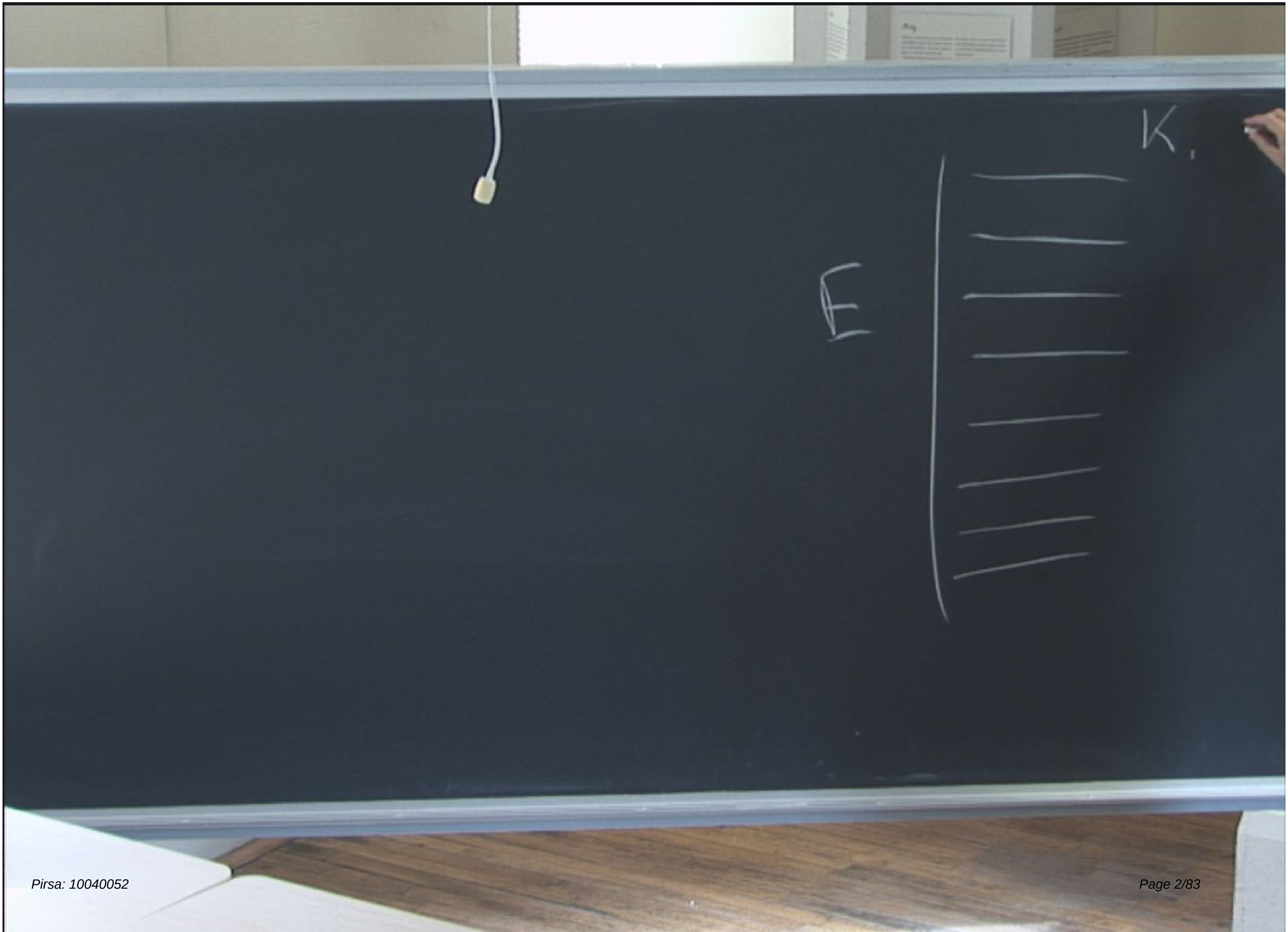
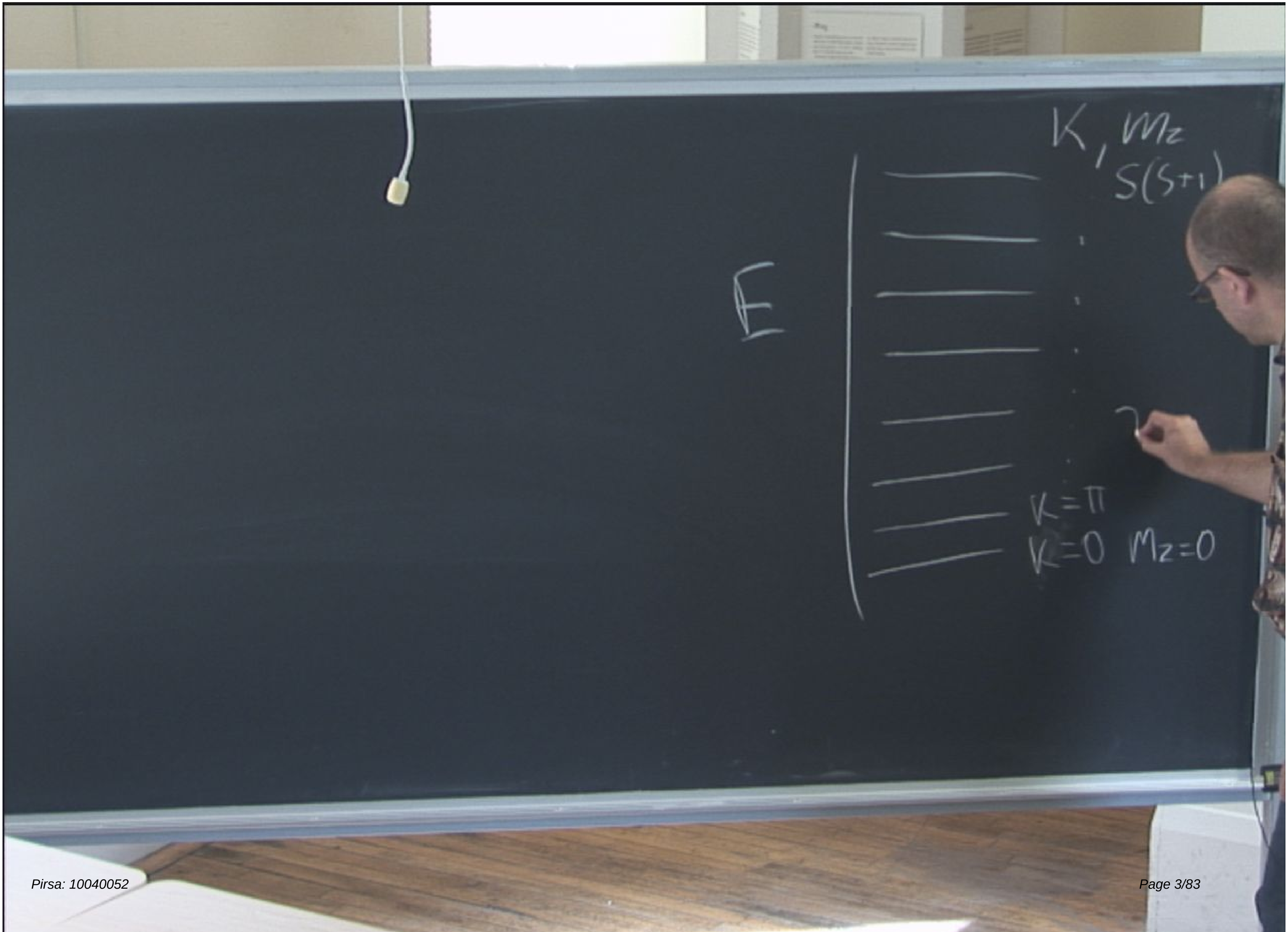
Title: Quantum Spin Simulations (PHYS 7380) - Lecture 10

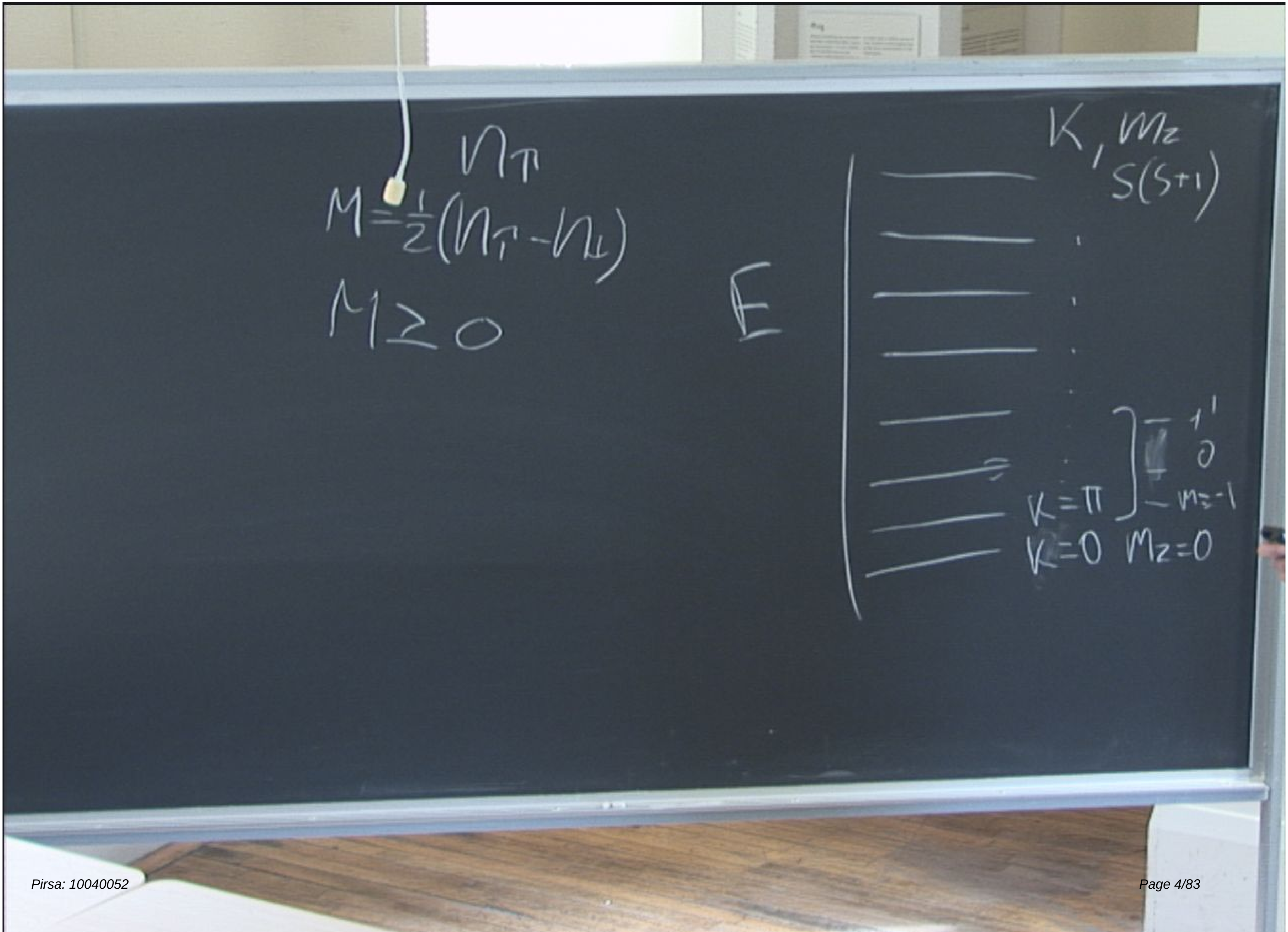
Date: Apr 16, 2010 11:00 AM

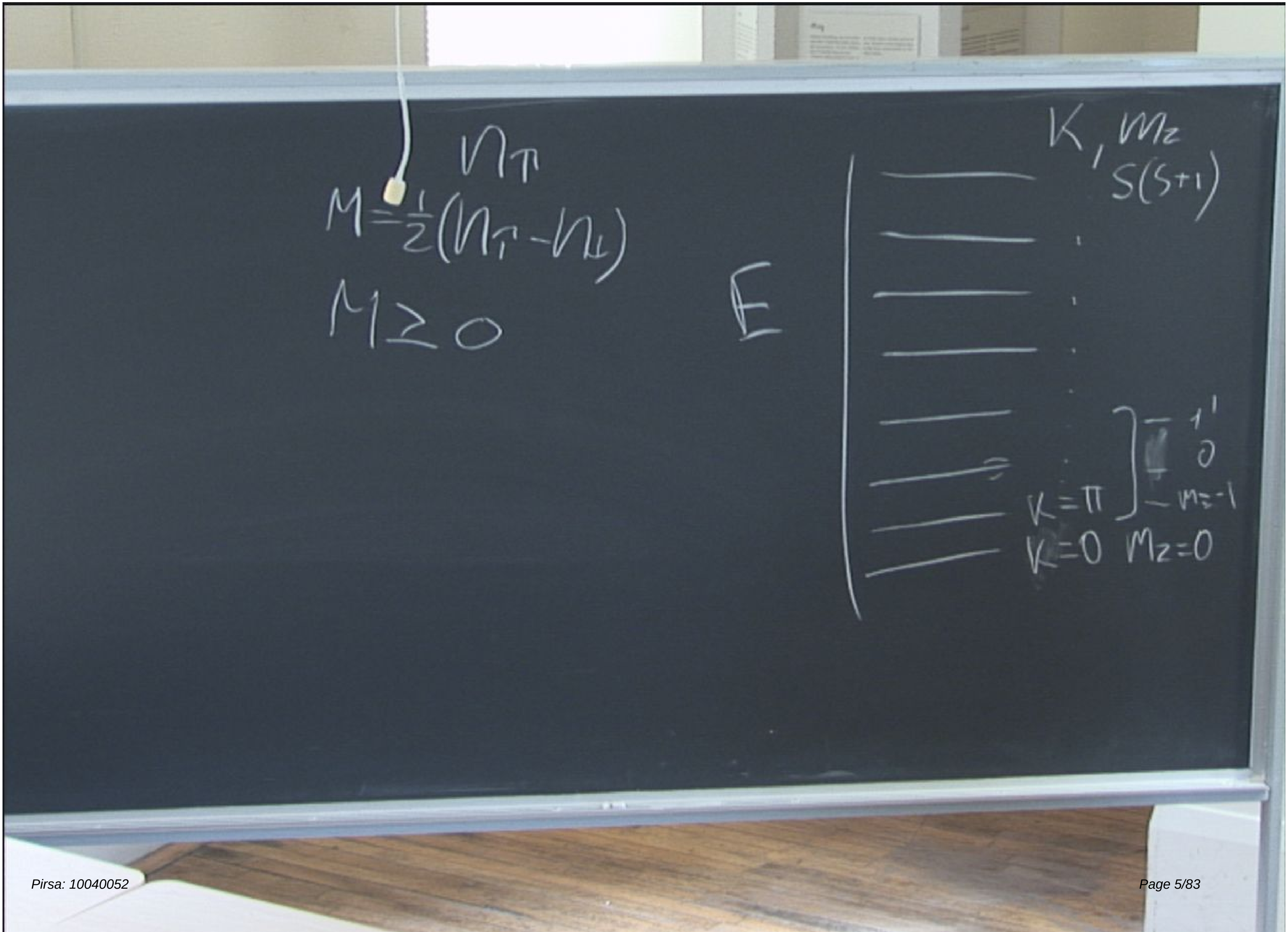
URL: http://pirsa.org/10040052

Abstract:


E
K,


K, mz
S(S+1)
E
K=π
K=0 Mz=0


$n_\uparrow$
$M = \frac{1}{2}(n_\uparrow - n_\downarrow)$
$M \geq 0$
E
$K, m_z, S(S+1)$
1
0
$m_z = -1$
$K = \pi$
$K = 0 \quad M_z = 0$


n↑
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M ≥ 0
E
K, m_z
S(S+1)
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K = π
K = 0 M_z = 0

Spin correlations in the Heisenberg chain

Let's look at the (staggered) spin correlation function

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle (-1)^r$$

versus the distance r and at r=N/2 versus system size N

Theory (bosonization, conformal field theory) predicts (for large r, N)

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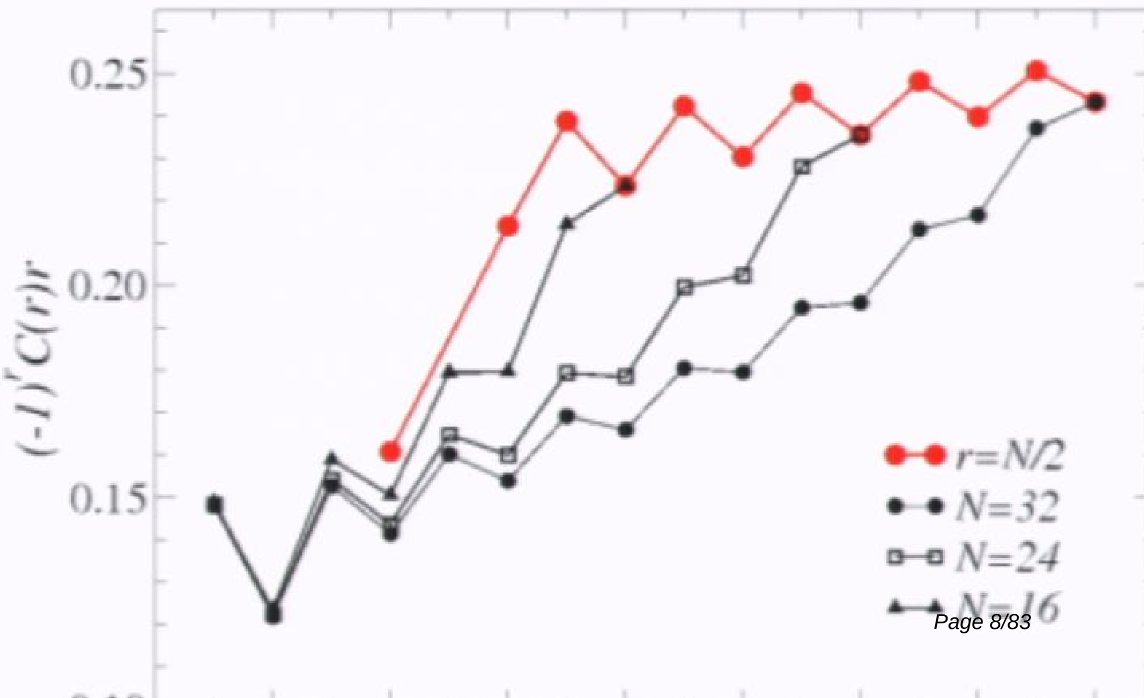
Plausible based on N up to 32
- other methods for larger N

Power-law correlations are a sign of a "critical" state; at the boundary between
- ordered (antiferromagnetic)
- disordered (spin liquid)



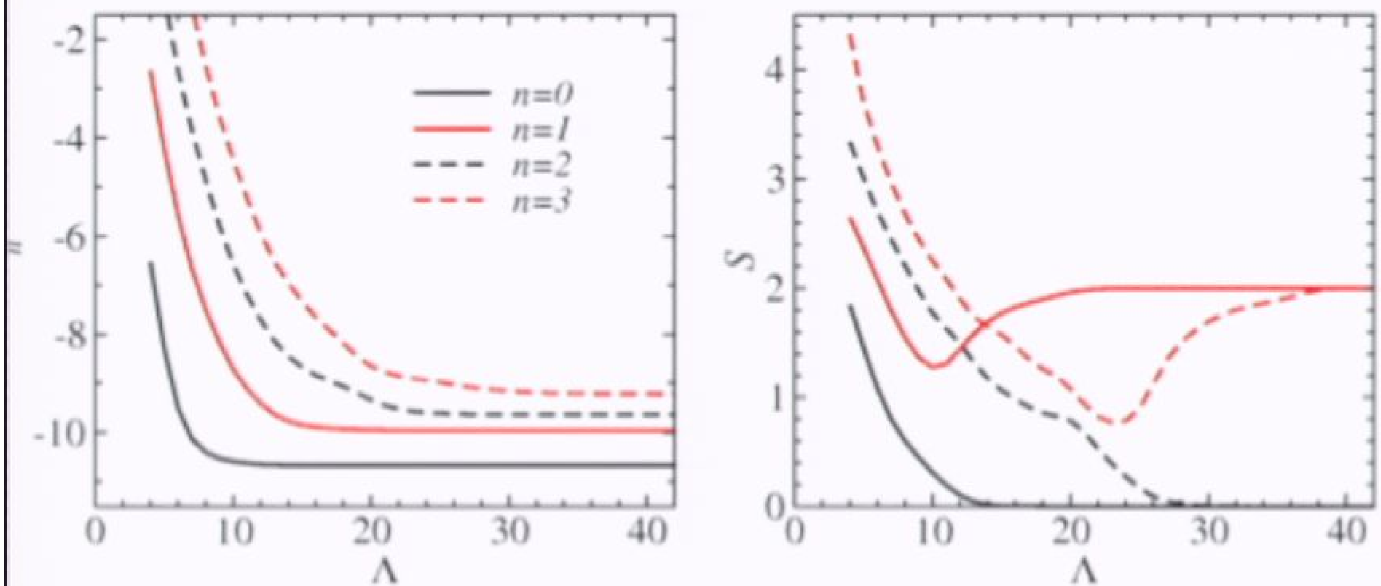
Re-orthogonalization procedure

For each state generated, remove all components of prior states, *i=1,...,m*

- easy if we work with the normalized basis and all states are stored

$$|\phi_m\rangle \rightarrow \frac{|\phi_m\rangle - q|\phi_i\rangle}{1-q^2}, \qquad q = \langle\phi_i|\phi_m\rangle$$

Convergence properties of the Lanczos method



Example; 24-site chain
$m_z = 0$, $k = 0$, $p = 1$, $z = 1$
block size M=28416

Ground state converges first, then successively excited states

Pseudocode; hamiltonian operation with compact storage

$$
\begin{aligned}
&\textbf{subroutine hoperation}(\phi, \gamma) \\
&\gamma = 0;\ i = 0 \\
&\textbf{do}\ a = 1, M \\
&\quad \textbf{do}\ j = 1, e_a \\
&\quad\quad i = i + 1 \\
&\quad\quad \gamma(B(i)) = \gamma(B(i)) + H(i)\phi(a) \\
&\quad\quad \gamma(a) = \gamma(a) + H(i)\phi(B(i)) \\
&\quad \textbf{enddo} \\
&\textbf{enddo}
\end{aligned}
$$

$$H|\phi\rangle = |\gamma\rangle = \sum_{a=1}^{M}\sum_{b=1}^{M}\phi(a)\langle b|H|a\rangle|b\rangle$$

Operator expectation values

Diagonalizing the tri-diagonal matrix → eigenstates in the Lanczos basis

- eigenvectors v_n, energies E_n
- only some number of low-energy states (<< Λ) are correct eigenstates of H

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To compute expectation values we normally go back to the original basis

$$\psi_n(a) = \sum_{m=0}^{\Lambda} v_n(m)\phi_m(a), \qquad a = 1,\ldots,M$$

To compute $\langle\psi_\mathbf{n}|\mathbf{O}|\psi_\mathbf{n}\rangle$ first construct

$$\begin{aligned} O|\psi_n\rangle = |\psi_n^O\rangle &= \sum_{a=1}^{M}\psi_n(a)O|a\rangle \\ &= \sum_{a=1}^{M}\sum_{b=1}^{M}\psi_n(a)|b\rangle\langle b|O|a\rangle \\ &= \sum_{b=1}^{M}\psi_n^O(b)|b\rangle \end{aligned}$$

<b|O|a> done exactly as when constructing of the H matrix

$$\psi_n^O(b) = \sum_{a=1}^{M}\psi_n(a)\langle b|O|a\rangle$$

Then evaluate the scalar product

M

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Pseudocode: modify state generation

```
do m = 1, Λ − 1
    call hoperation(φ_m, φ_{m+1})
    a_m = ⟨φ_m|φ_{m+1}⟩; φ_{m+1} = φ_{m+1} − a_m φ_m − n_m φ_{m−1}
    call normalize(φ_{m+1}, n_{m+1})
    do i = 1, m
        q = ⟨φ_{m+1}|φ_i⟩; φ_{m+1} = (φ_{m+1} − q φ_i)/(1 − q^2)
    enddo
enddo
```

