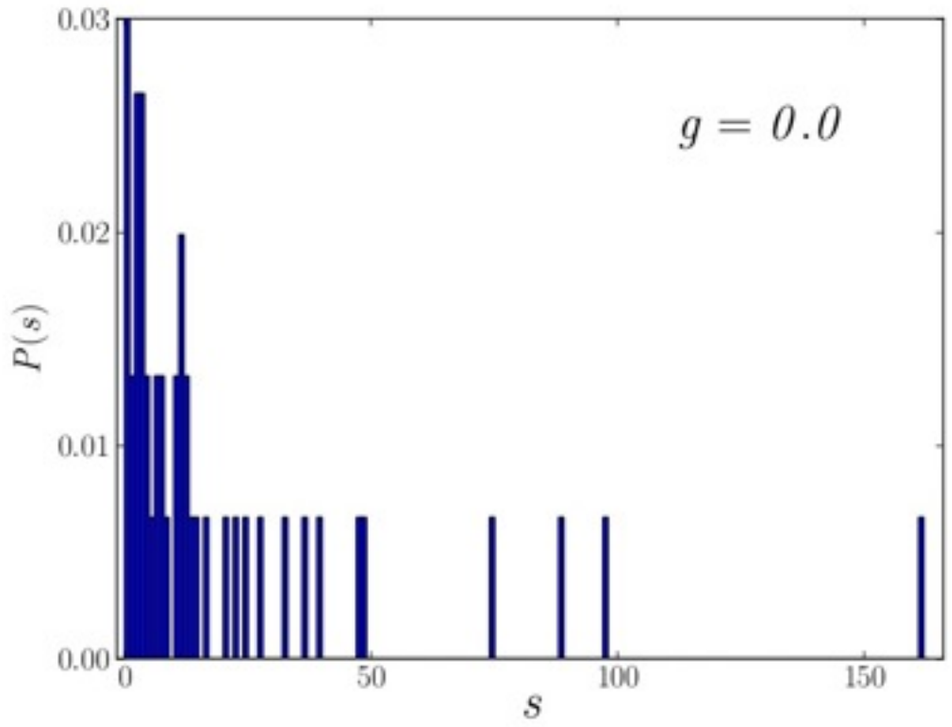
N=16

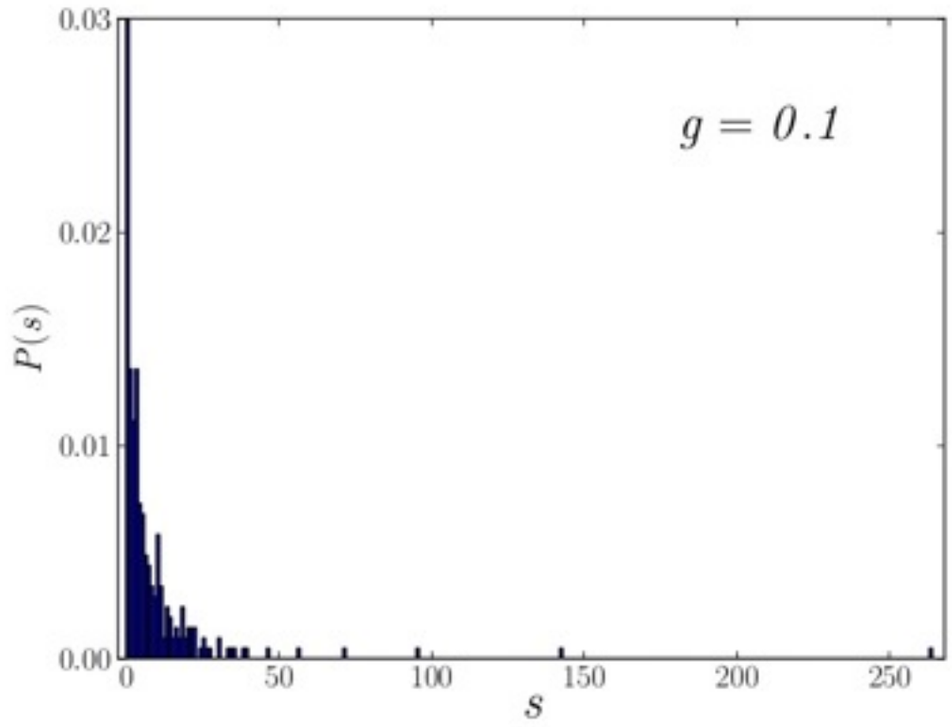


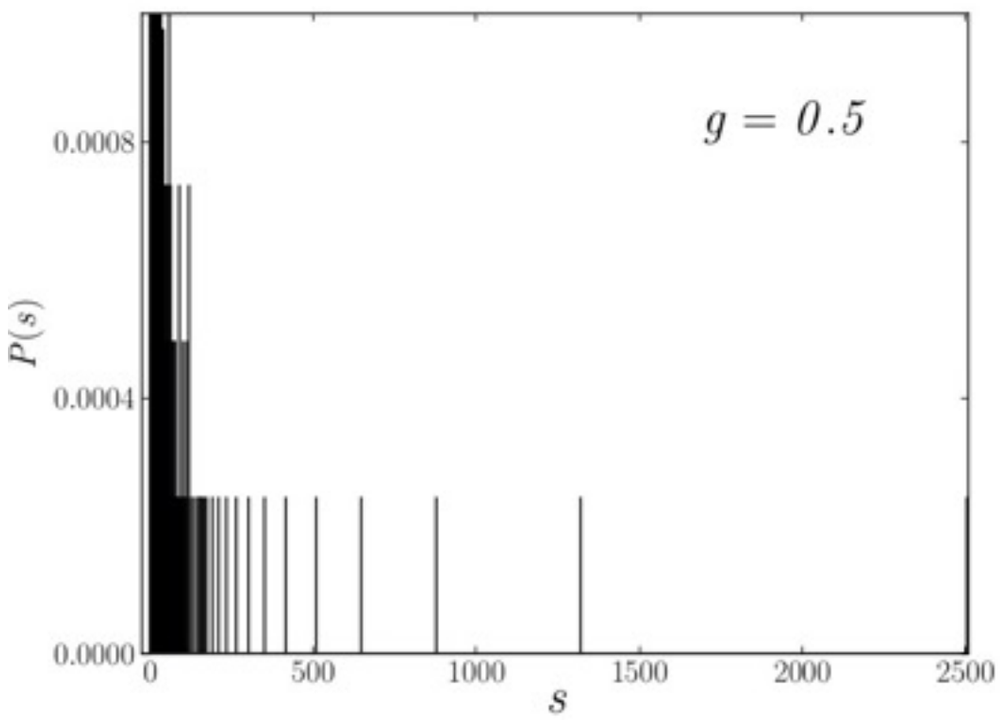


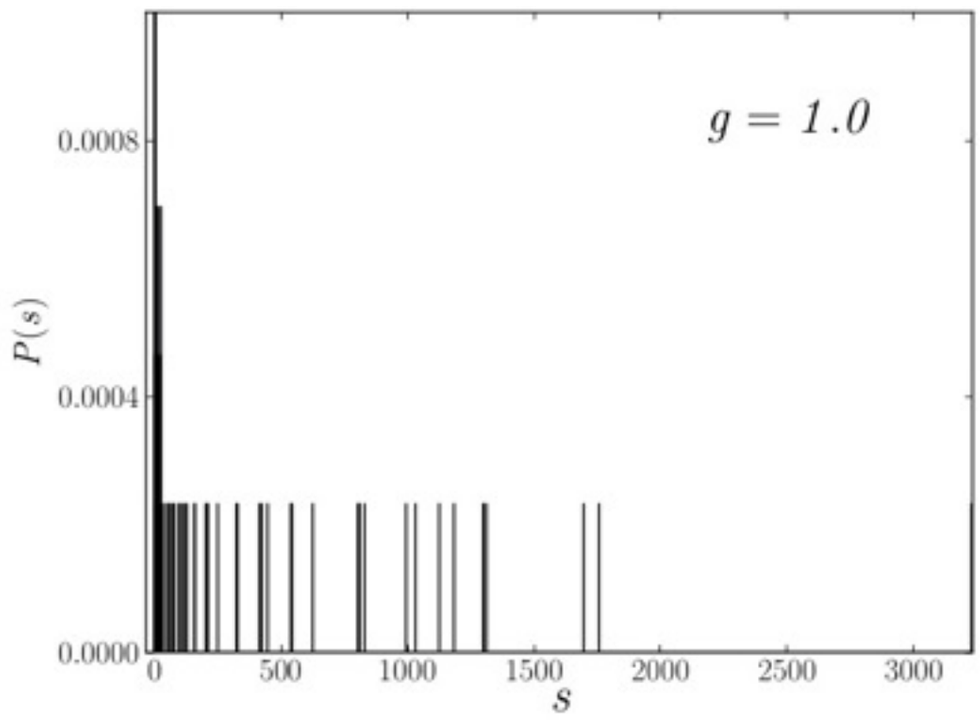


Spacing Distribution $P(s) = \sum_i \delta(s - \tilde{\epsilon}_i + \tilde{\epsilon}_{i+1})$ $\tilde{\epsilon} = I_0(2\sqrt{-b_0 ln(\frac{\epsilon}{\epsilon_{max}})})$









Unlike the above, Energy level spacing: Wigner (GSE) in metallic, Poisson in insulating state

Metal-Insulator Crossover Transition in Nano-Chains

$$y_0 = N^{\frac{1}{3}} g \approx 0.24$$

For a fixed size, transition can occur at

$$g \simeq 0.24/N^{1/3}$$

Gutzwiller state successful to explain band structure (ARPES) in Ni

Buenemann et al PRB67, 075103 (2003)

$$g \log g = -\frac{4t}{\pi U}$$

t~ 0.5 ev for $dd\sigma$ band U~10 ev

Nano-chains 2-3 microns
Antiferromagnetic and Insulating

Bliznyuk et al, Nanotechnology, 20, 105606 (2009)

a~0.3 nM N~10000

This implies from the crossover formula: g~ 0.01

$$\frac{t}{U} \sim 0.4$$

Conclusions

Off-diagonal correlations should dominate for nonzero two-spin entanglement

Long-ranged correlations do not imply long-ranged entanglement

Diagonal Correlations, viz. Coulomb interactions decrease global entanglement

Optimal double occupancy maximizes Ent: Metallic states

Discourage or encourage double occupancy lowers Ent

Multi-species Ent: between up and down electrons can track quantum phase transitions

Nonzero only for correlated states

Block Entaglement Entropy for Gutzwiller state: Deviations from CFT

Scaling form entanglement for metal-insulator crossover

Double occpancy in insulating regime, Jump at fermi surface in metallic regime

Entanglment spectrum deviates from CFT near crossover

Spacing Distribution shows wider range in the metallic regime