

Correlation Effects and DMRG

Talk in the seminar
„Condensed Matter Theory“

Augsburg University, 18.11.2003

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Agenda

1. The DMRG algorithm
2. Spincluster-Model for NaV_2O_5
3. Dimerized Spinsystems and scaling arguments
4. Hubbard-Ladders
5. Aspects of quantum chemistry with the DMRG
6. Misc / Discussion

DMRG algorithm

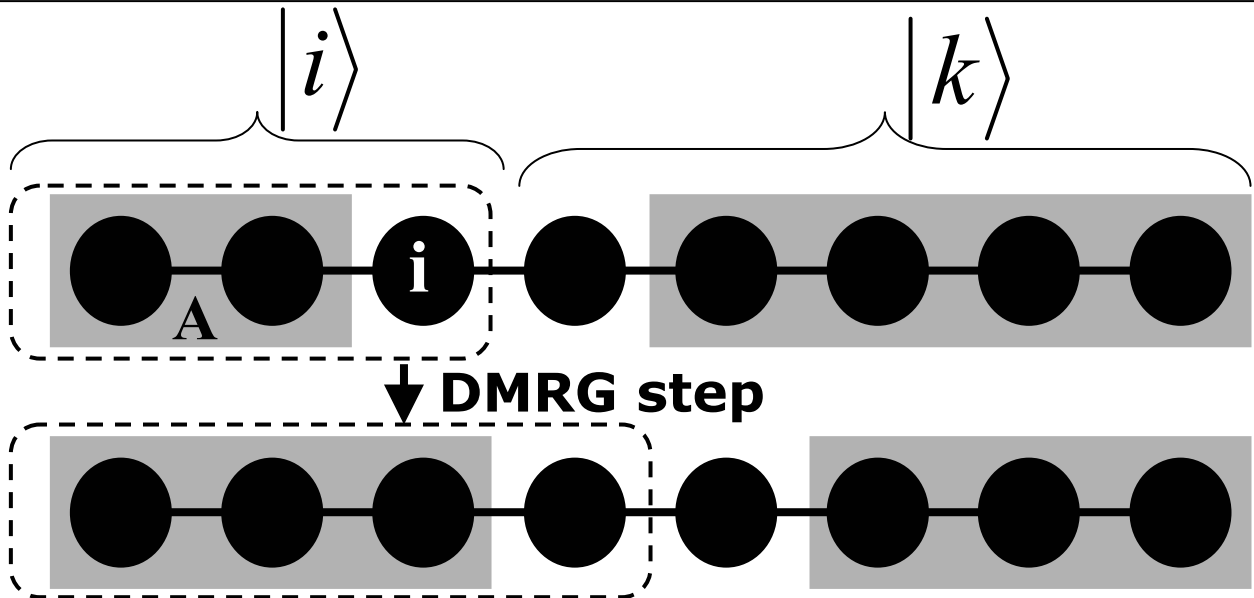
Idea

RG: selection by energy (e.g.

Kondo: exp. decrease in energy)