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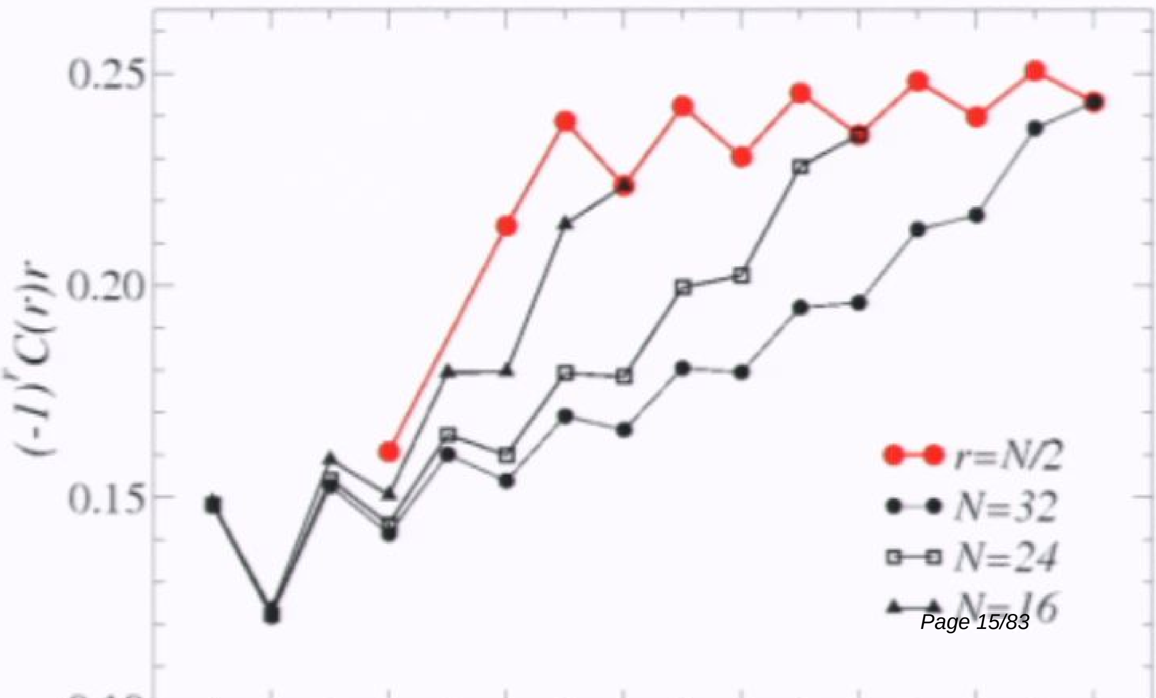

Excitations of the Heisenberg chain

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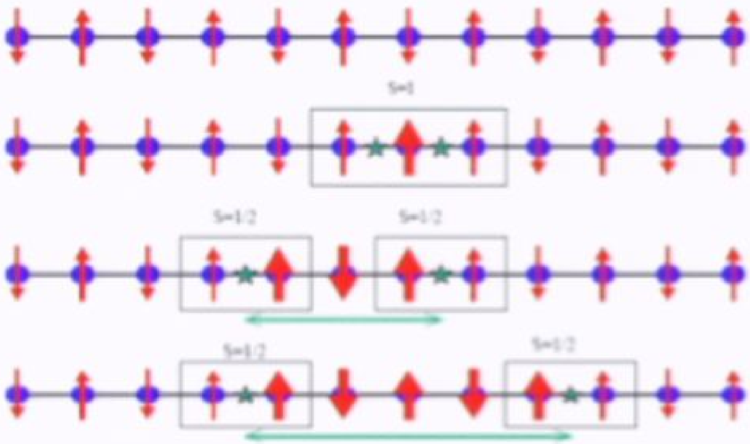
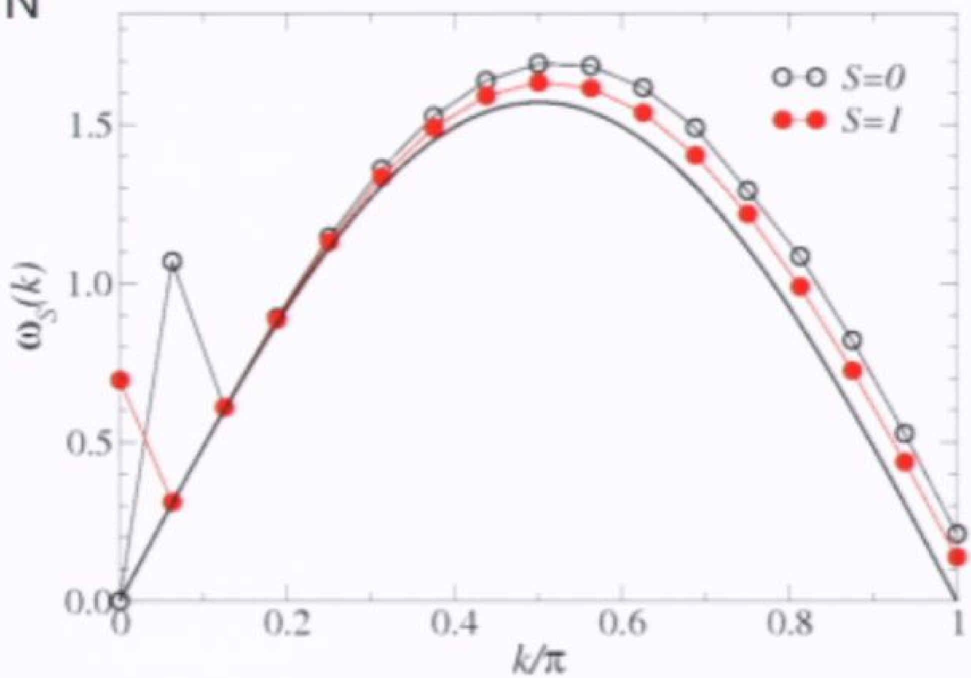
- the ground state is a singlet (S=0) for even N
- the first excited state is a triplet (S=1)
- can be understood as pair of "spinons"





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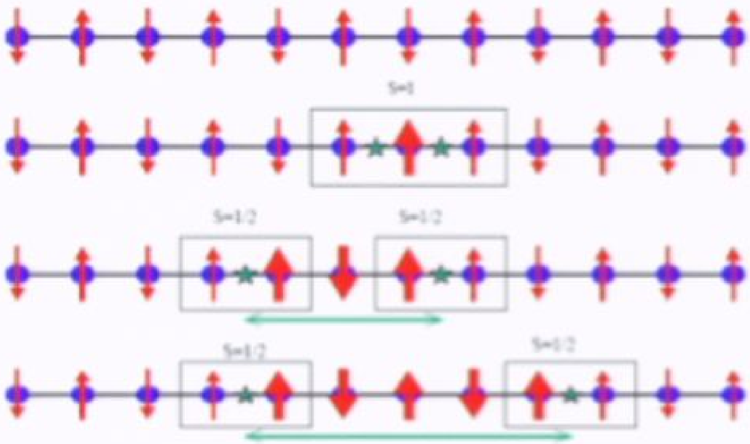
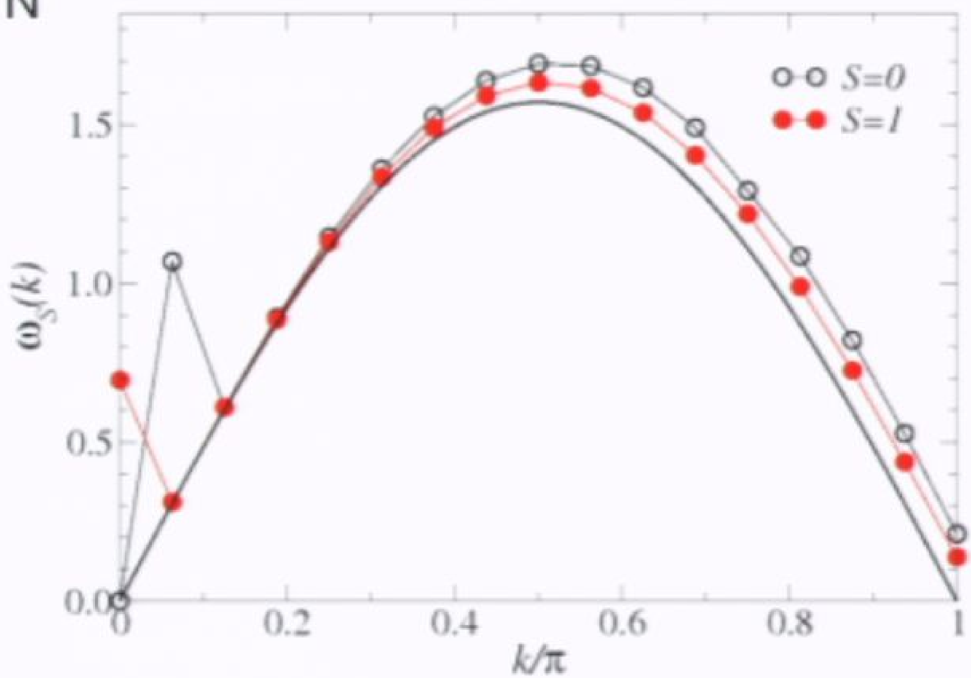
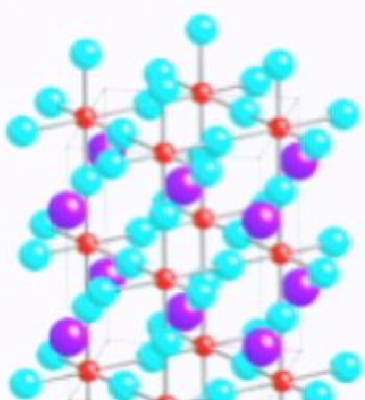


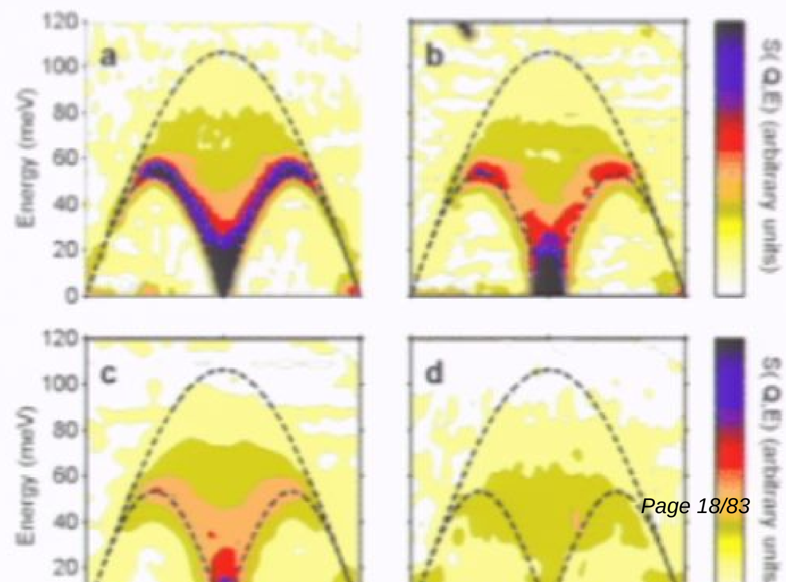


Neutron scattering experiments

- quasi-one-dimensional $KCuF_3$

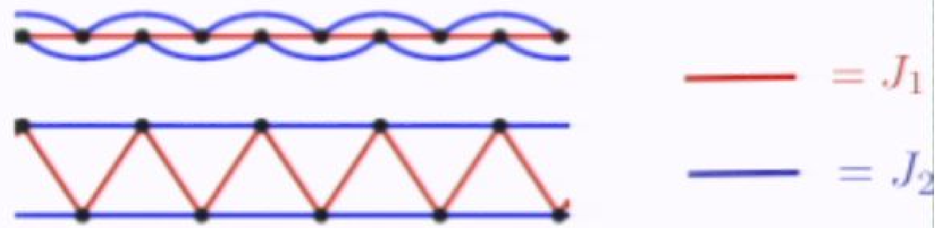
B. Lake et al., Nature Materials 4 329-334 (2005)





Heisenberg chain with frustrated interactions

$$H = \sum_{i=1}^{N} \left[J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right]$$



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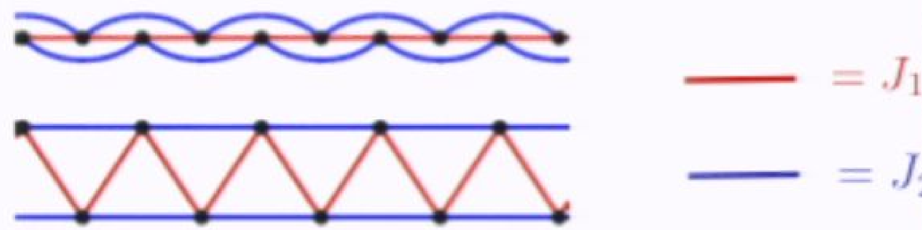

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$$|\Psi_A\rangle = |(1,2)(3,4)(5,6)\cdots\rangle$$

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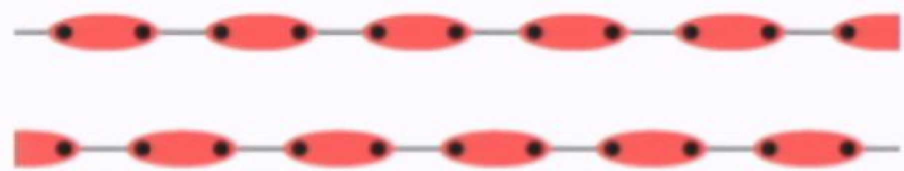

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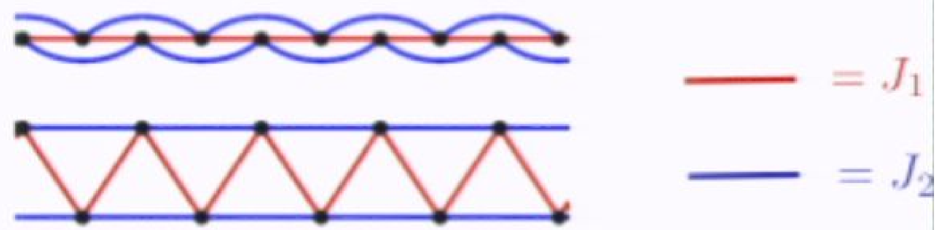

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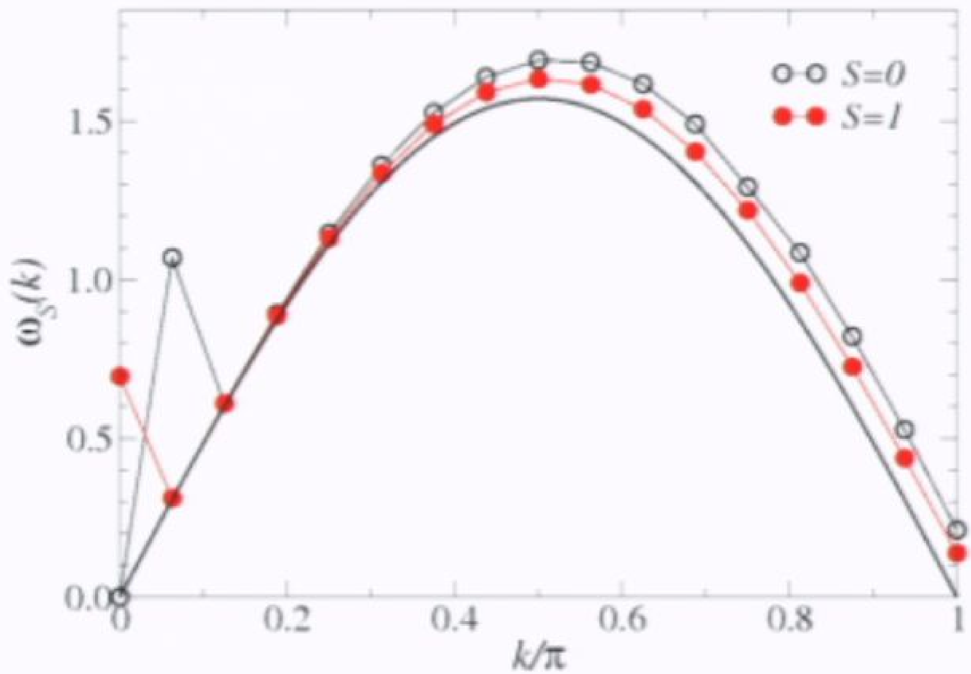

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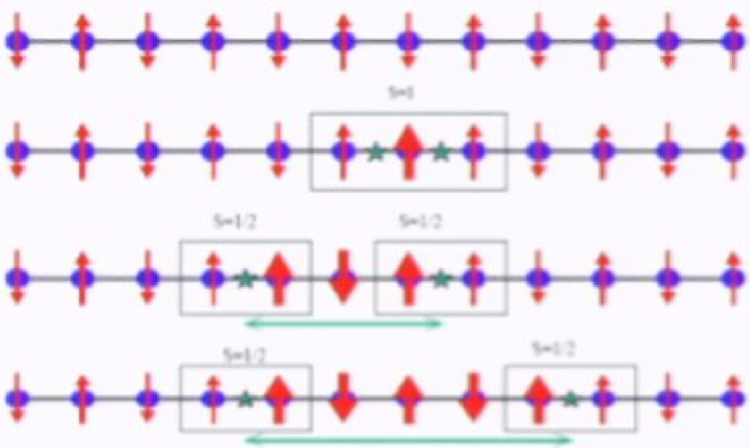

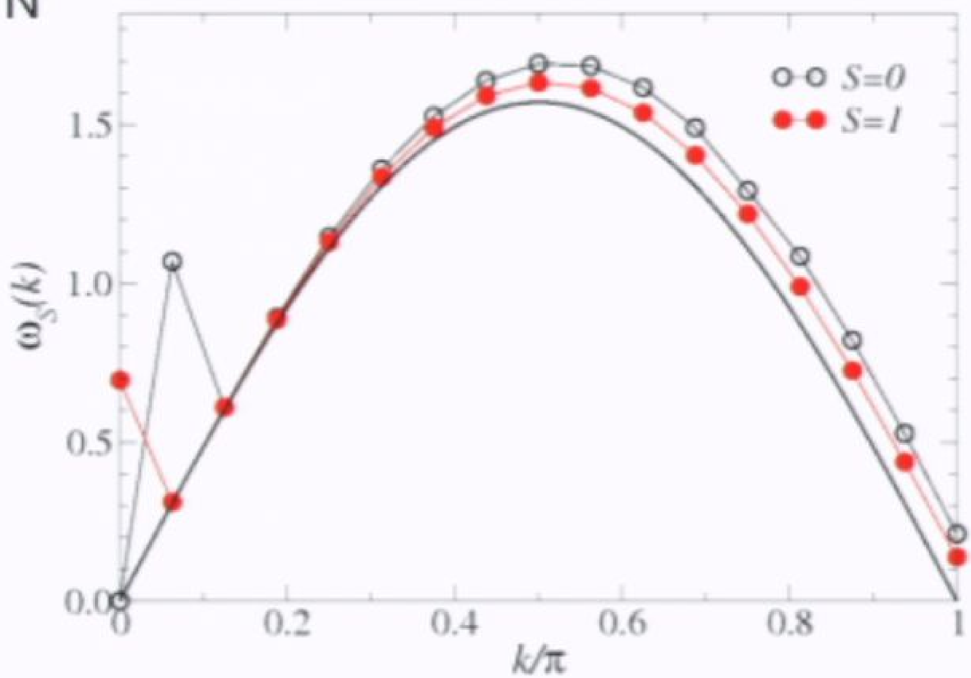

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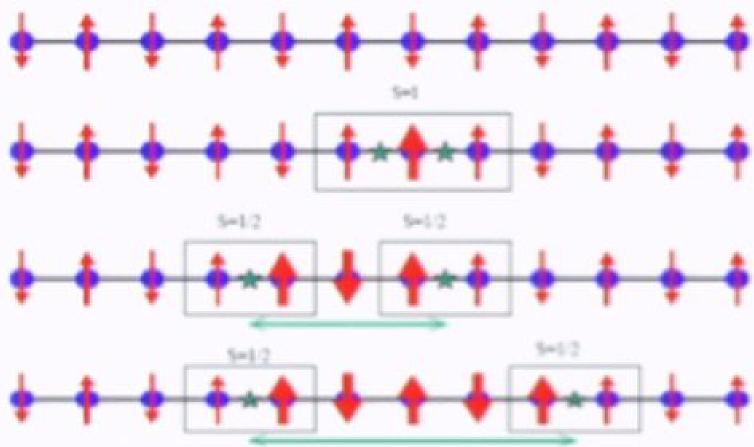

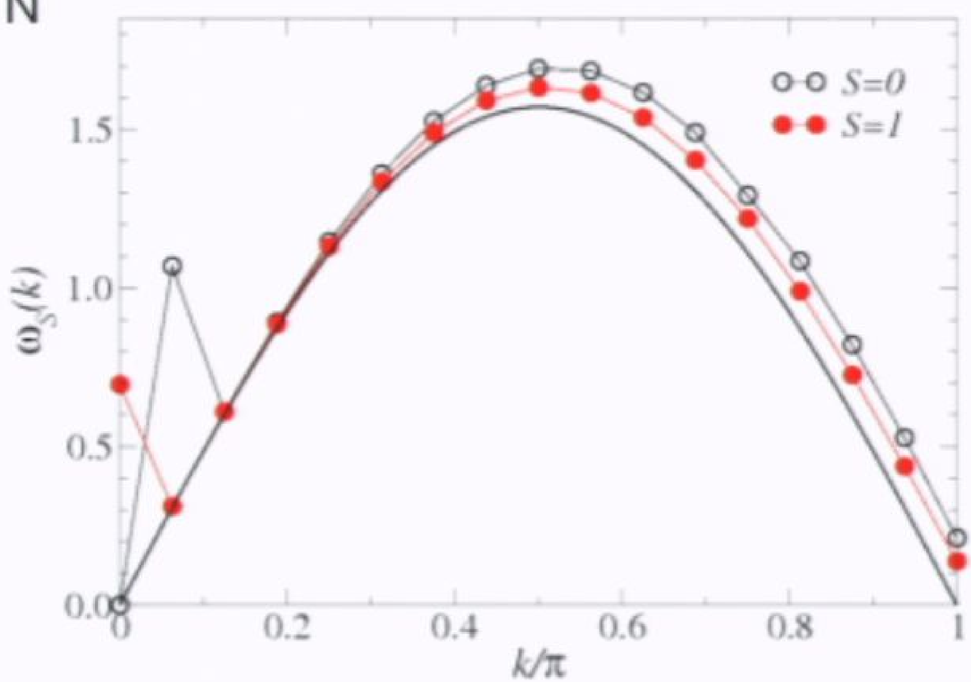

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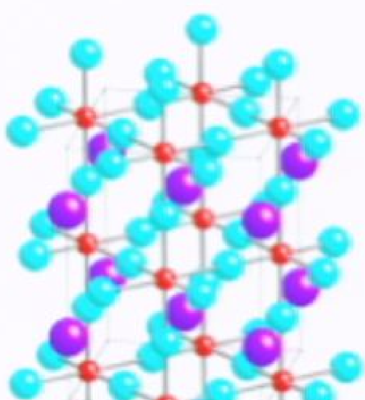

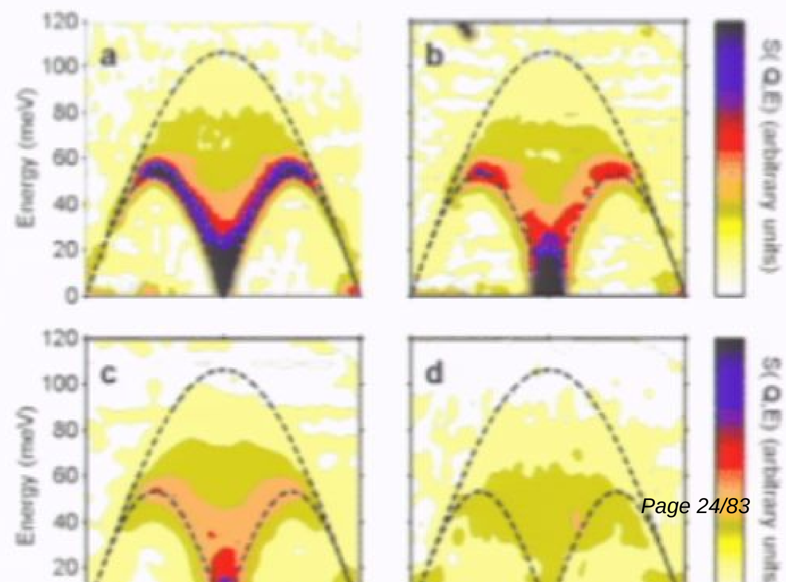

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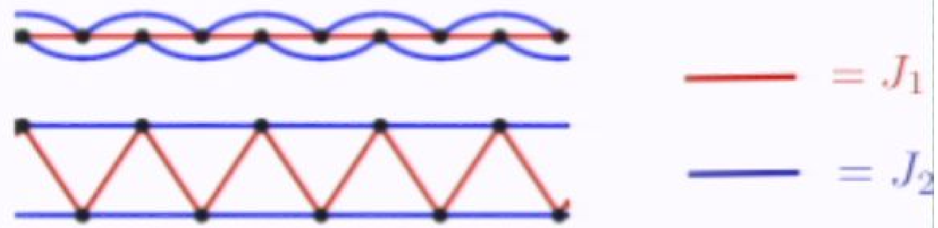