DMRG: selection by DM-weight, optimal basis

selection, 1D: exp. decrease in DM-weights

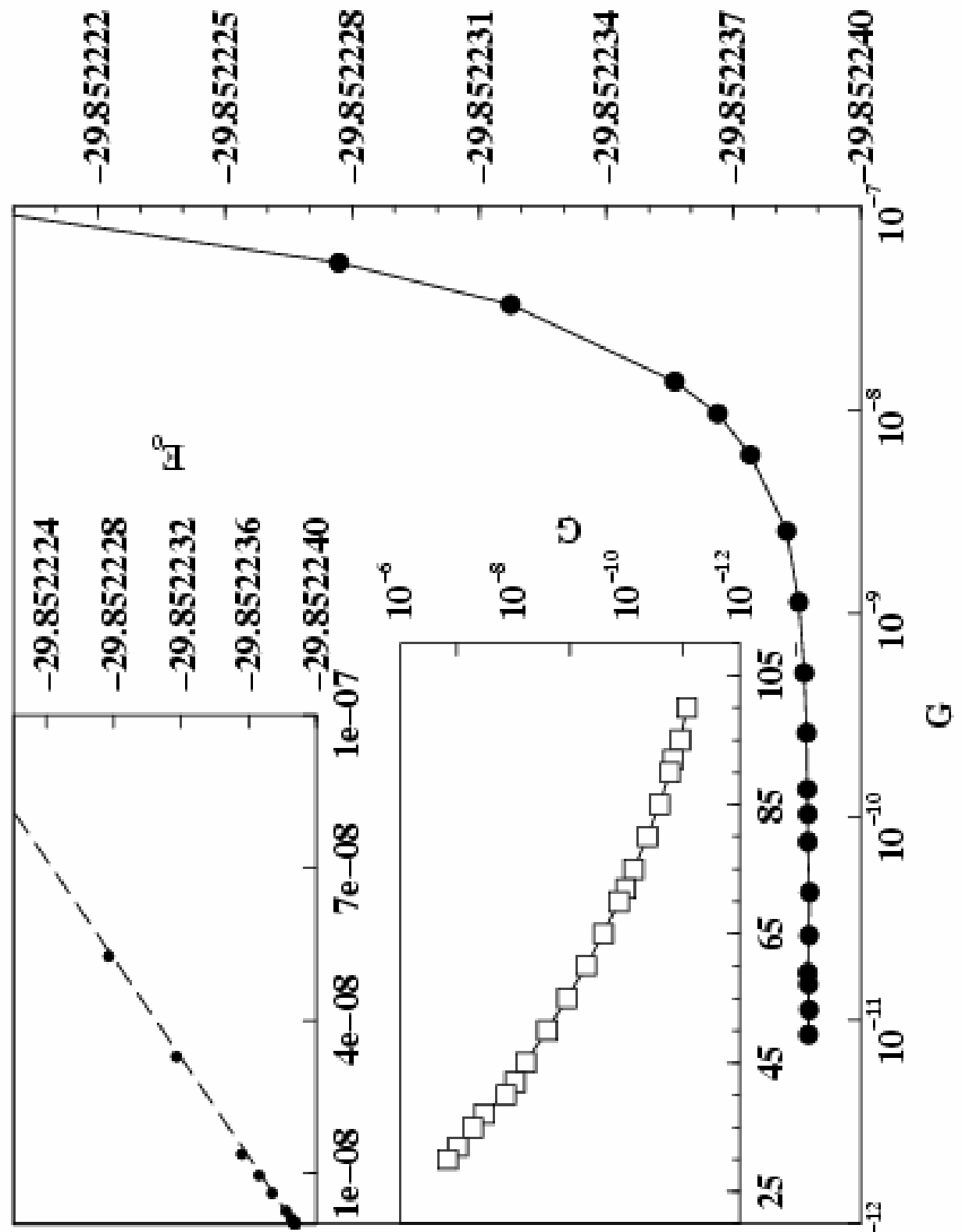


1. Diagonalize H_{total}
2. Build $\rho_{ij} = \sum_k |i, k\rangle \langle k, j|$
3. Diagonalize Density-Matrix ρ , select m „heaviest“ eigenstates
4. Build bigger system by
 - transforming operators
 - building $H = H_A + H_i$ for bigger fragment
5. Iterate beginning with 1.