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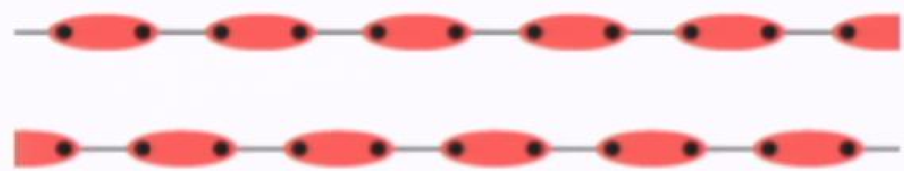

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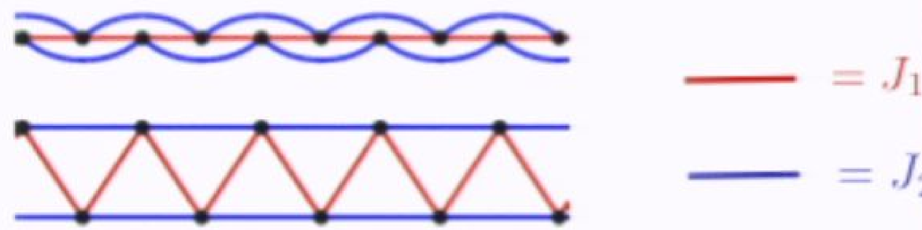

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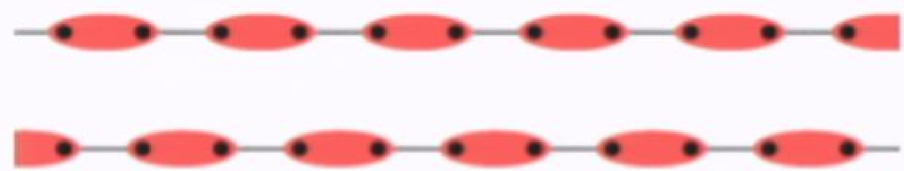

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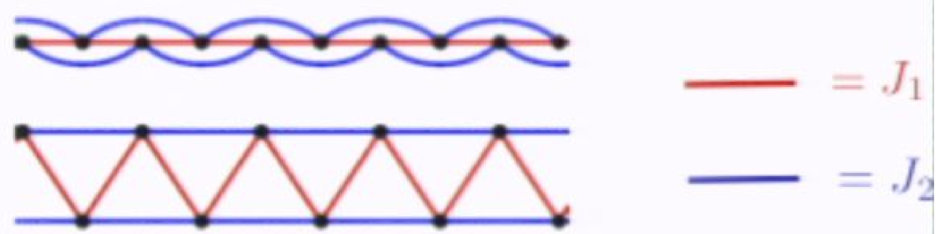

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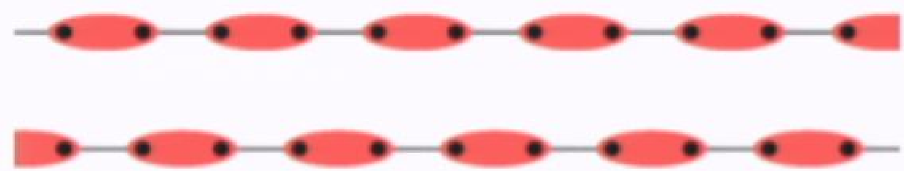

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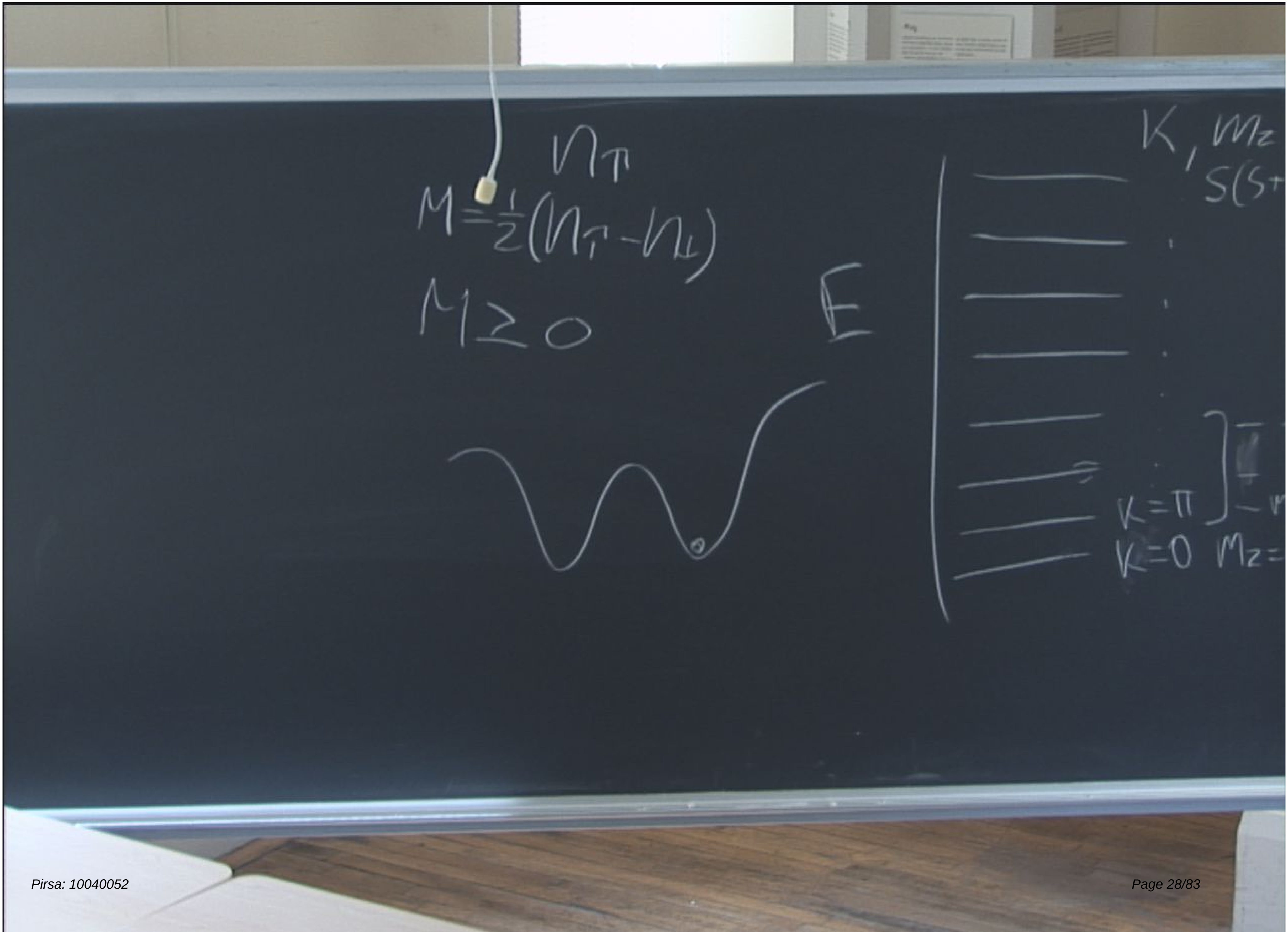
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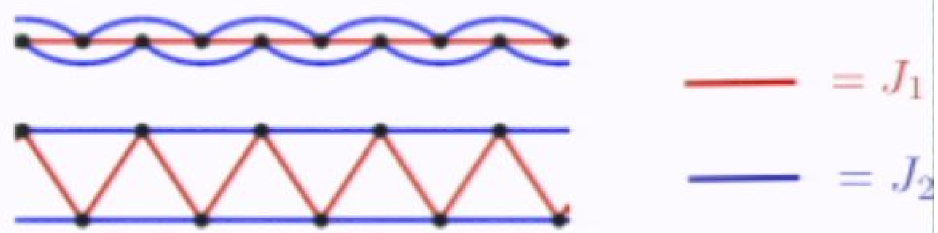

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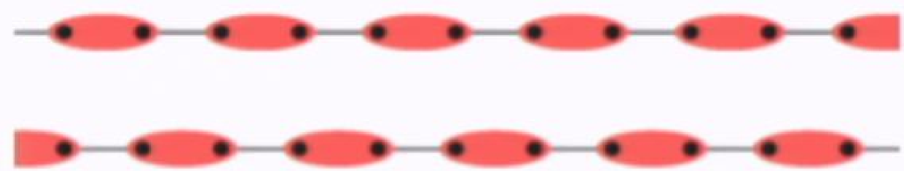

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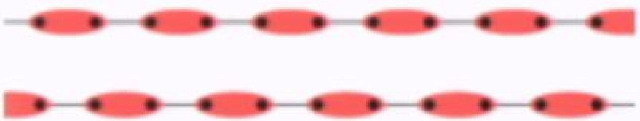

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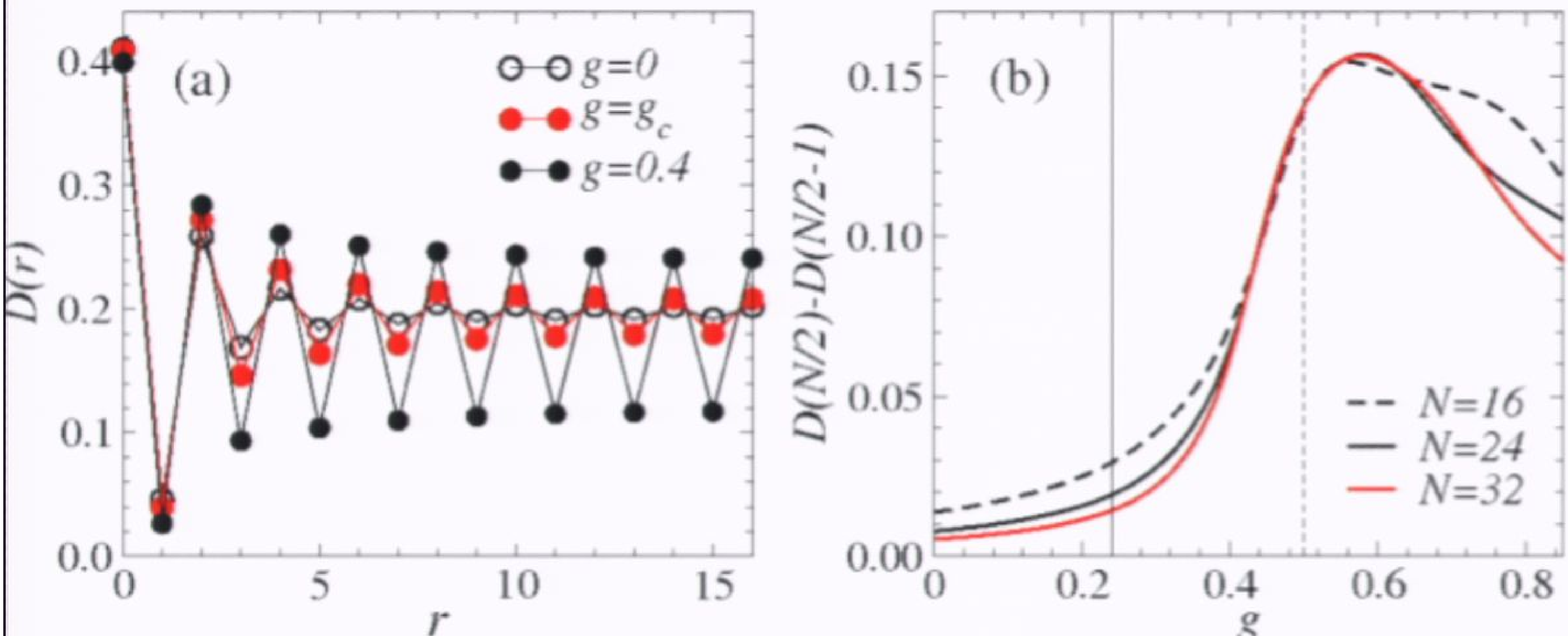

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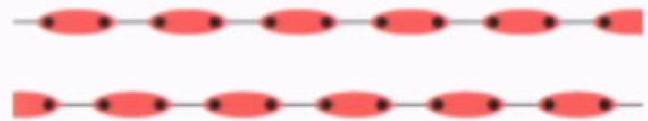

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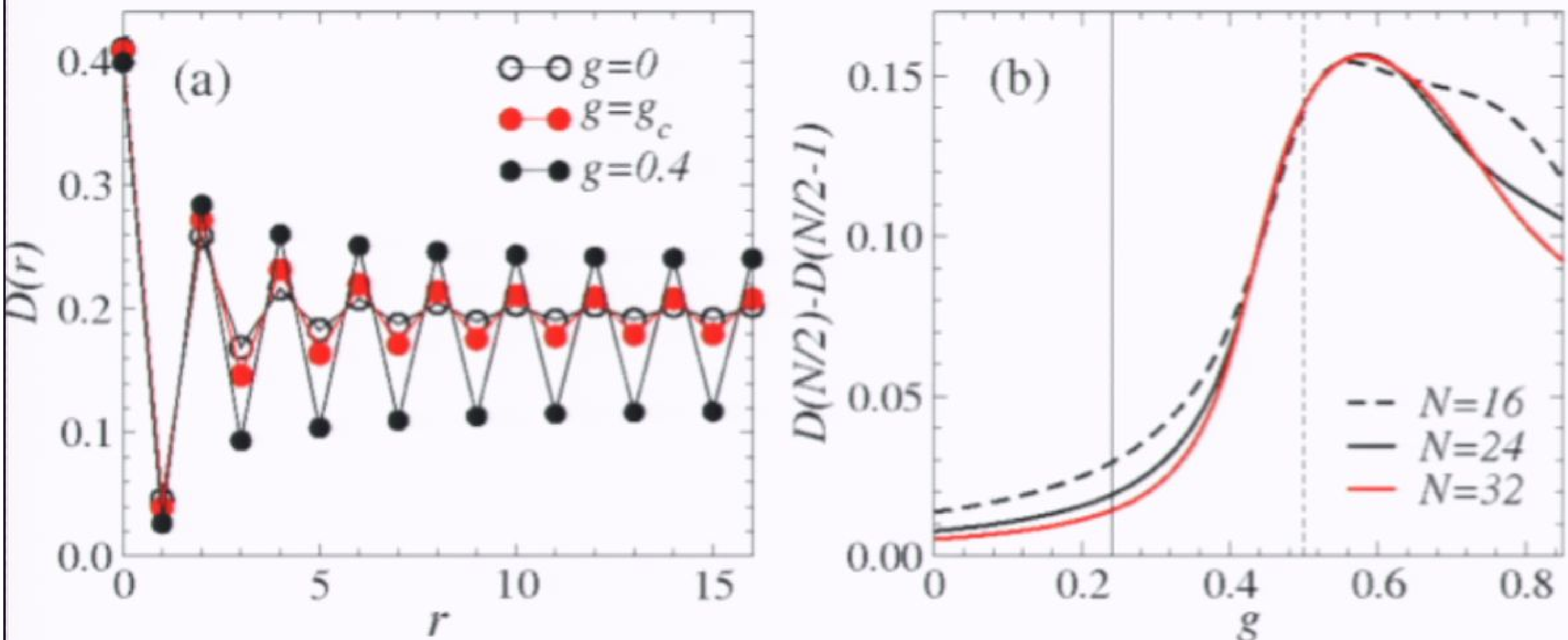

It is not easy to detect the transition this way

- "infinite-order" transition; exponential (slow) growth of the VBS order
- much larger systems are needed for observing a sharp transition

Determining the transition point using level crossings

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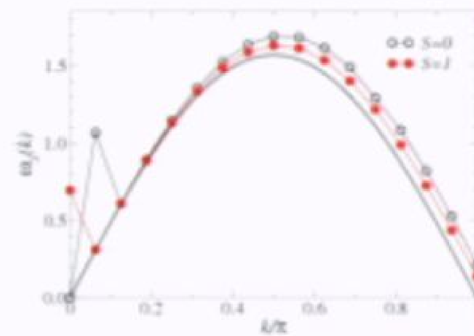
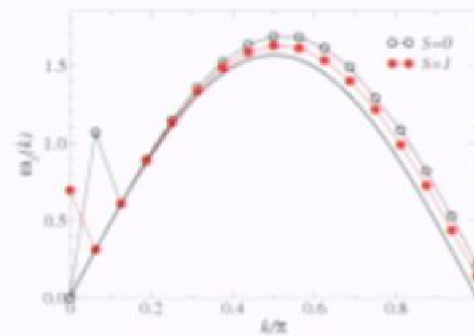


Lowest excitation for the g=0 Heisenberg chain is a triplet

- this can be expected for all $g<g_c$

Determining the transition point using level crossings



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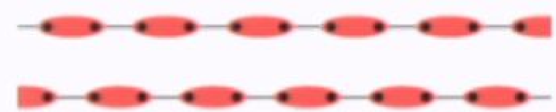

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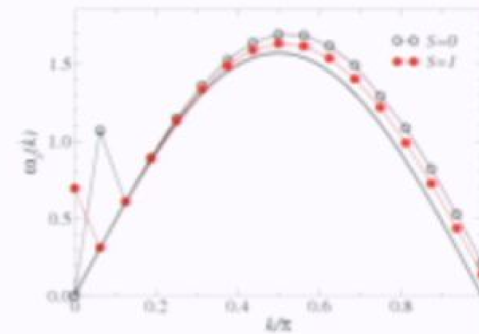

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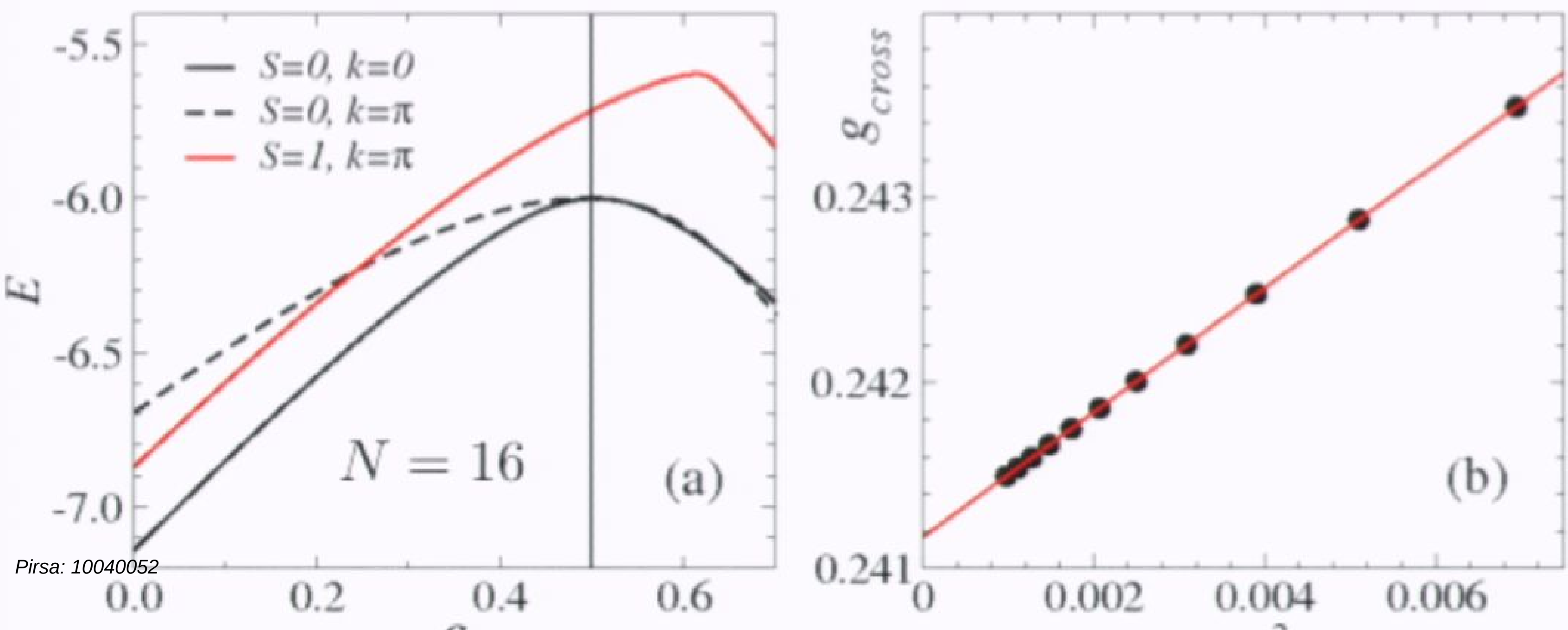

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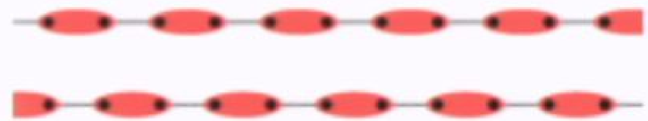

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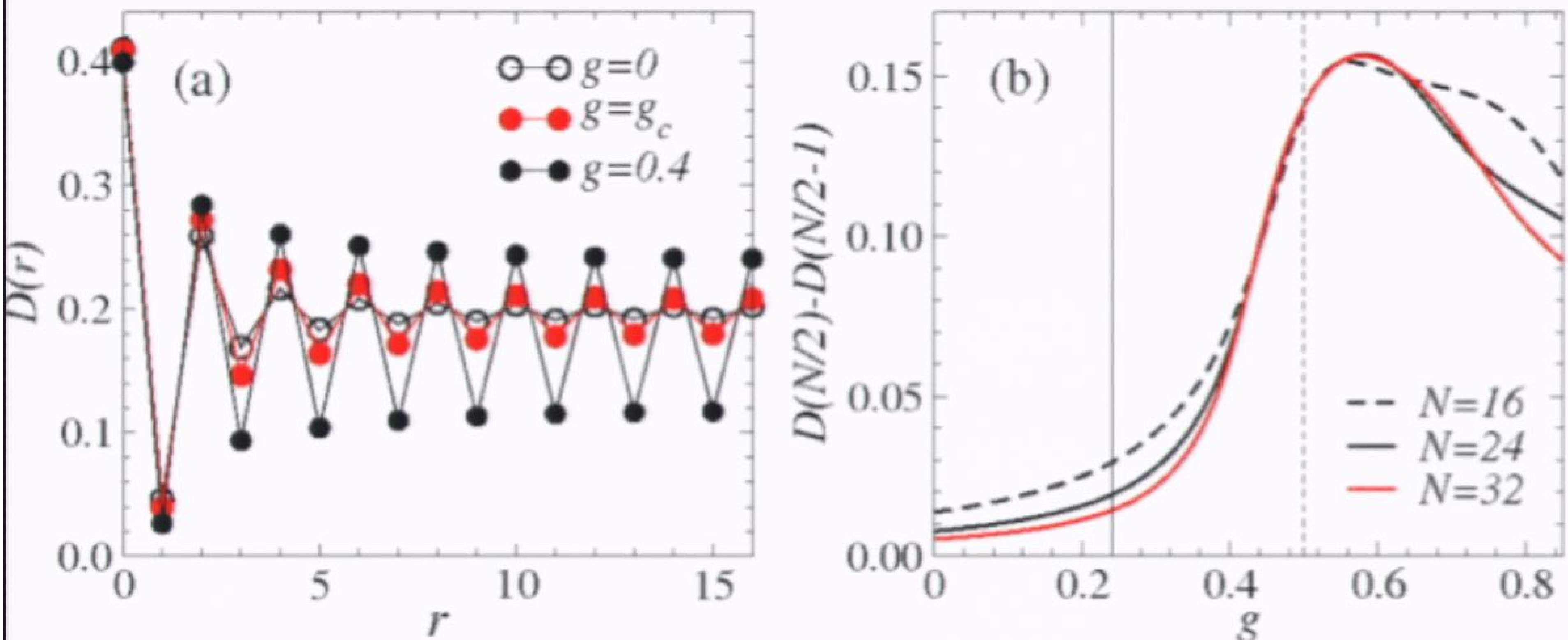

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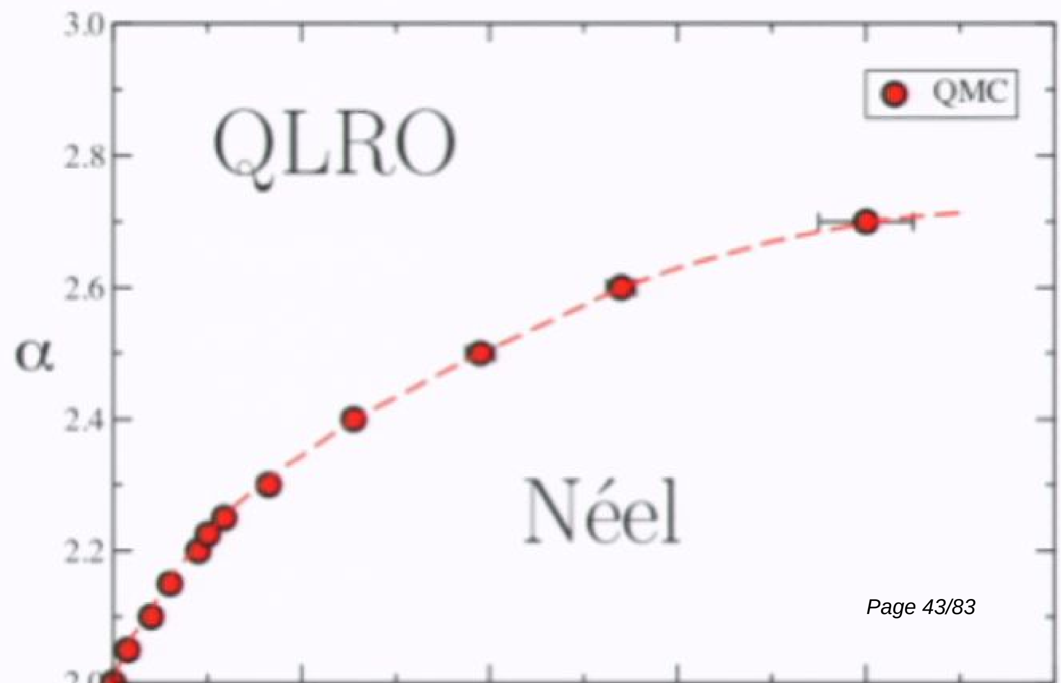

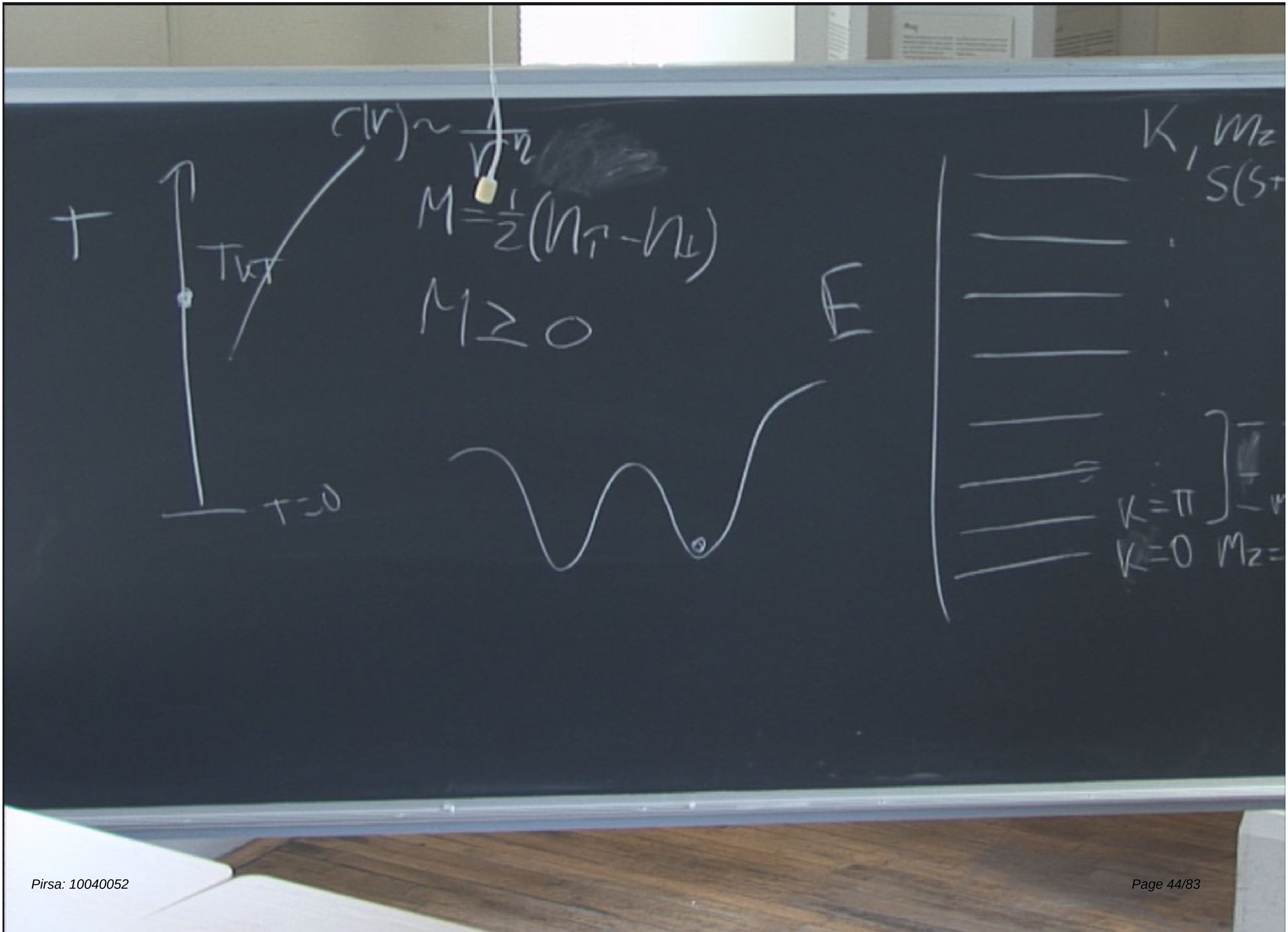

C(r) ~ 1/r^η
M = 1/2 (n↑ − n↓)
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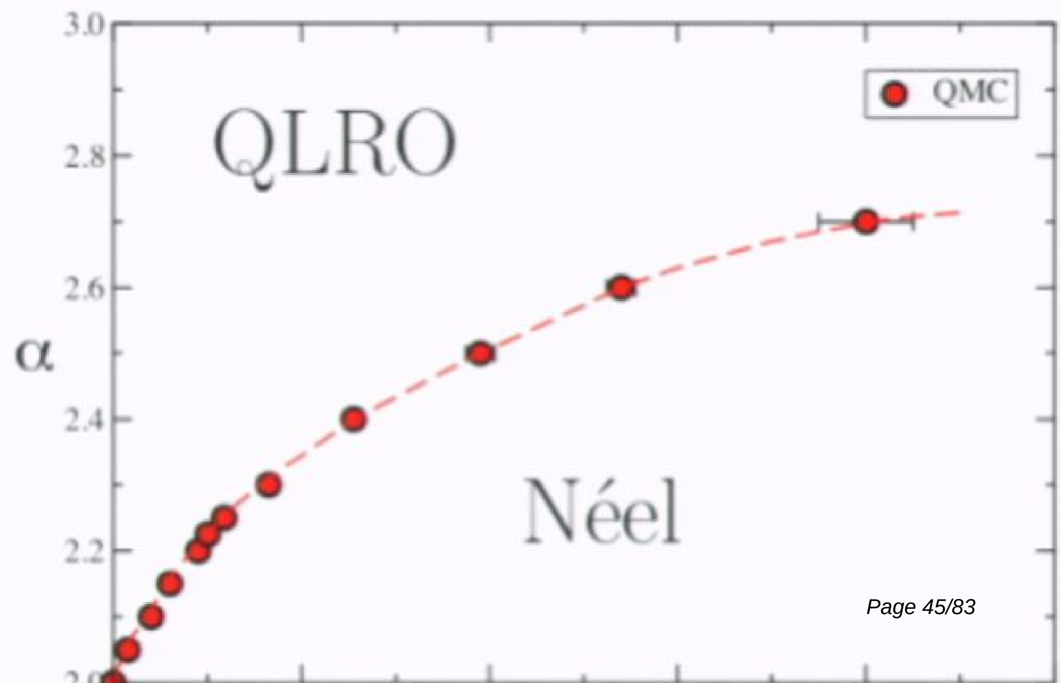

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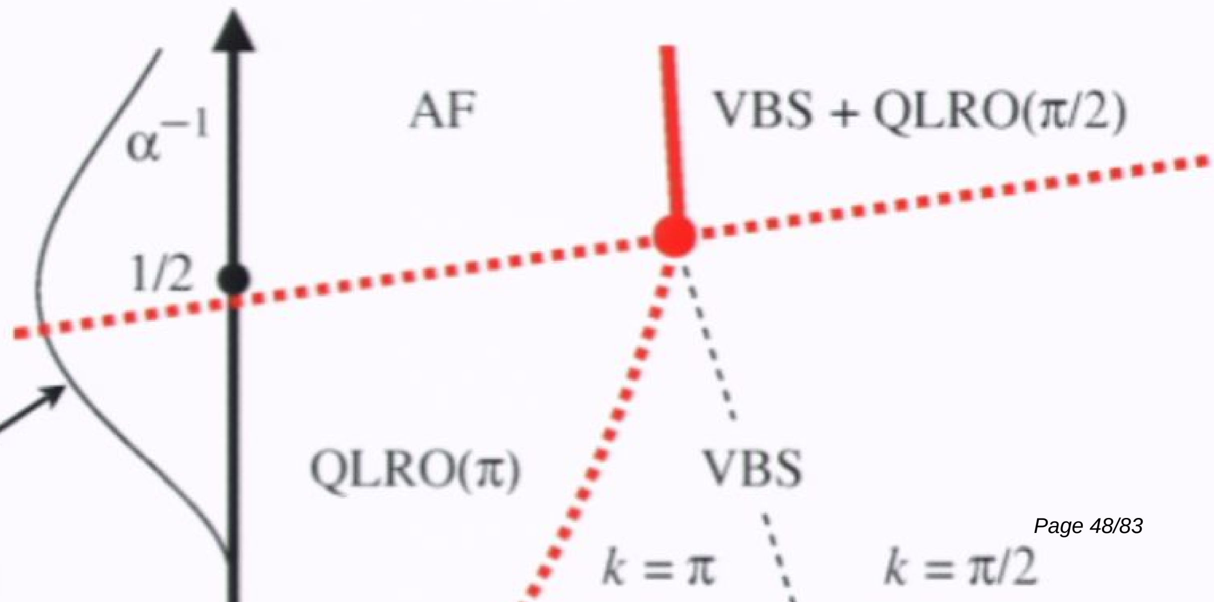

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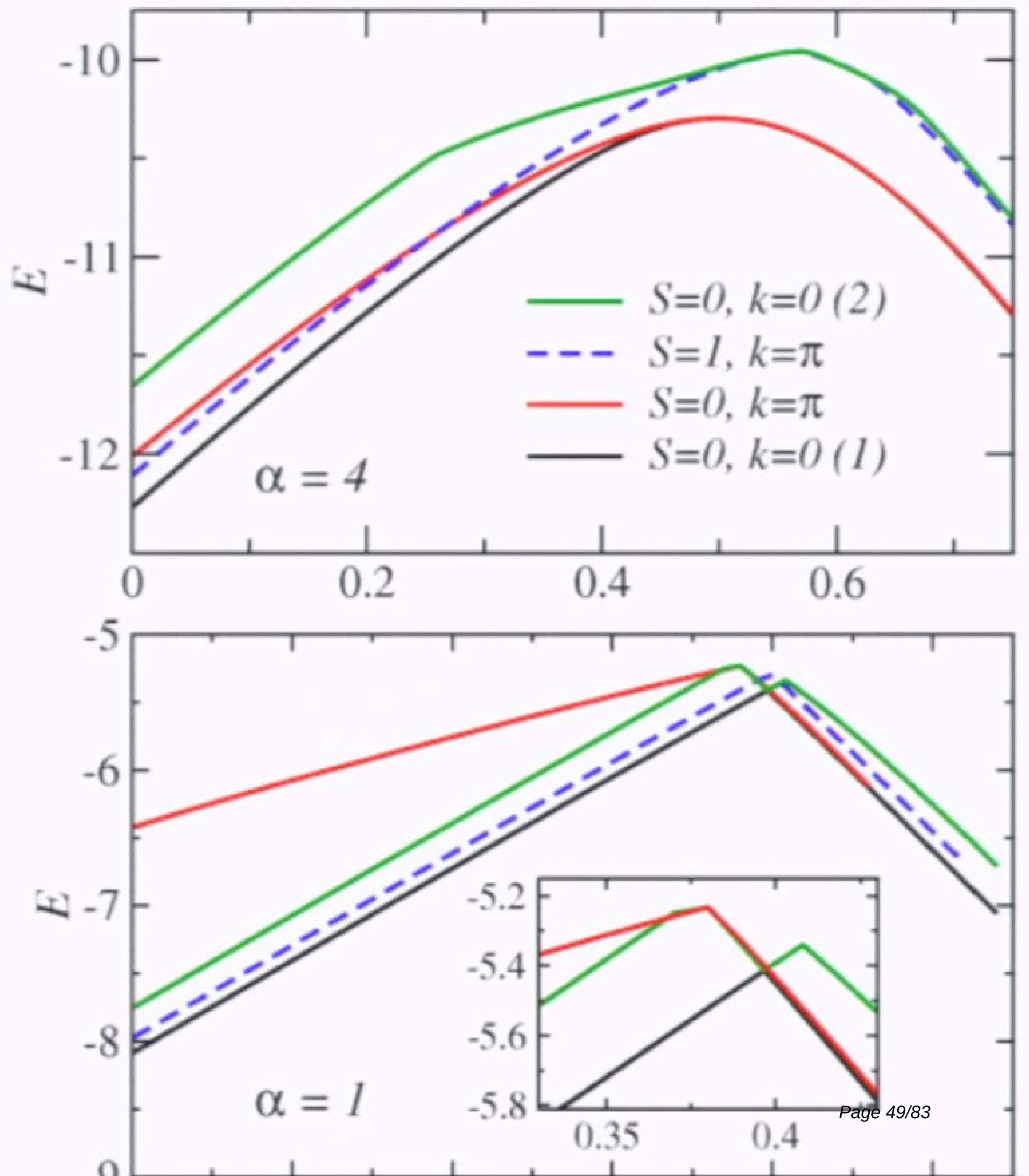

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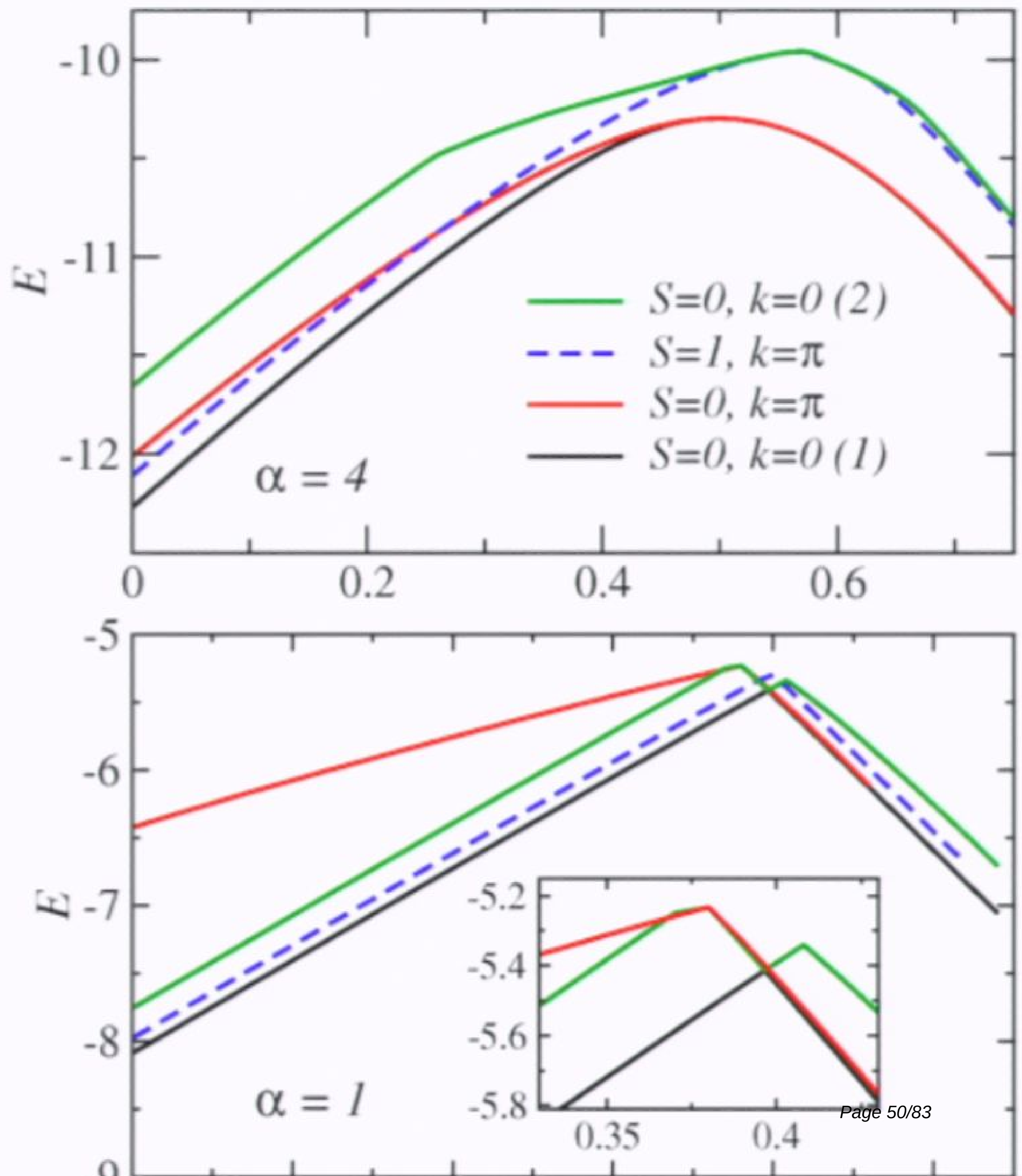

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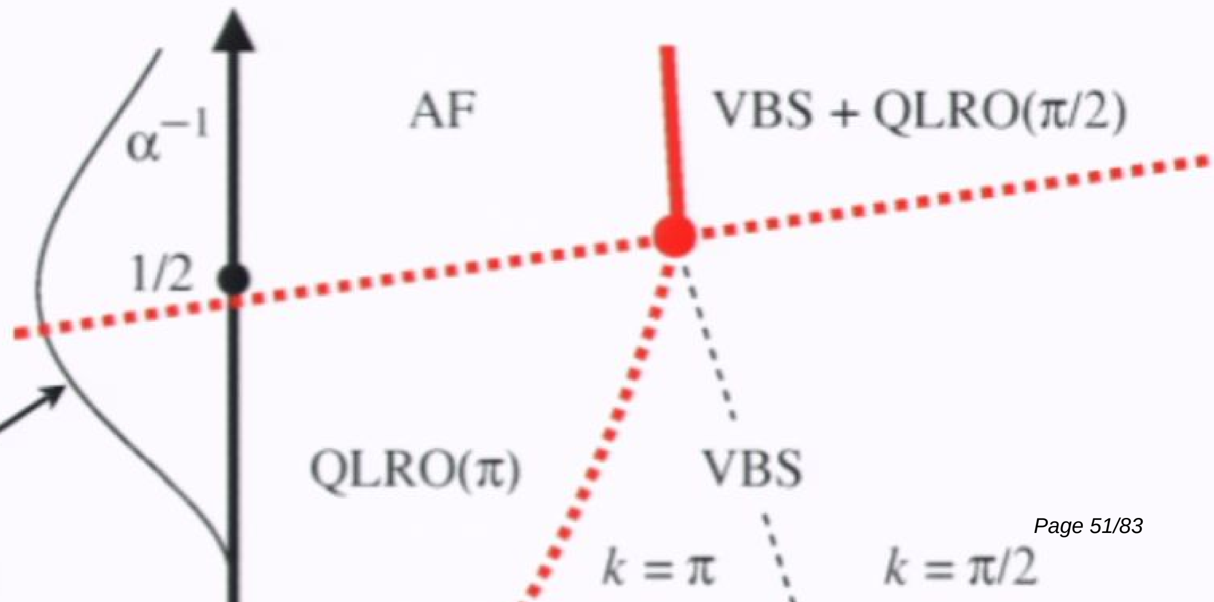

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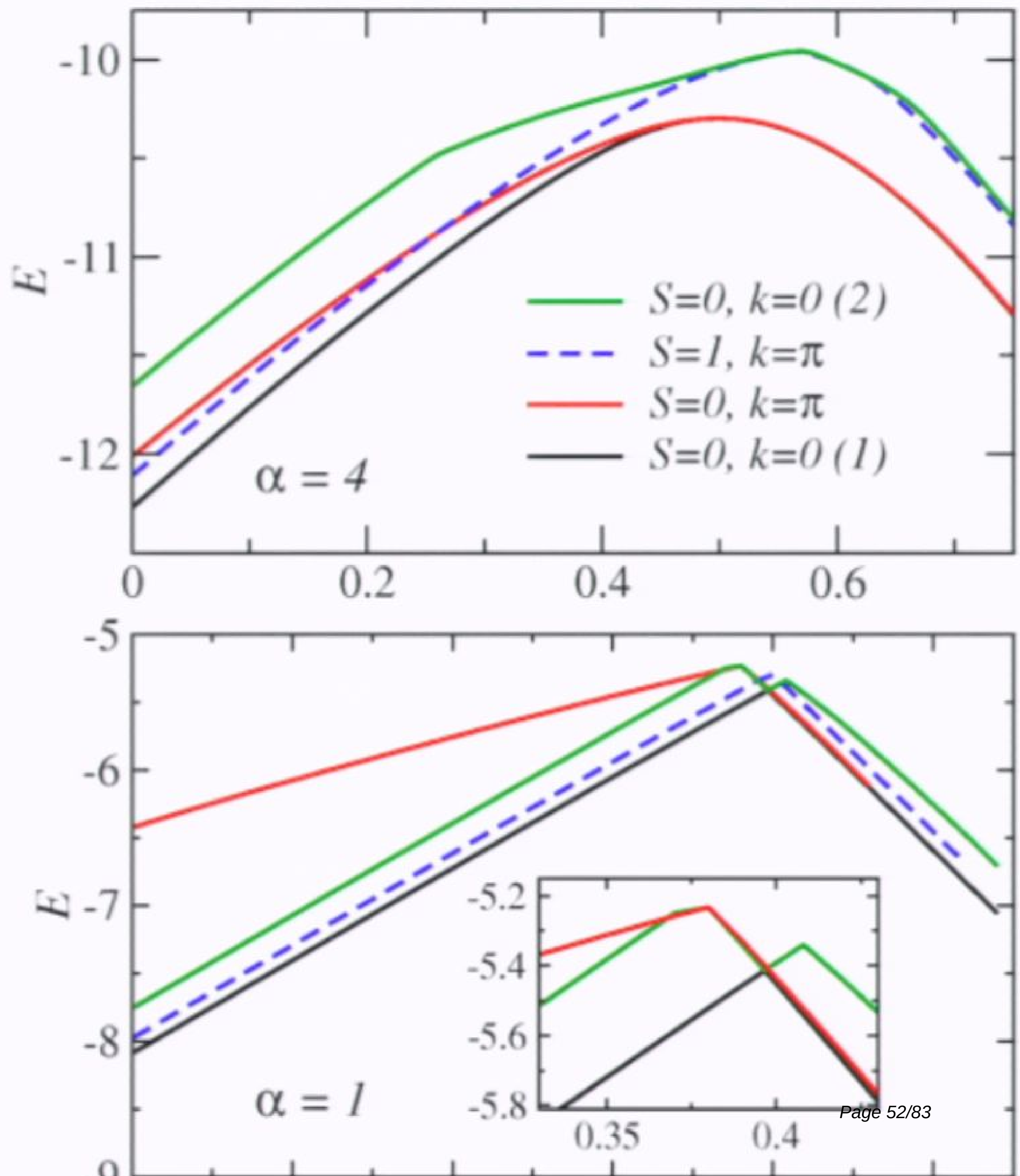

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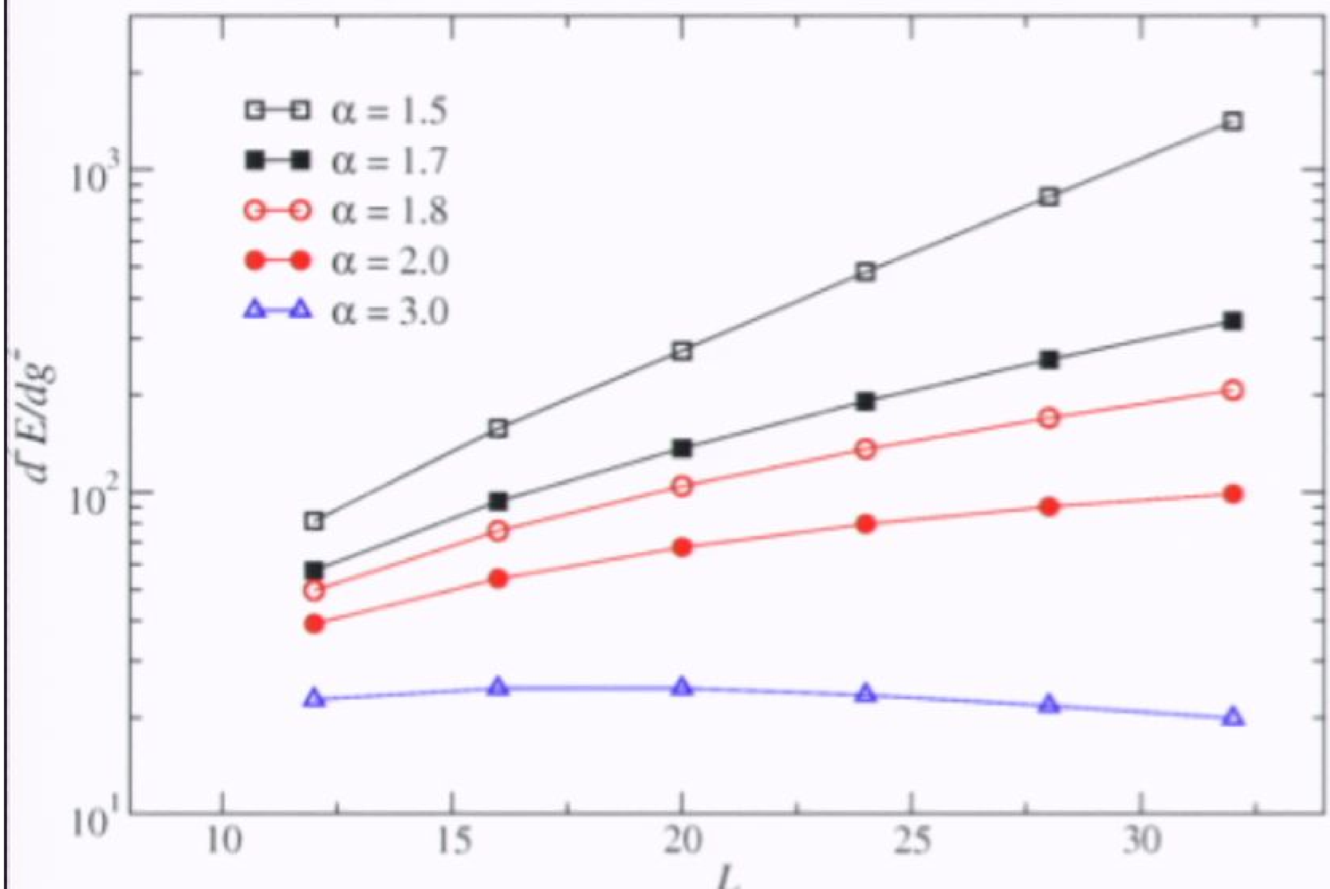

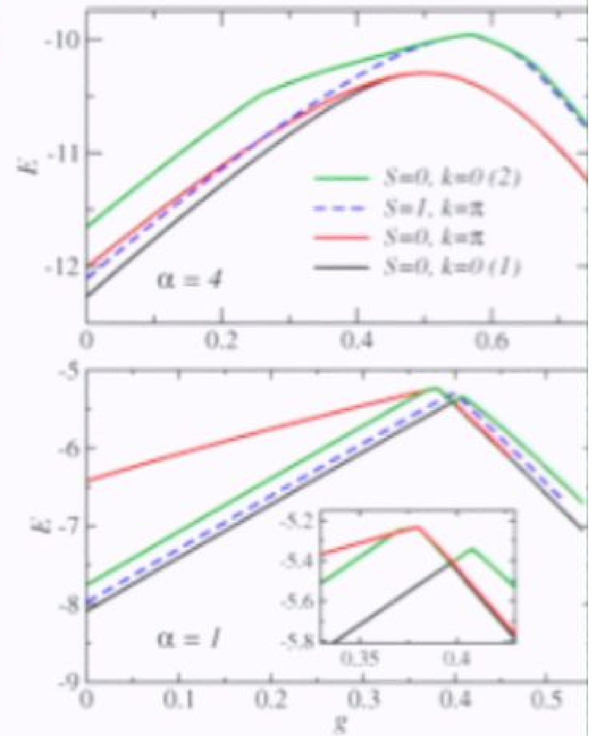

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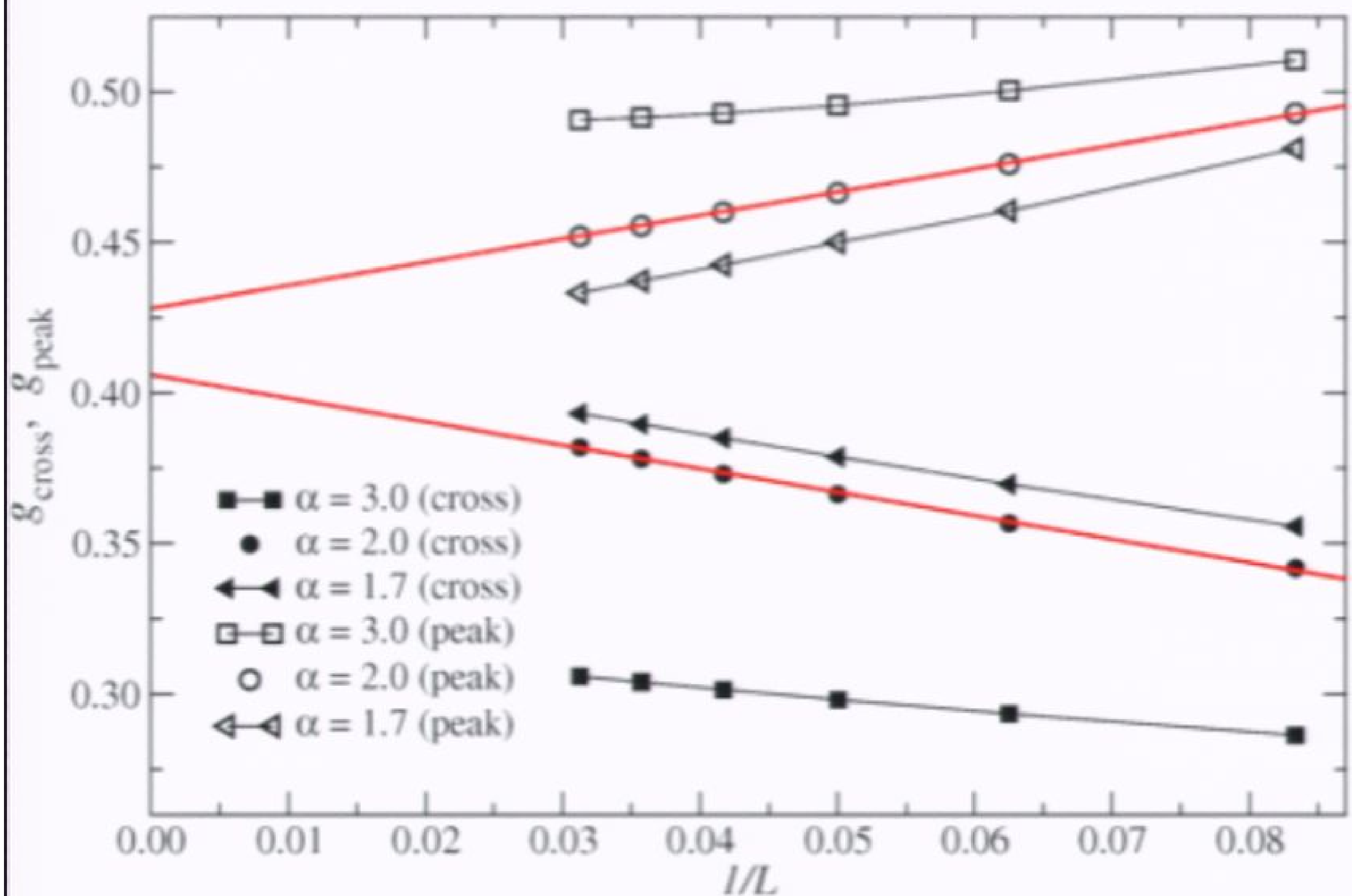

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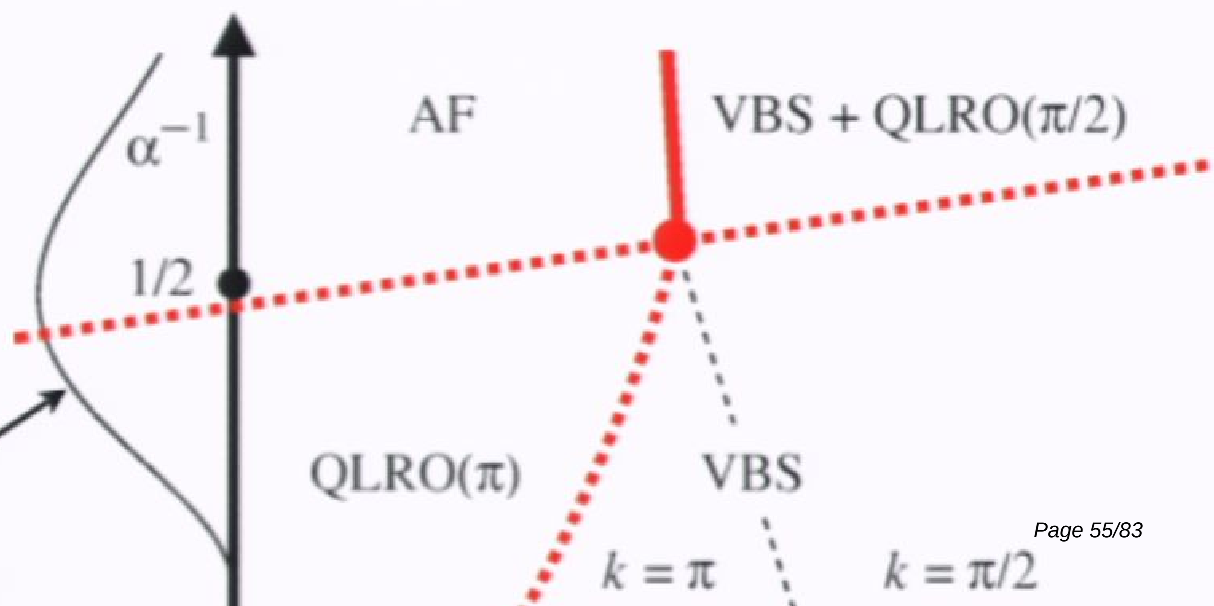

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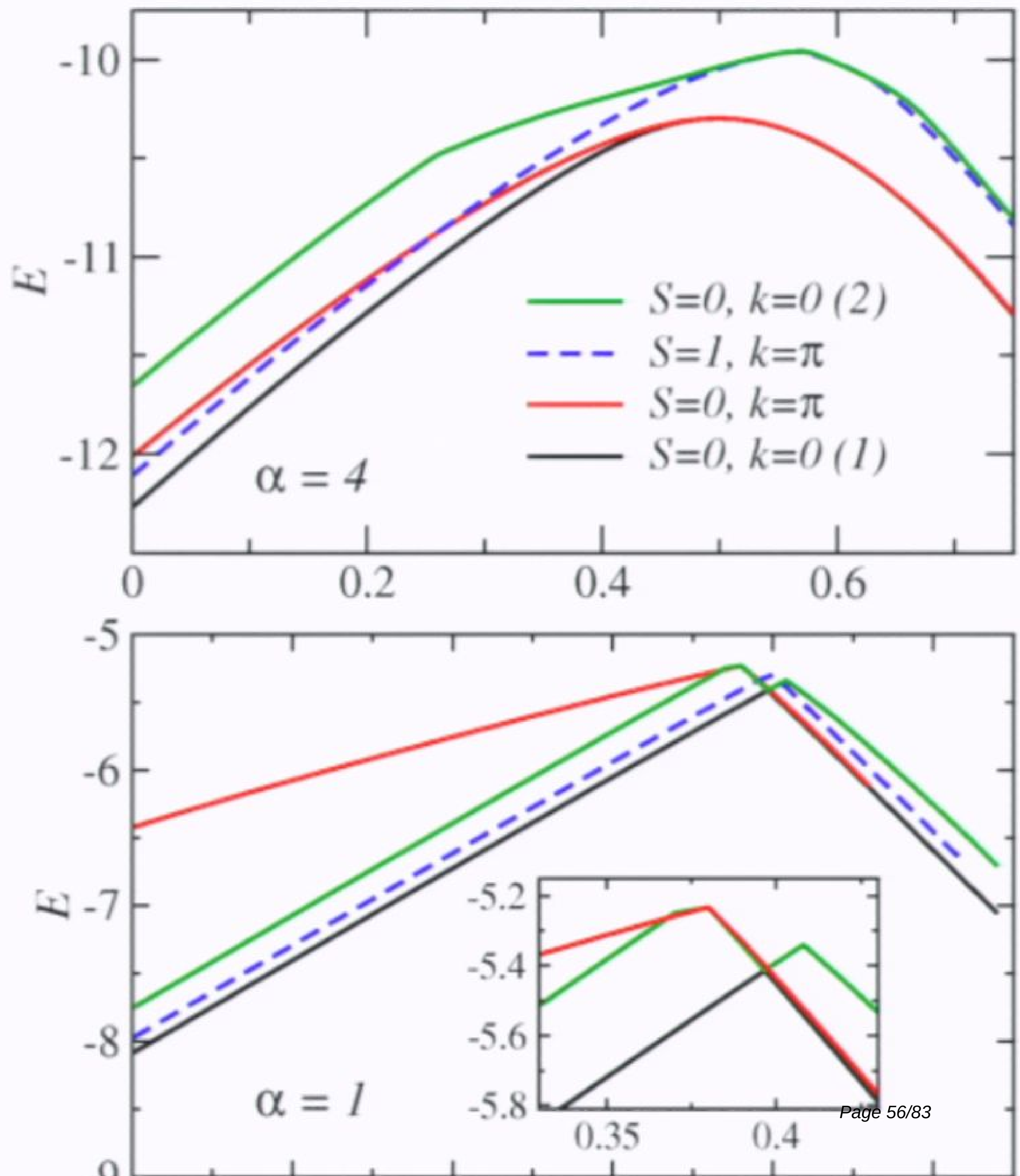

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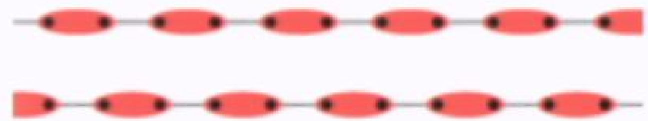

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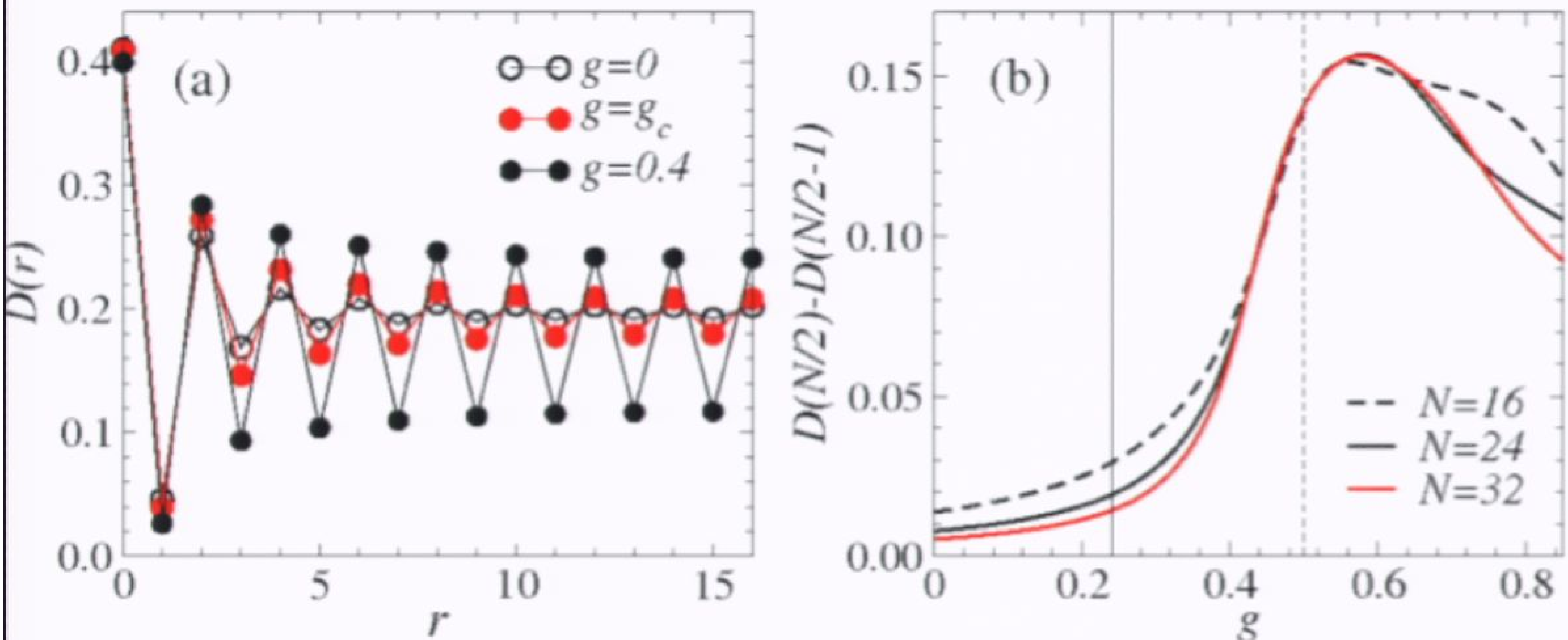

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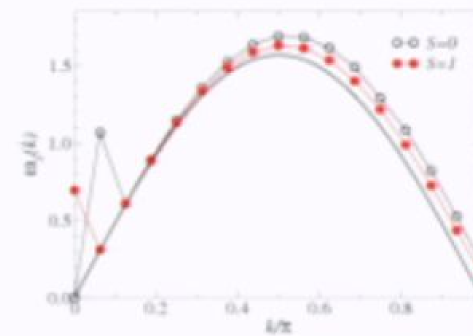

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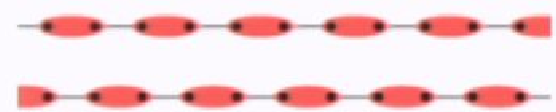

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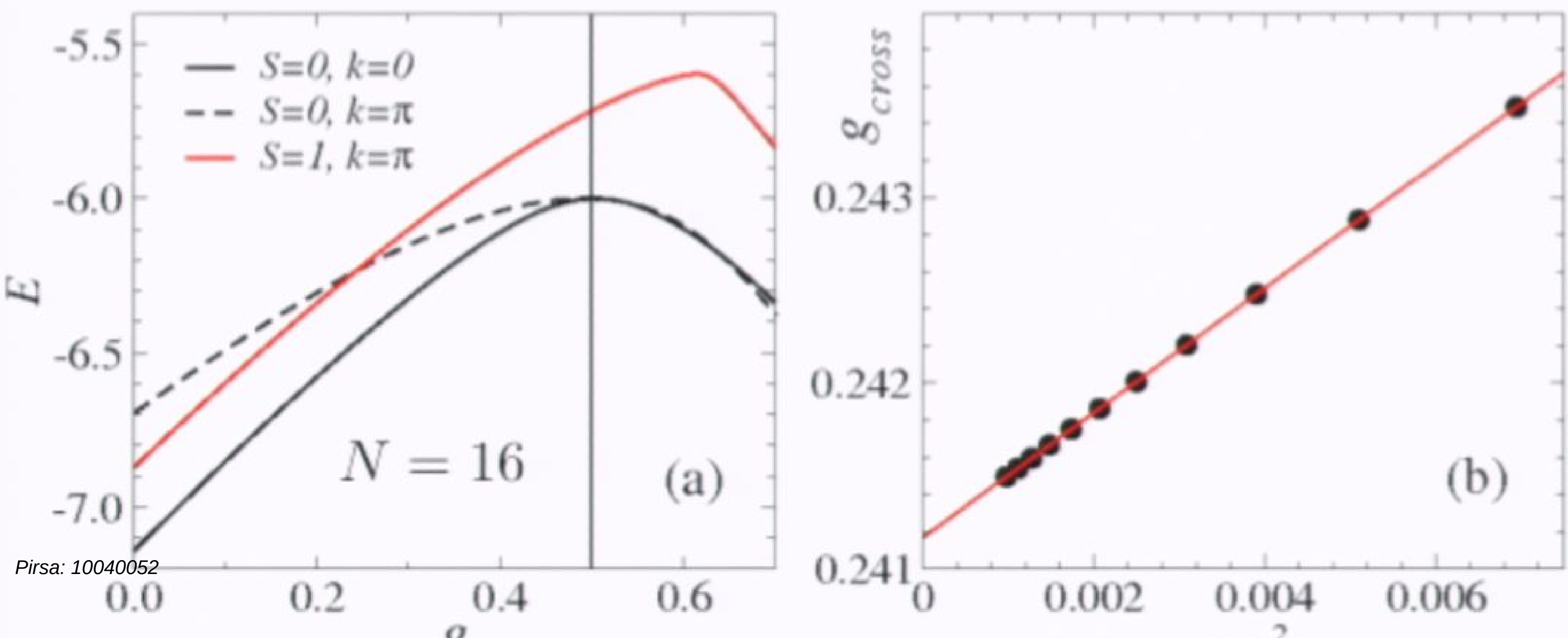

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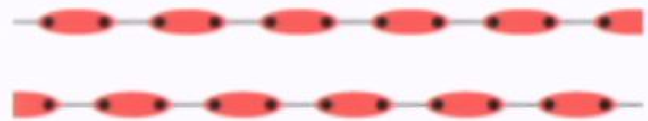

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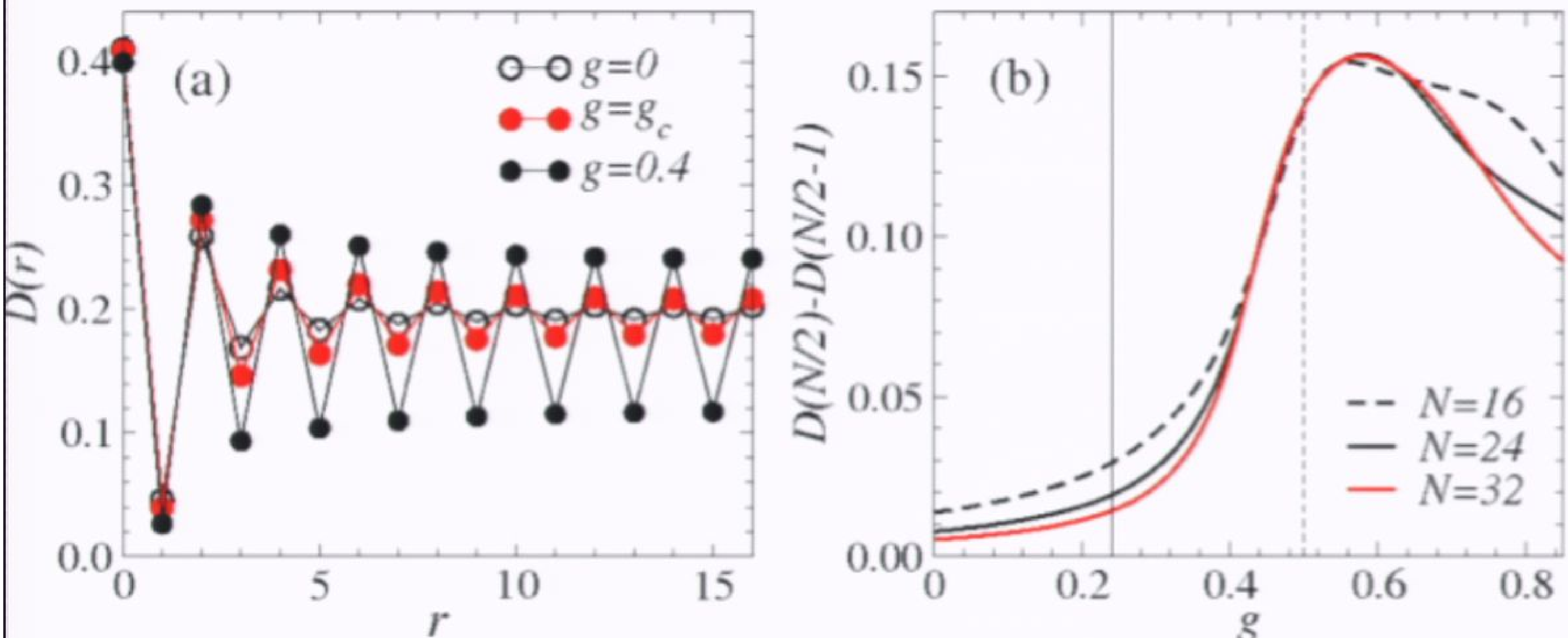

It is not easy to detect the transition this way

- "infinite-order" transition; exponential (slow) growth of the VBS order
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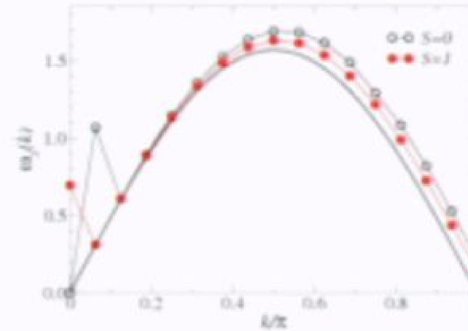

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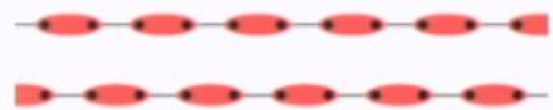

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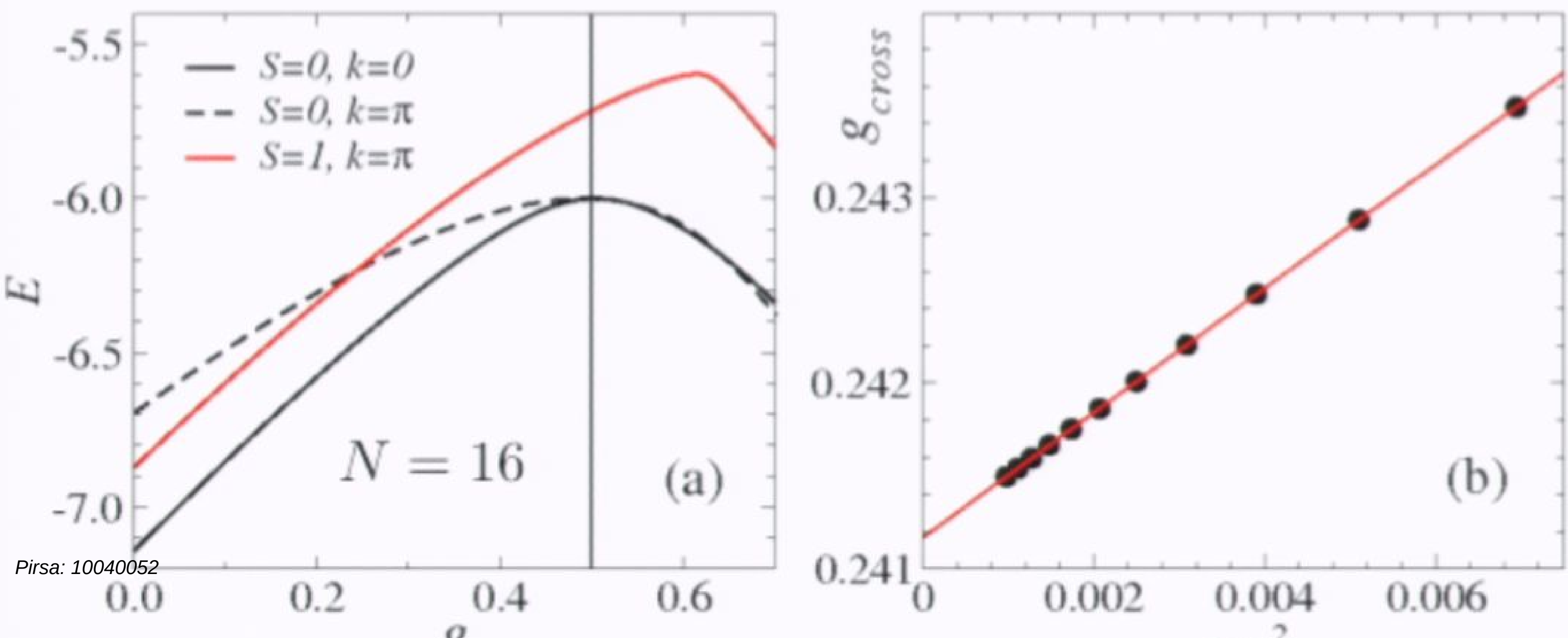

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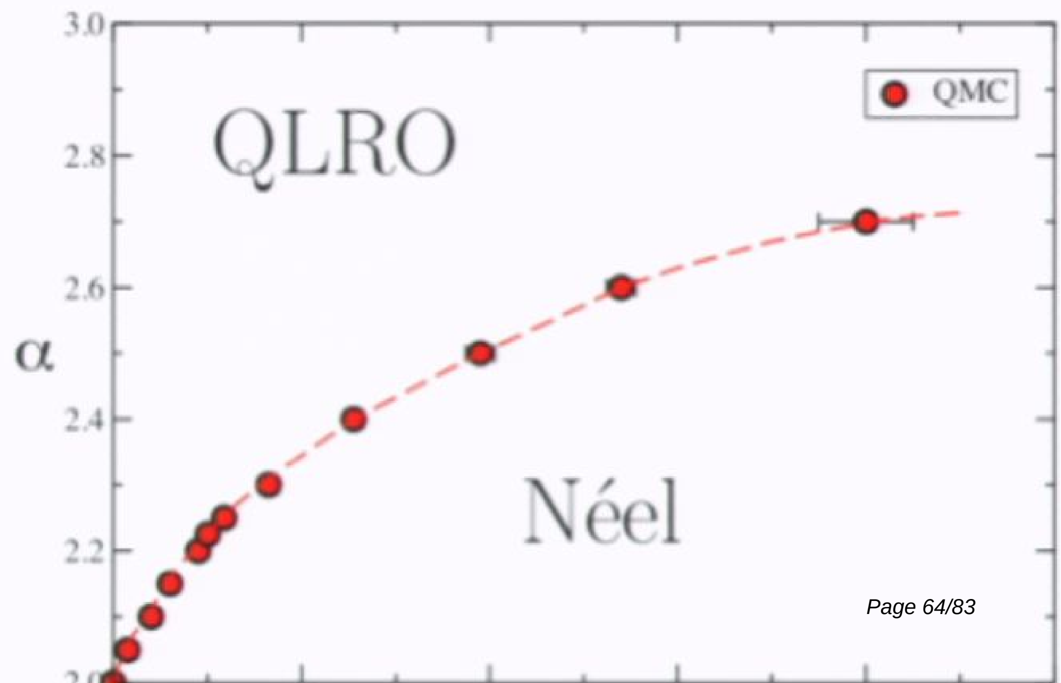

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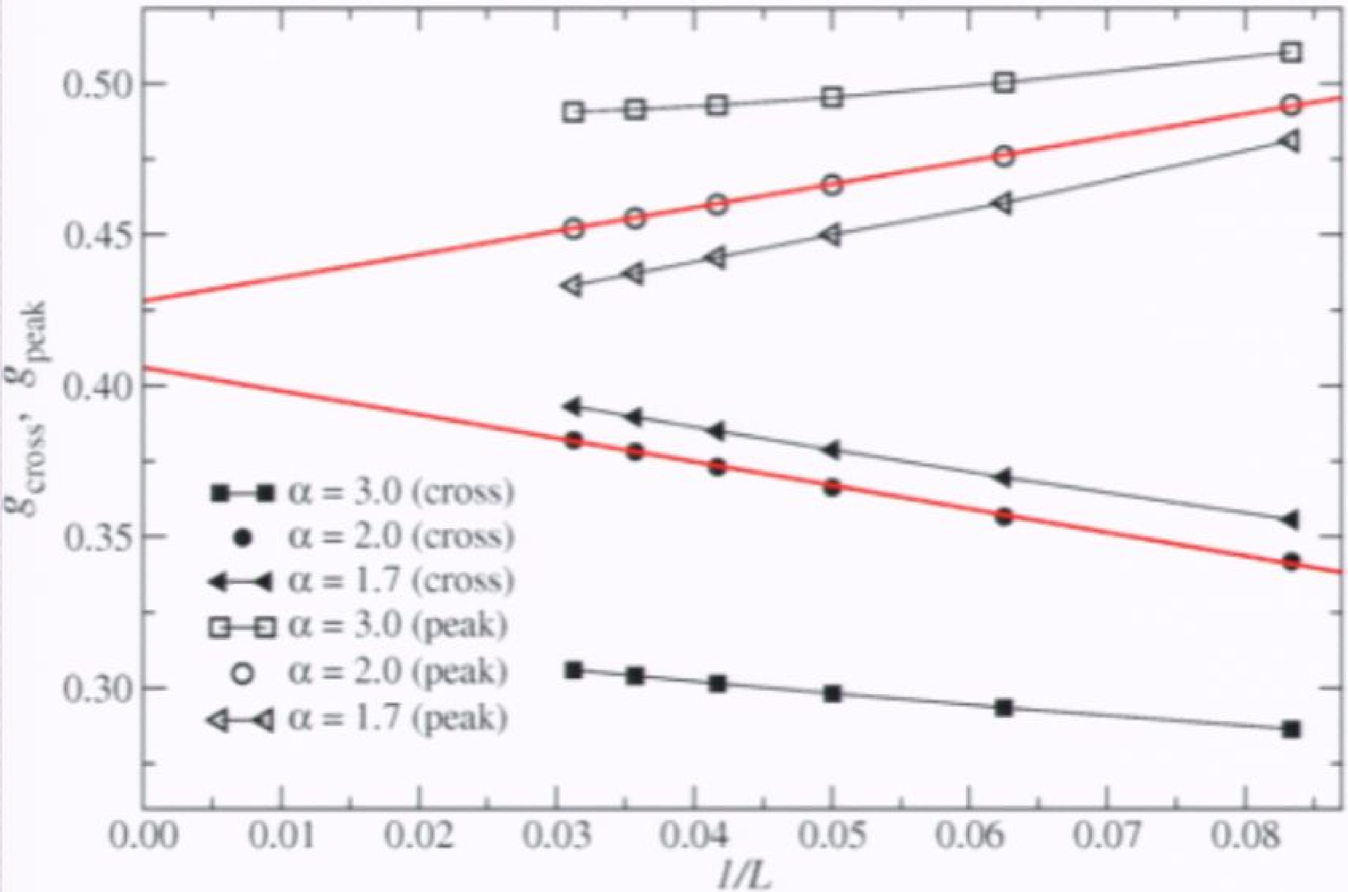

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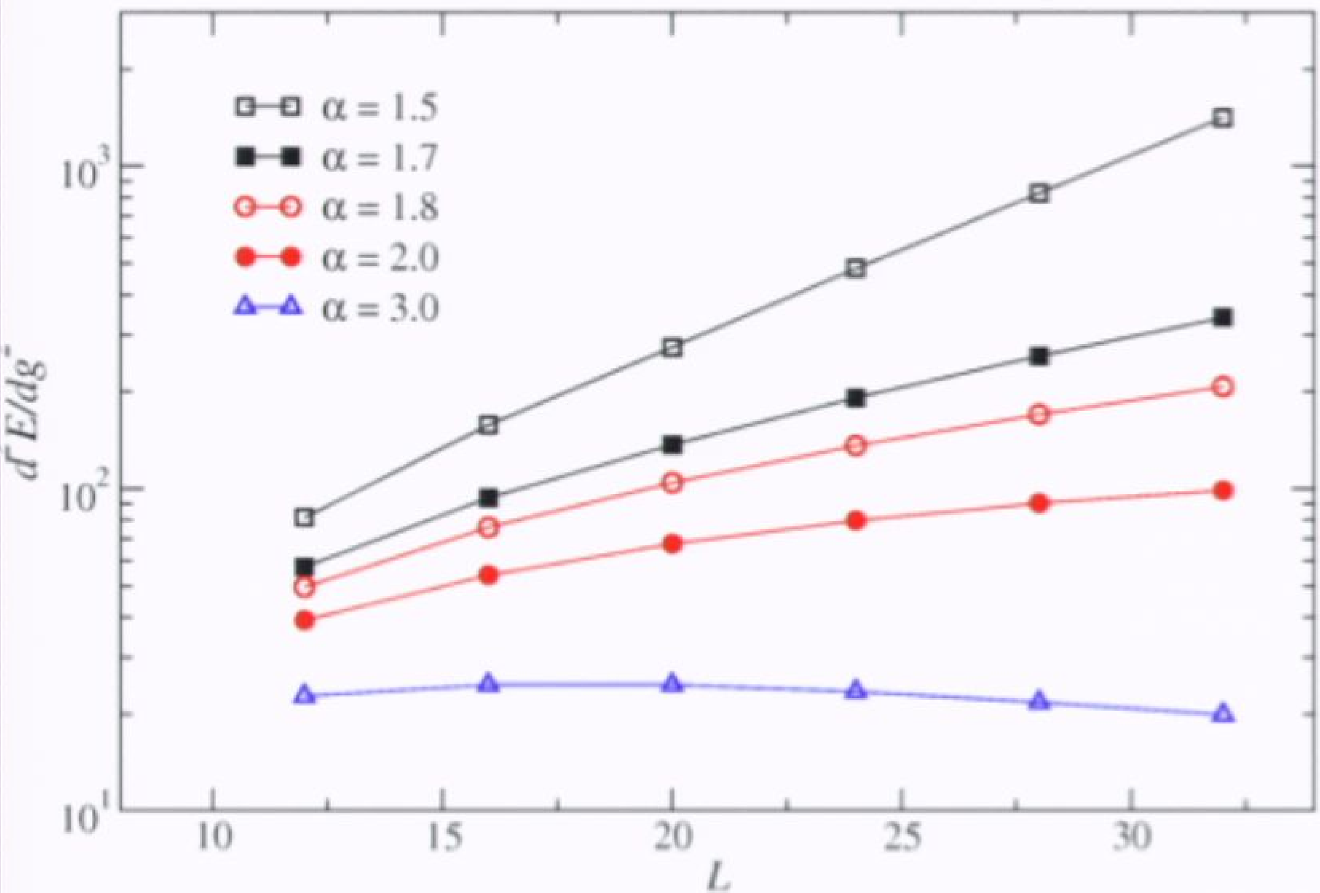

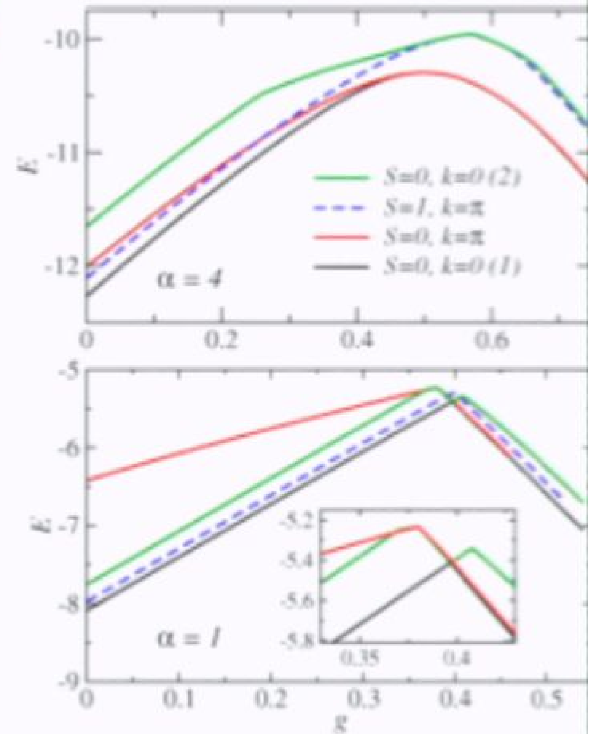

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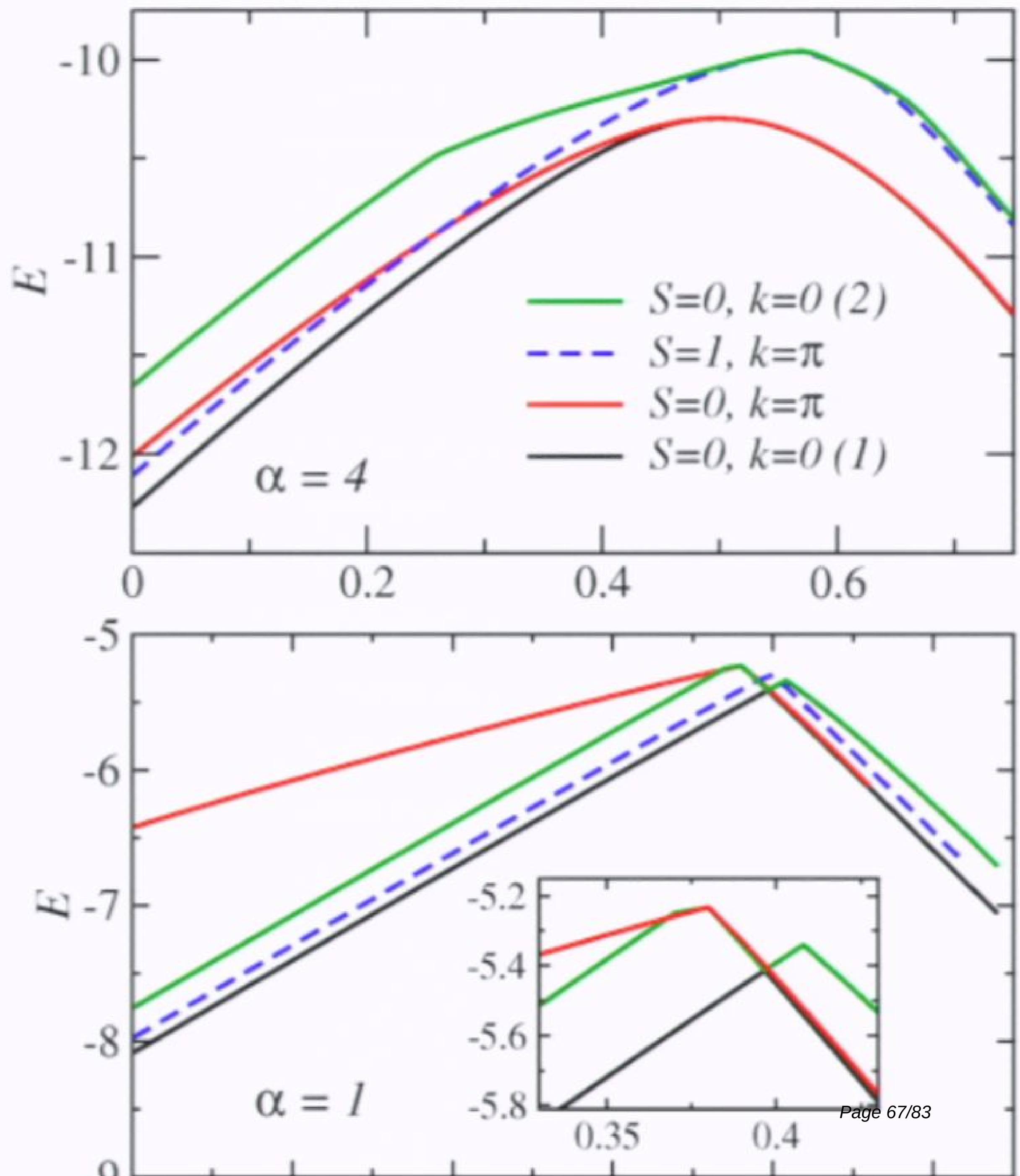

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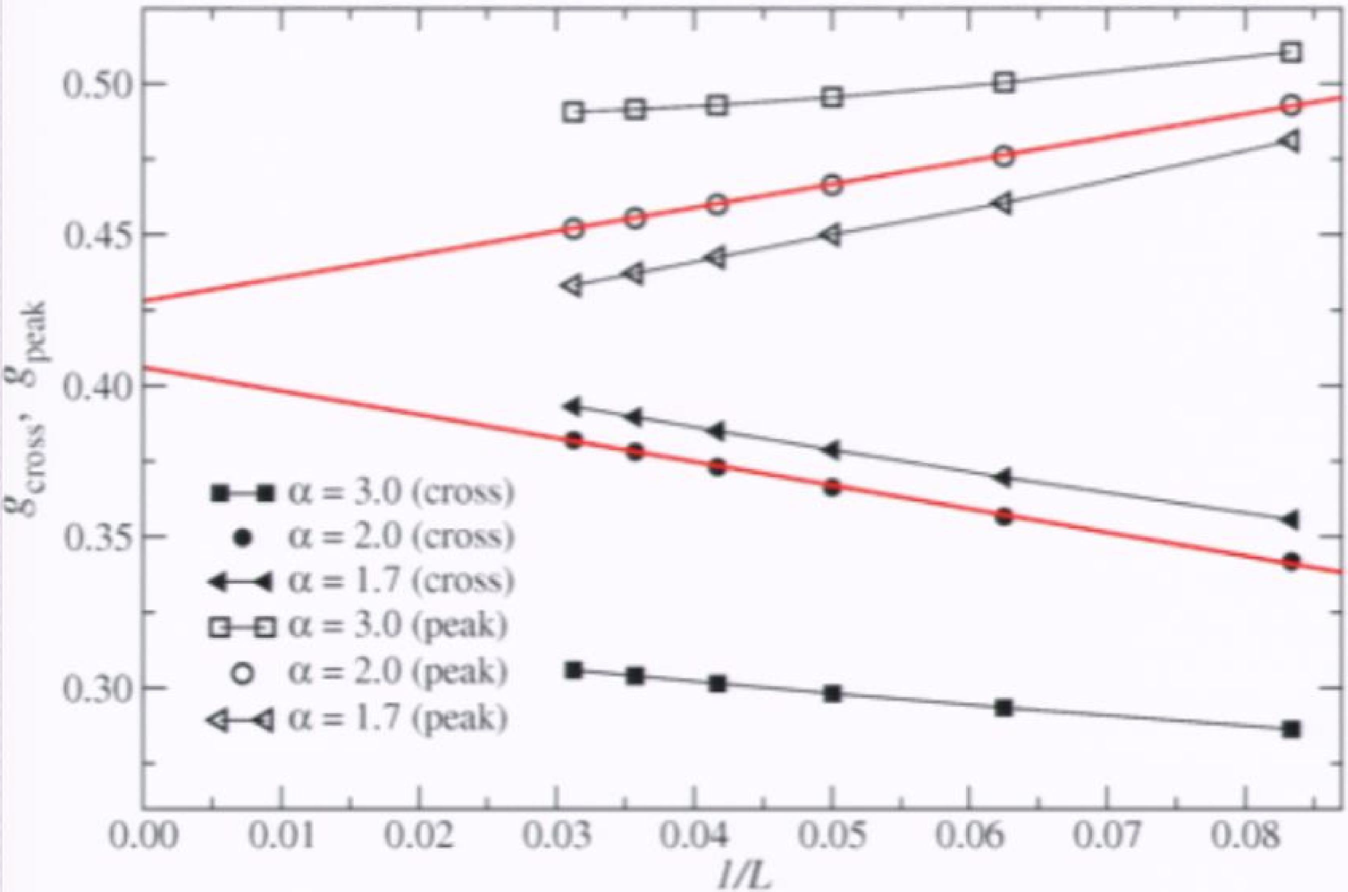

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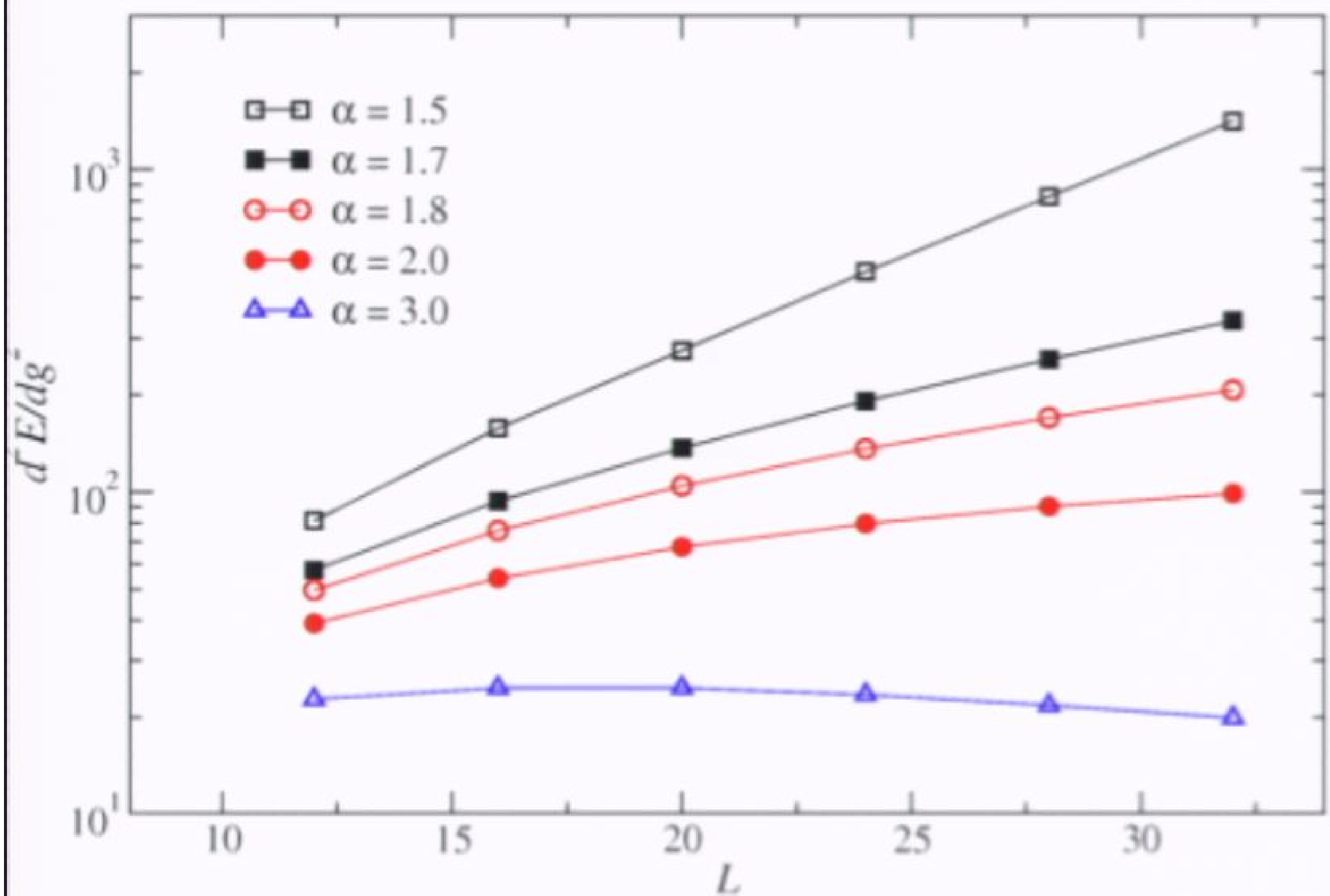
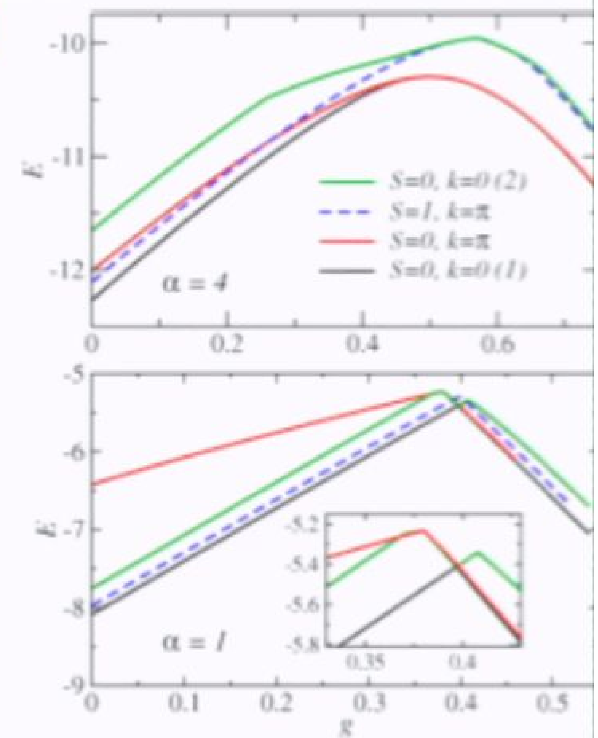




Exponentially divergent peak curvature for α<2

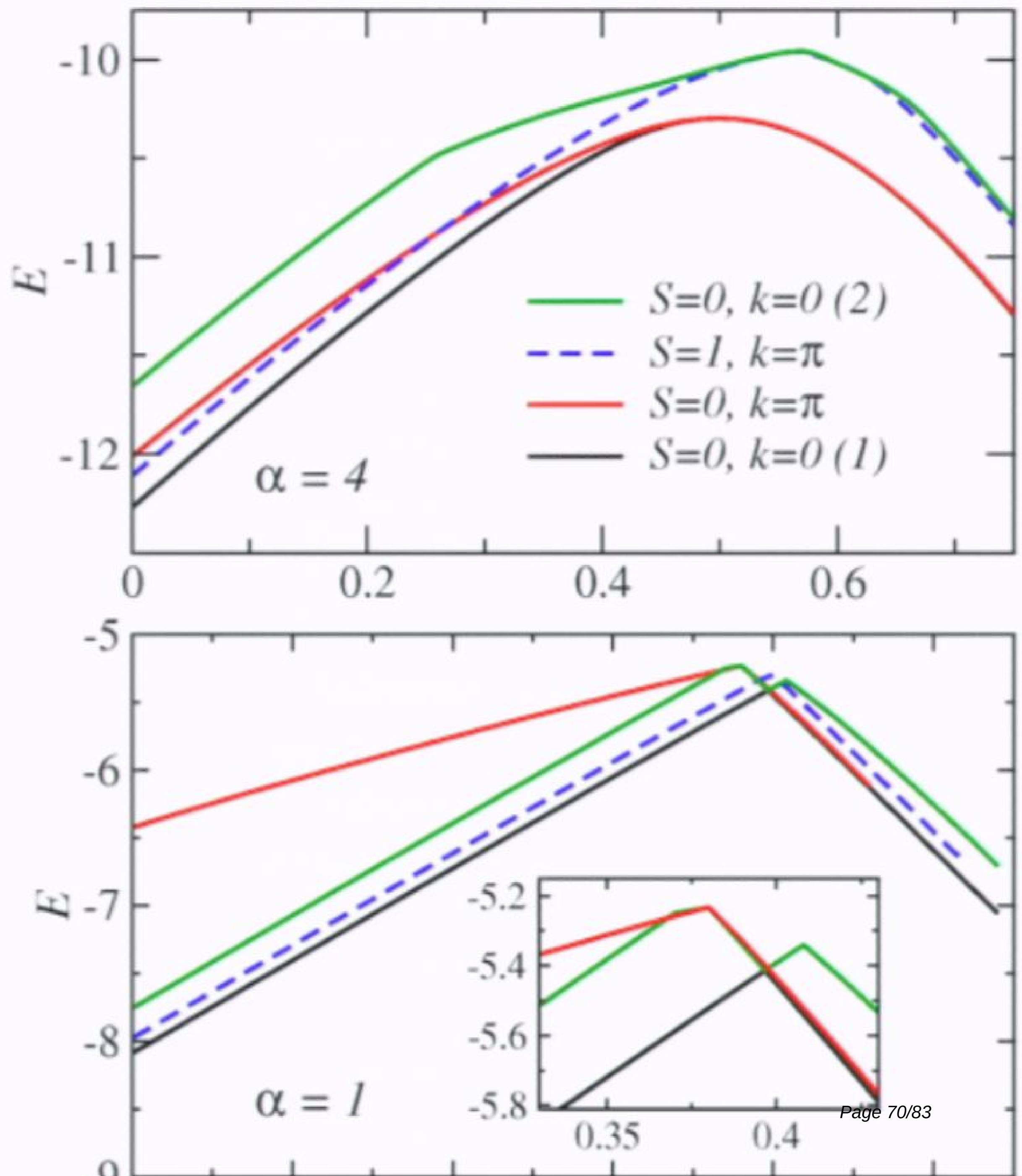
Lanczos results for ground state and excitation **energies**

Similar to the J_1-J_2 chain for large α (>2)

- singlet-triplet crossing
- rounded E_0 maximum

Different curve shapes for small α (<2)

- sharp breaks
- avoided level crossings
- indicative of 1st order phase transition



Spin correlations C(r)

- staggered (Neel) for $g<g_c$
- period 4 for $g>g_c$ (critical?)

Dimer correlations D(r)

- short-ranged for $g<g_c$
- period-2 VBS for $g>g_c$

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle$$

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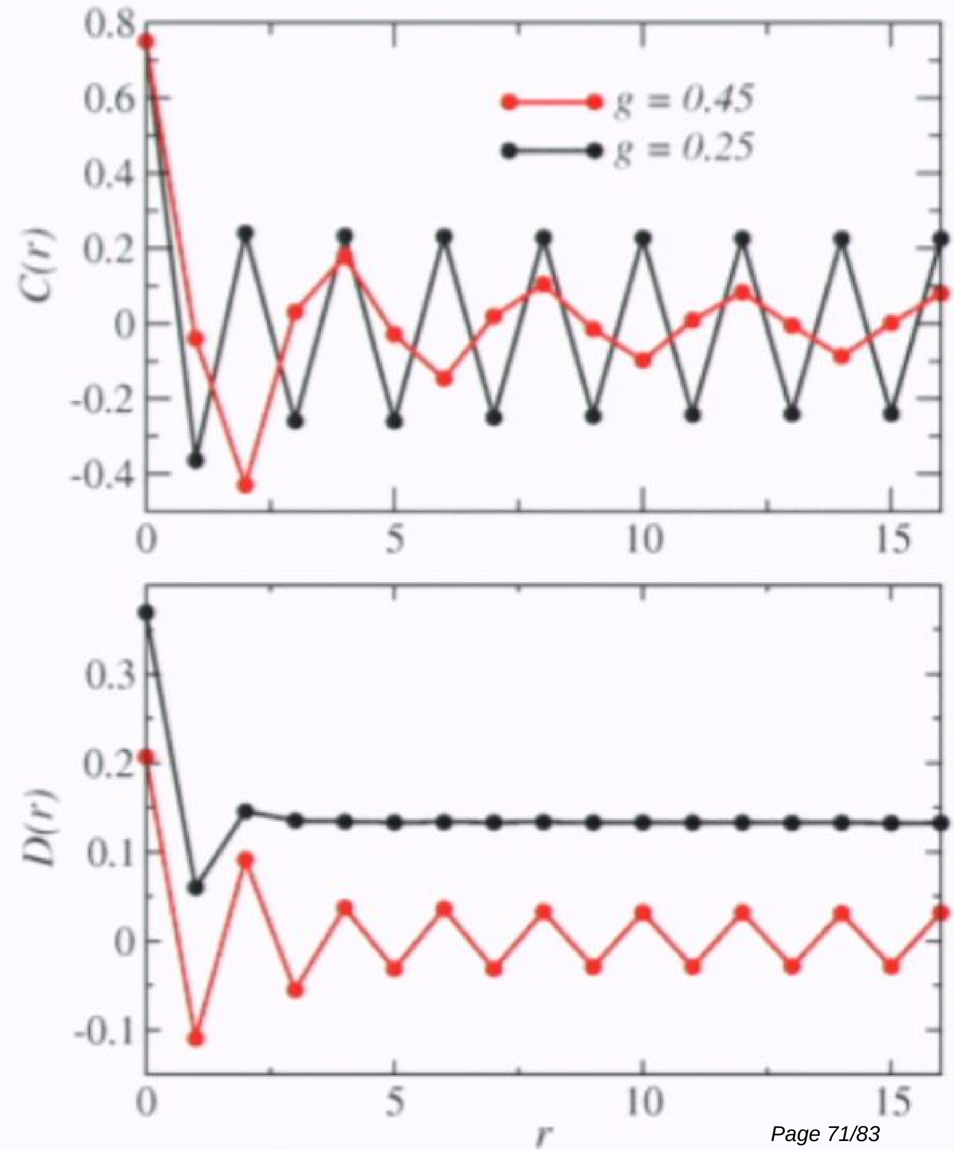

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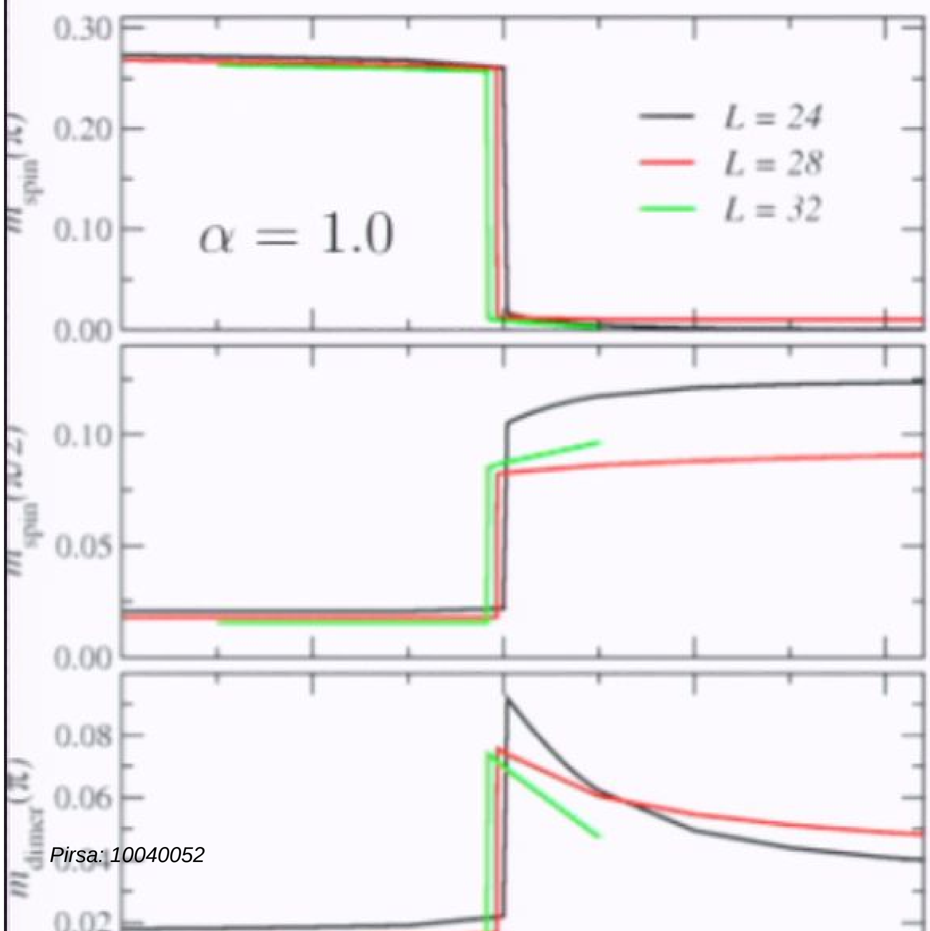
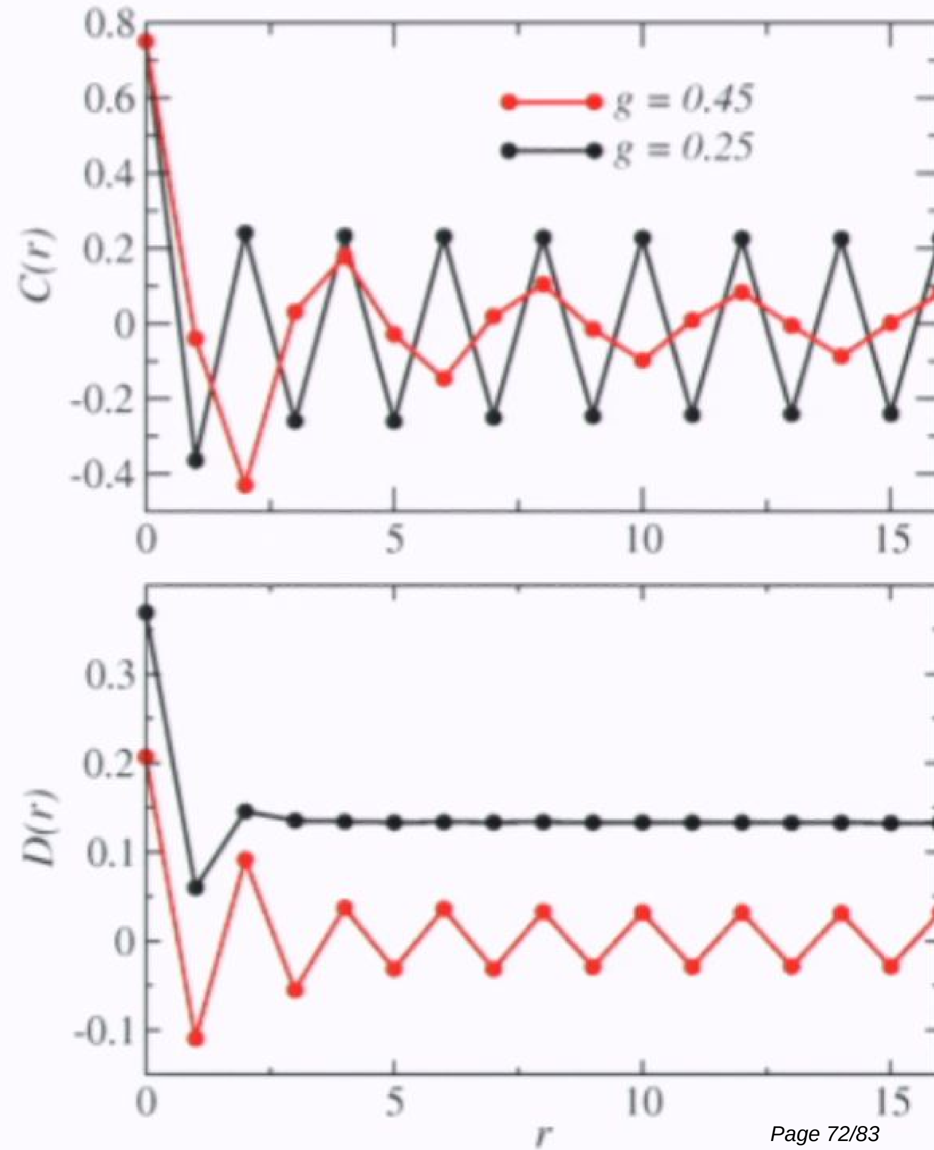


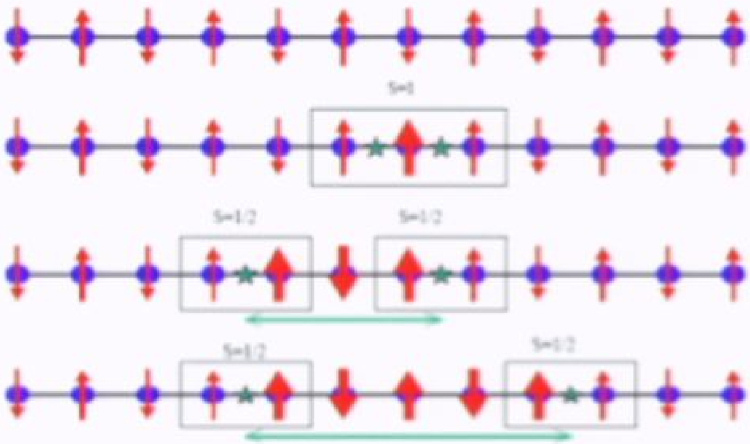


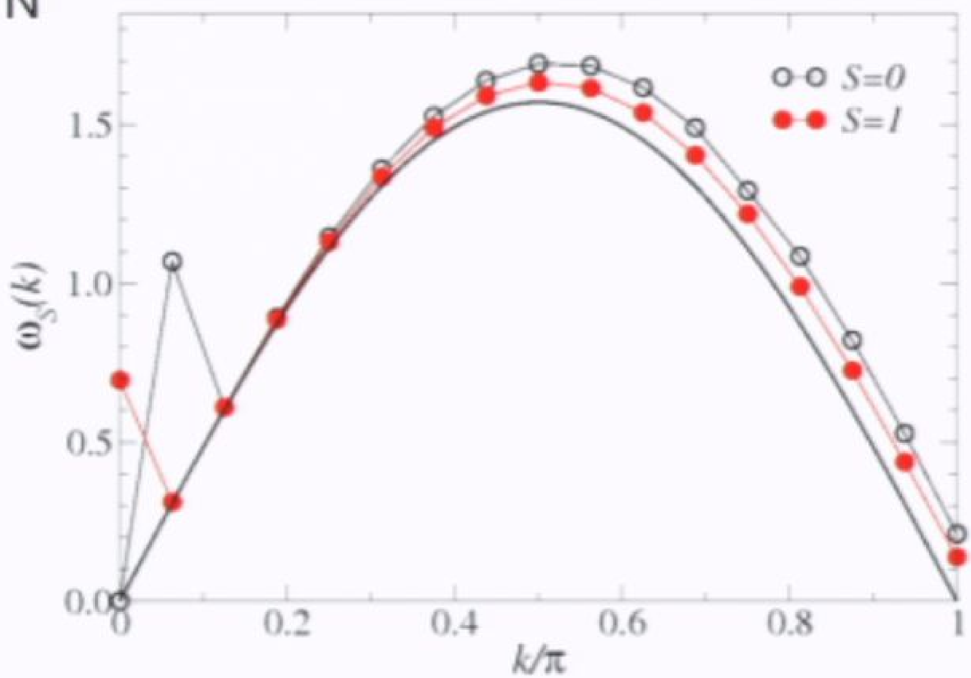
Heisenberg chains with long-range interactions

The spin-rotational symmetry cannot be spontaneously broken
n 1D Heisenberg systems with short-range interactions
with long-range interactions magnetic (e.g., Neel) order can form

Excitations of the Heisenberg chain

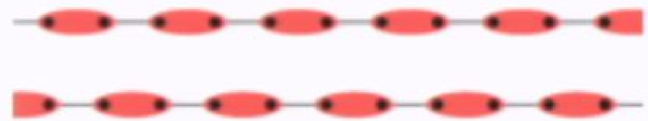
- the ground state is a singlet (S=0) for even N
- the first excited state is a triplet (S=1)
- can be understood as pair of “spinons”



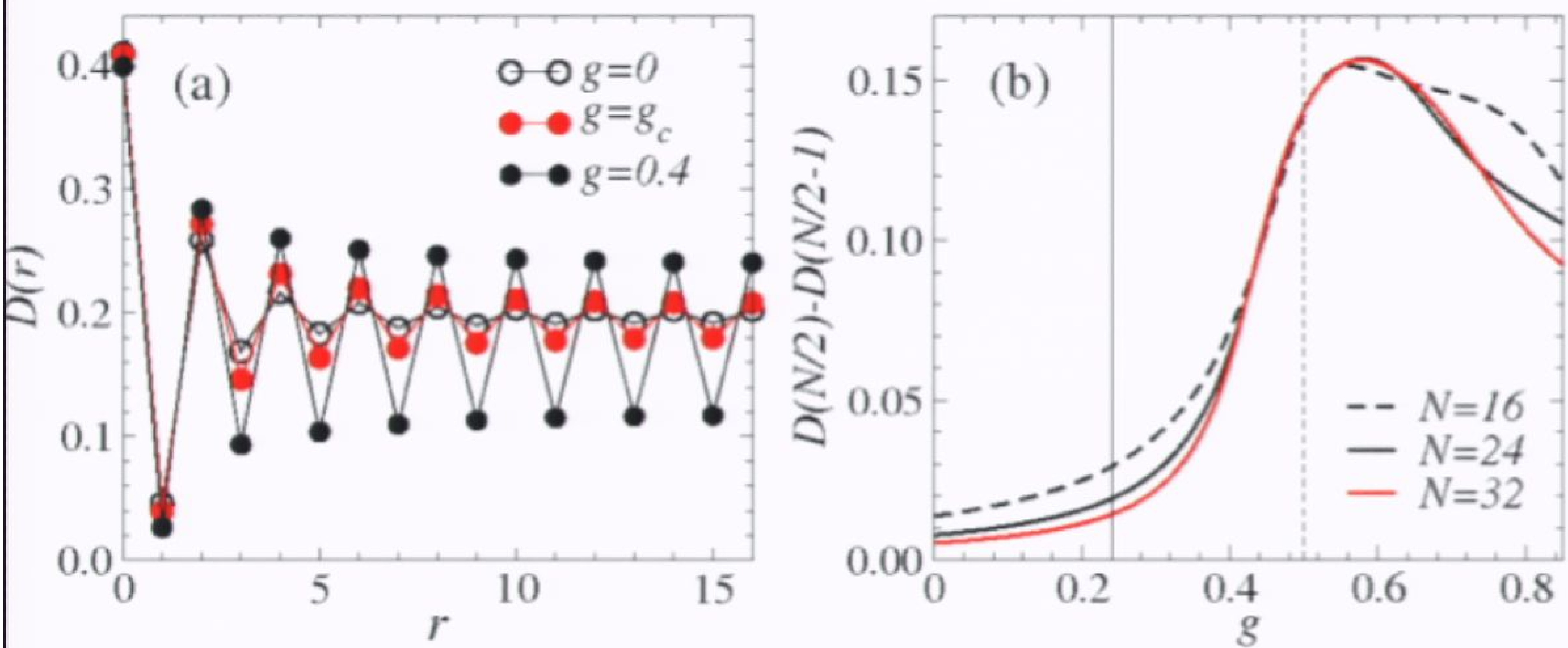


The VBS state can be detected in finite systems using "dimer" correlations

$$D(r) = \langle B_i B_{i+r} \rangle = \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_{i+r} \cdot \mathbf{S}_{i+1+r}) \rangle$$



Results from Lanczos diagonaization; different coupling ratios ***$g=J_2/J_1$***



Heisenberg chains with long-range interactions

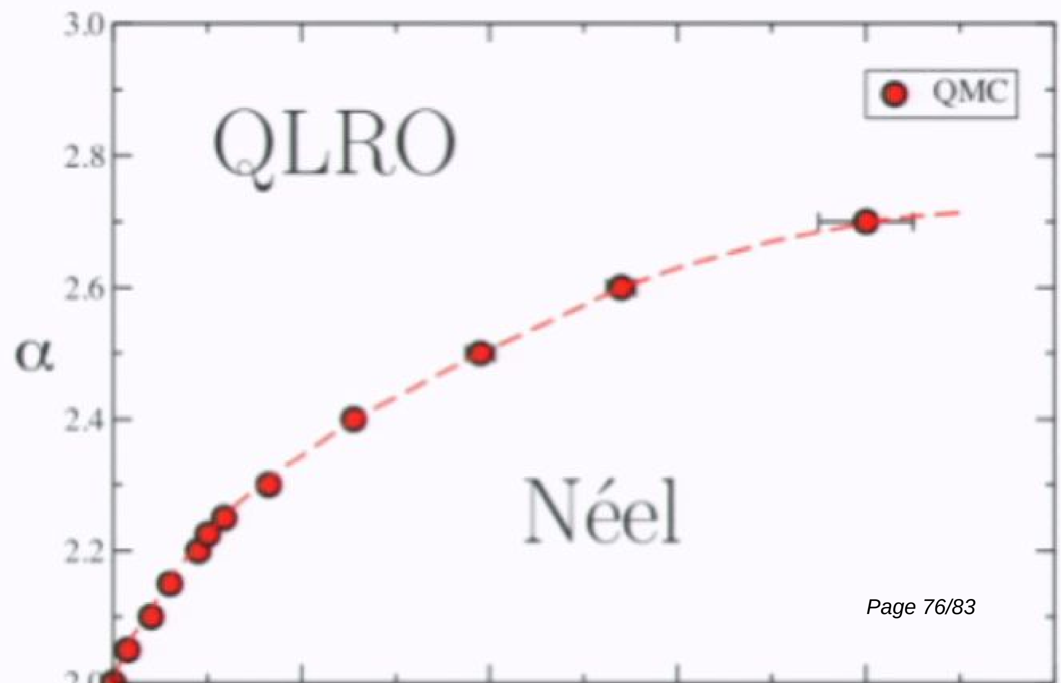
The spin-rotational symmetry cannot be spontaneously broken
in 1D Heisenberg systems with short-range interactions
- with long-range interactions magnetic (e.g., Neel) order can form

Consider power-law decaying unfrustrated antiferromagnetic interactions
[N. Laflorencie, I. Affleck, and M. Berciu, JSTAT (2006)]

$$H = \sum_{r=1}^{N/2} (-1)^{r-1} J_r \sum_{i=1} \mathbf{S}_i \cdot \mathbf{S}_{i+r} \qquad J_1 = \lambda, \quad J_{r>1} = \frac{1}{r^\alpha}$$

Phase transition between
- critritical state
- Neel-ordered state

The critical (or "quasi-long-range ordered") phase has the normal Heisenberg chain critical fluctuations/correlations

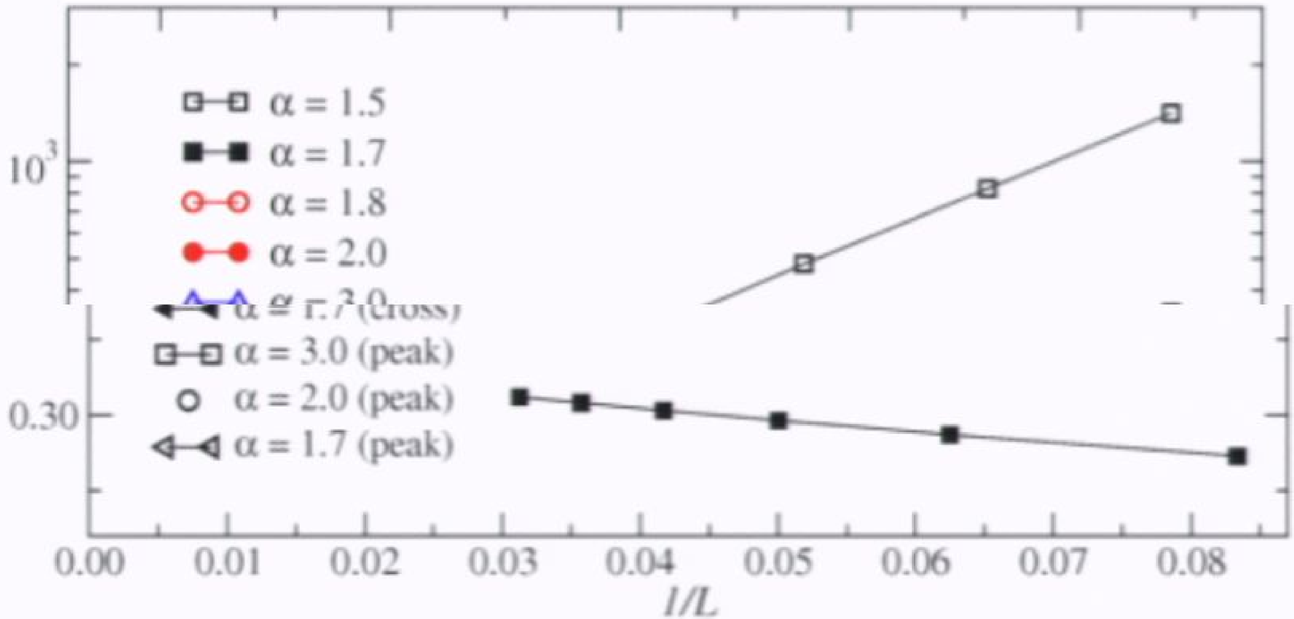


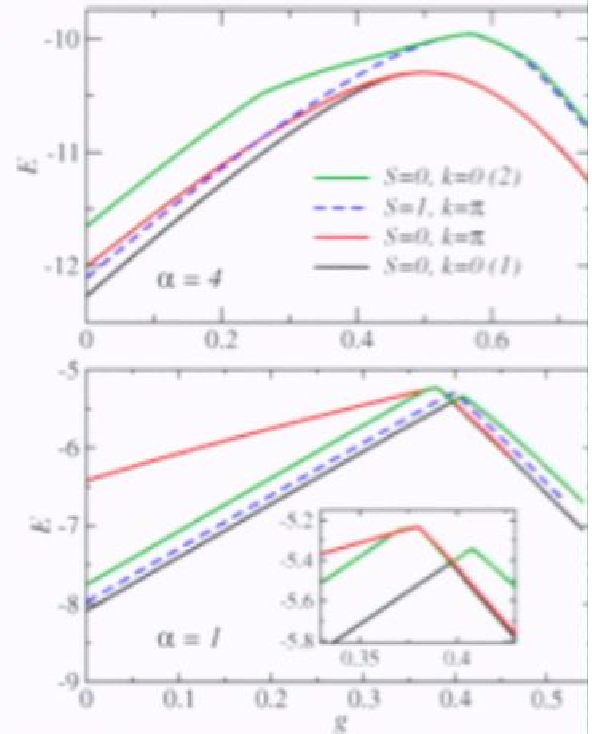
Transition curve $\alpha_c(\lambda)$

Analysis of the ground state energy curve $E_0(g)$

Characterize the sharpness of the maximum
by the second derivative versus chain length

$$\frac{d^2 E_0(g)}{dg^2} \quad \text{(at the peak value } g_{\text{peak}}\text{)}$$





transition as in
standard J_1-J_2
chain

For α<1.8

- the two special points coincide when L→∞
- what is the nature of the transition
- Neel state expected for small g

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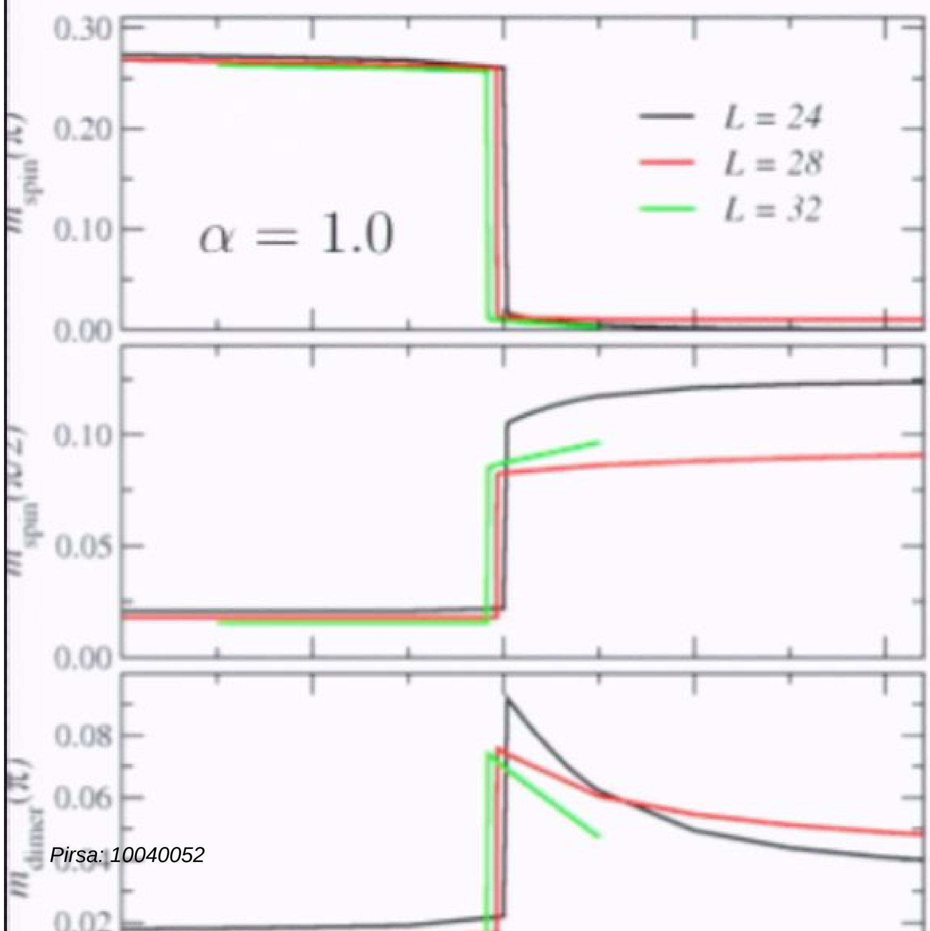

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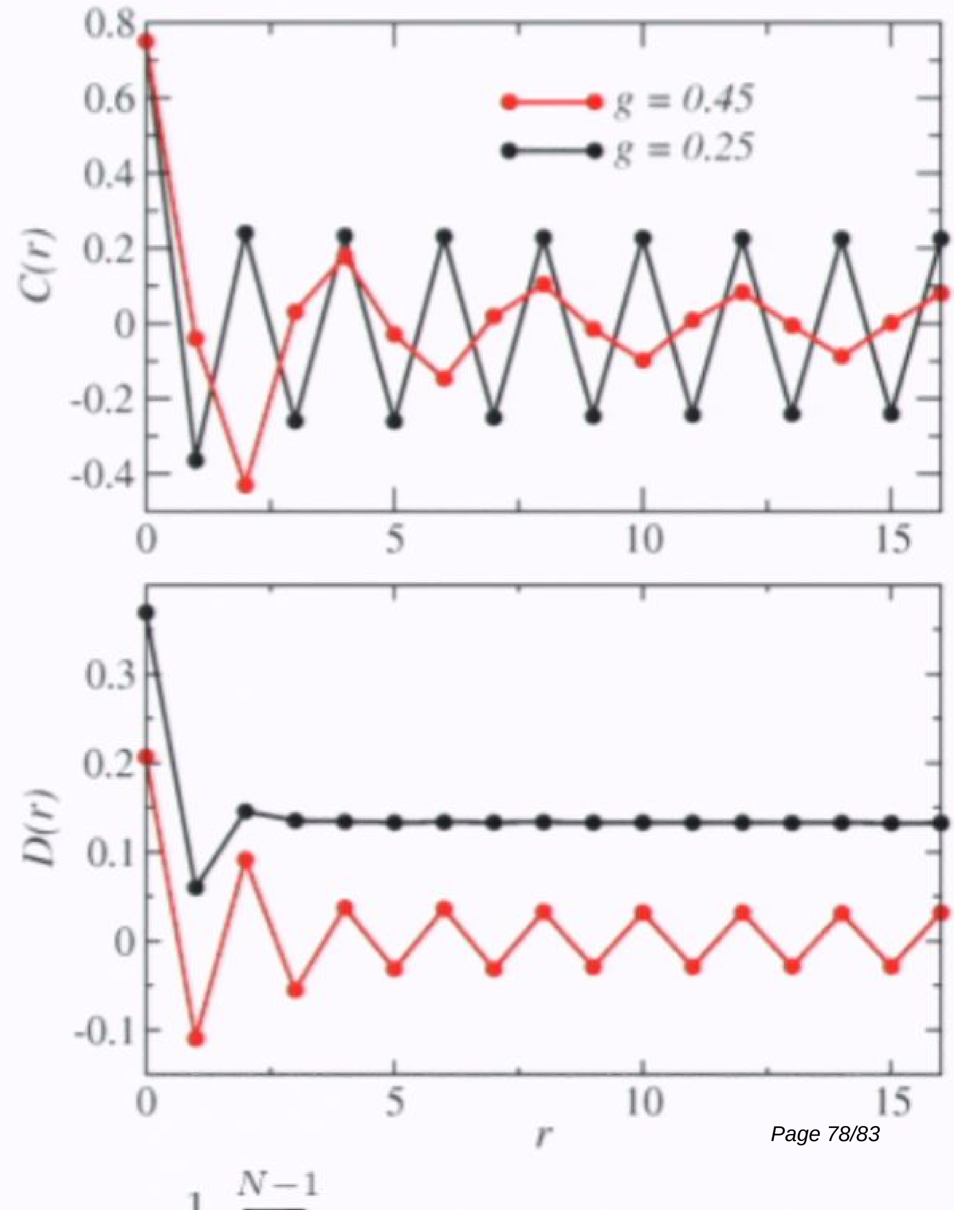
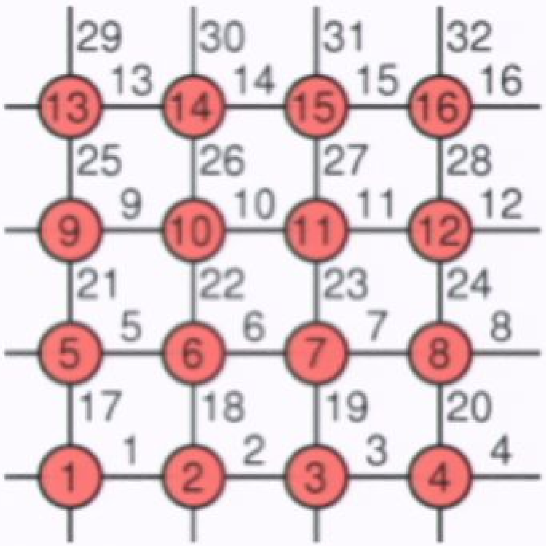


Exact diagonalization of 2D systems (simple square lattice)

- Label lattice sites and bonds
- hamiltonian construction very similar to 1D chains using site and bond maps



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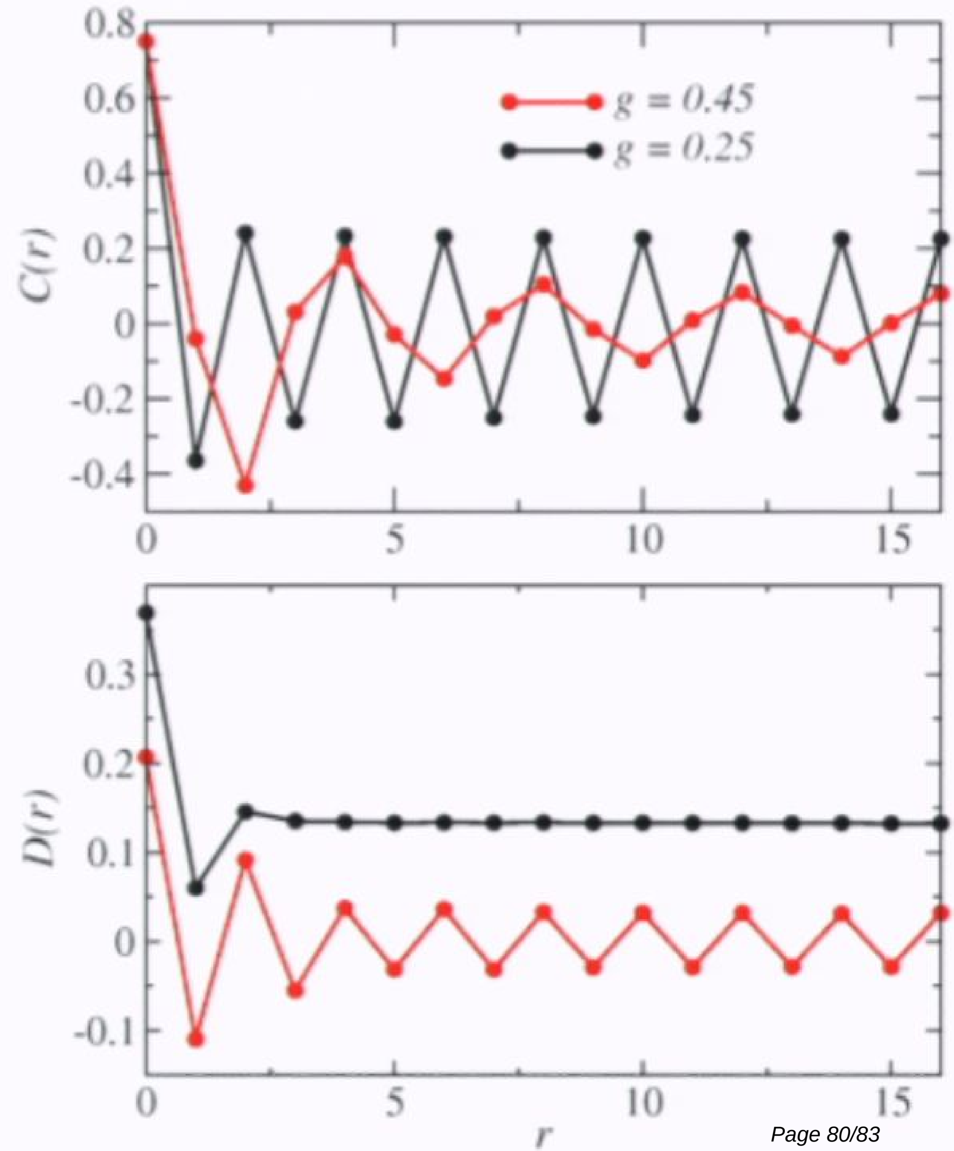

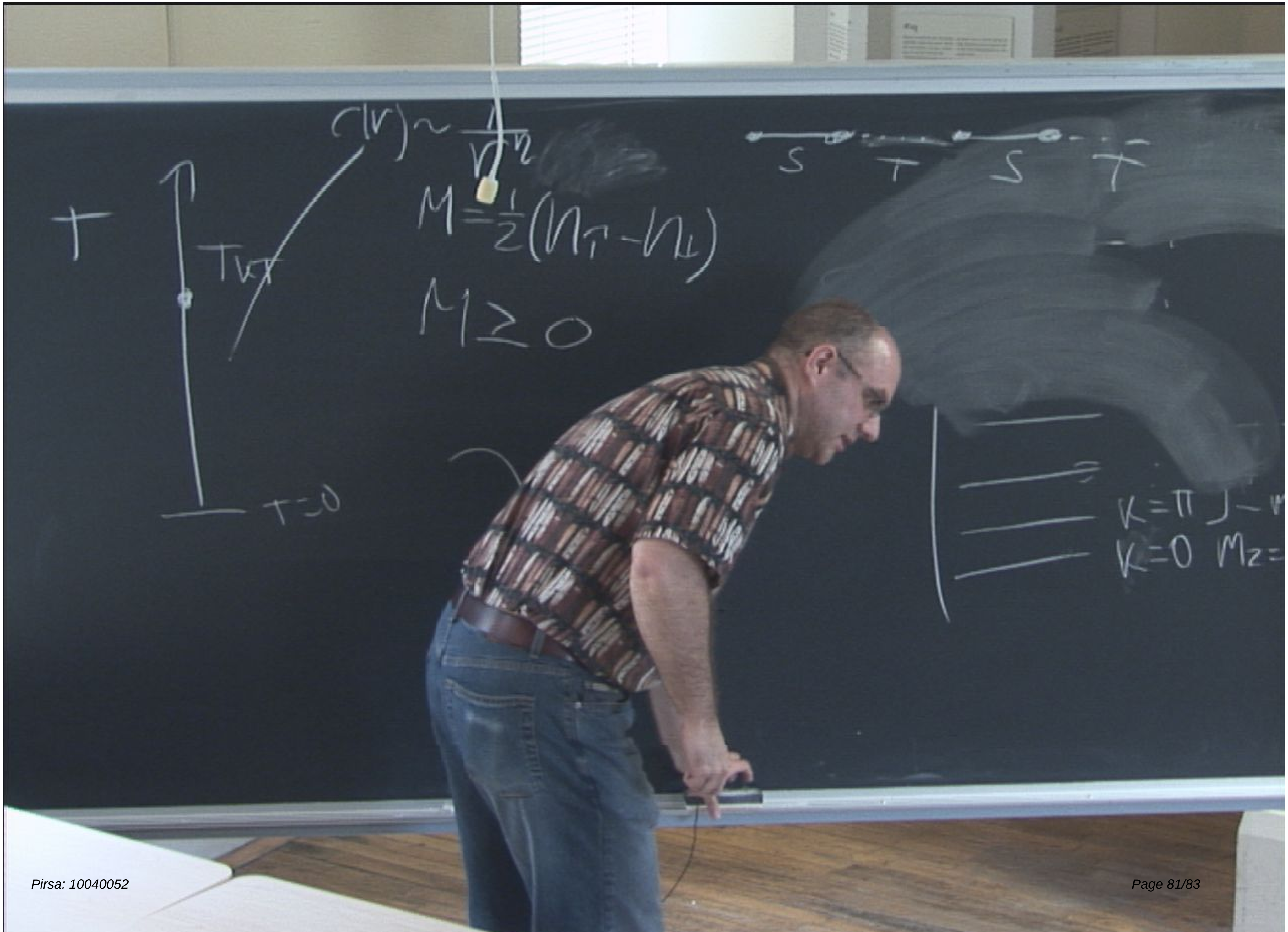

C(r) ~ 1/r^η
M = 1/2 (n↑ − n↓)
M ≥ 0
T
T_KT
T=0
S T S T
K=π
K=0 M_z=

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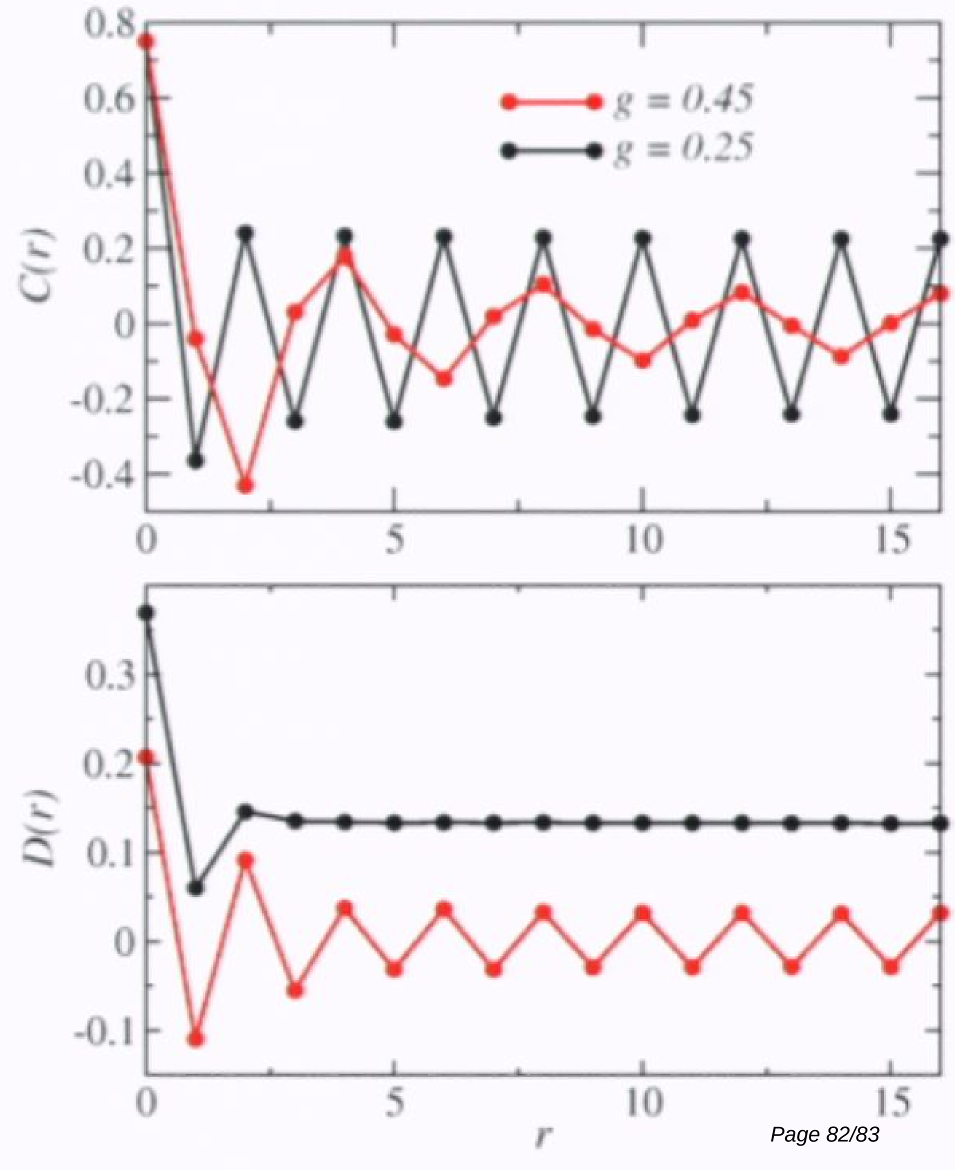

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