Discarded Weight G is a measure for precision

Spinchain
L=80

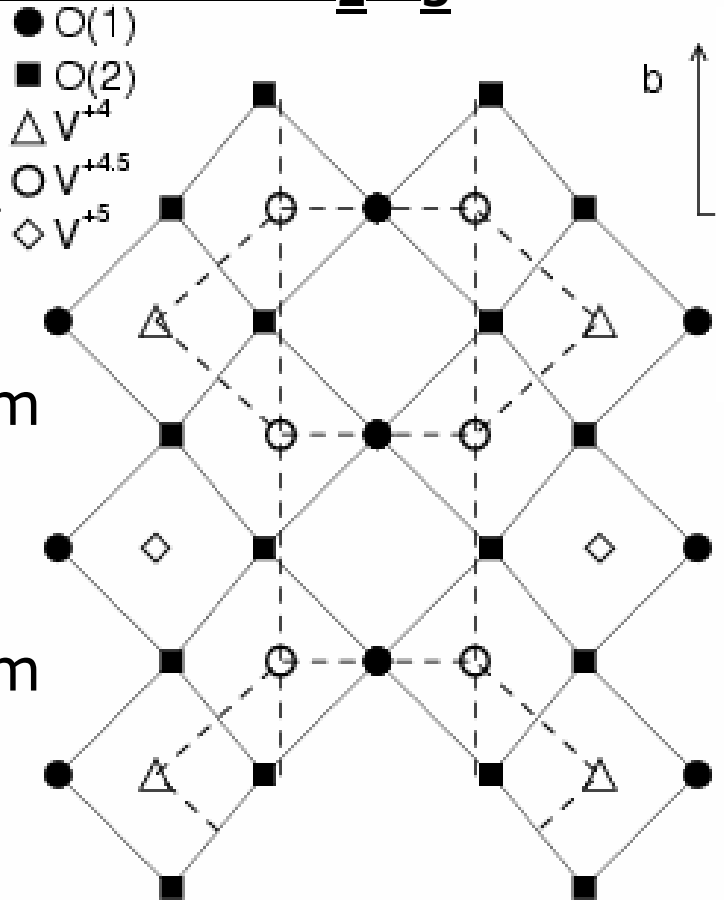
$$G := \sum_{l=m+1}^M w_l$$



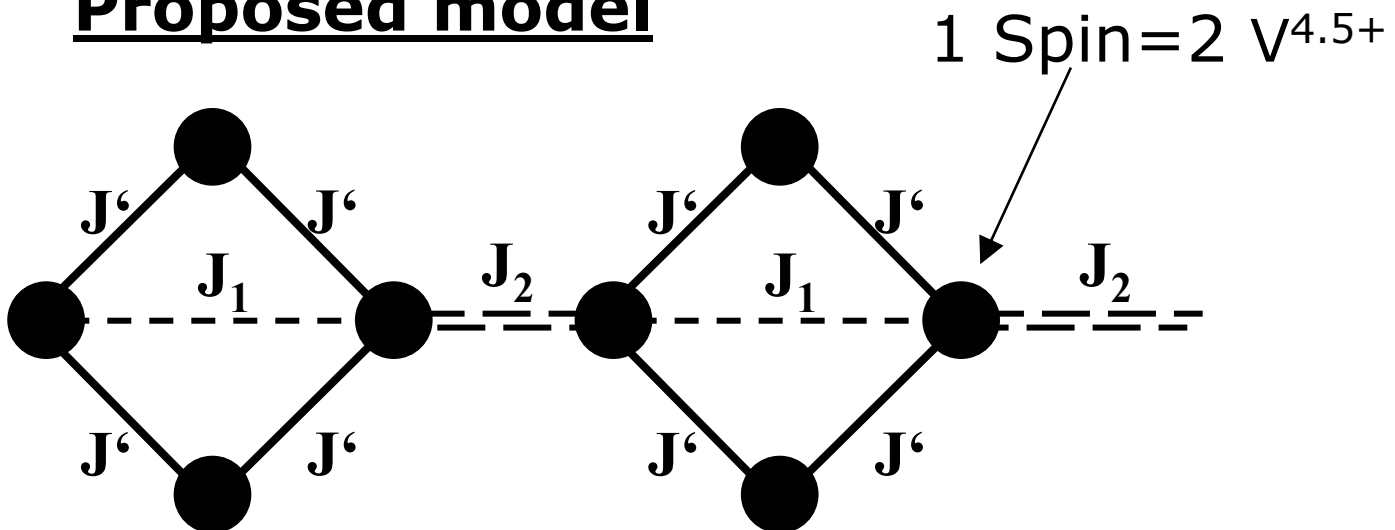
Spincluster-Model for NaV₂O₅

below $T_c = 34\text{K}$:

- $V^{4.5+} \rightarrow V^{4+}, V^{4.5+}, V^{5+}$
- Spin-Gap 10 meV
- dispersion maximum lowest magnon at $\pi/(2b)$, minima at $0, \pi/b$
- dispersion maximum is $\Delta_{\max} = 40\text{meV}$
- coupling along b is $J = 38\text{ meV}$



Proposed model



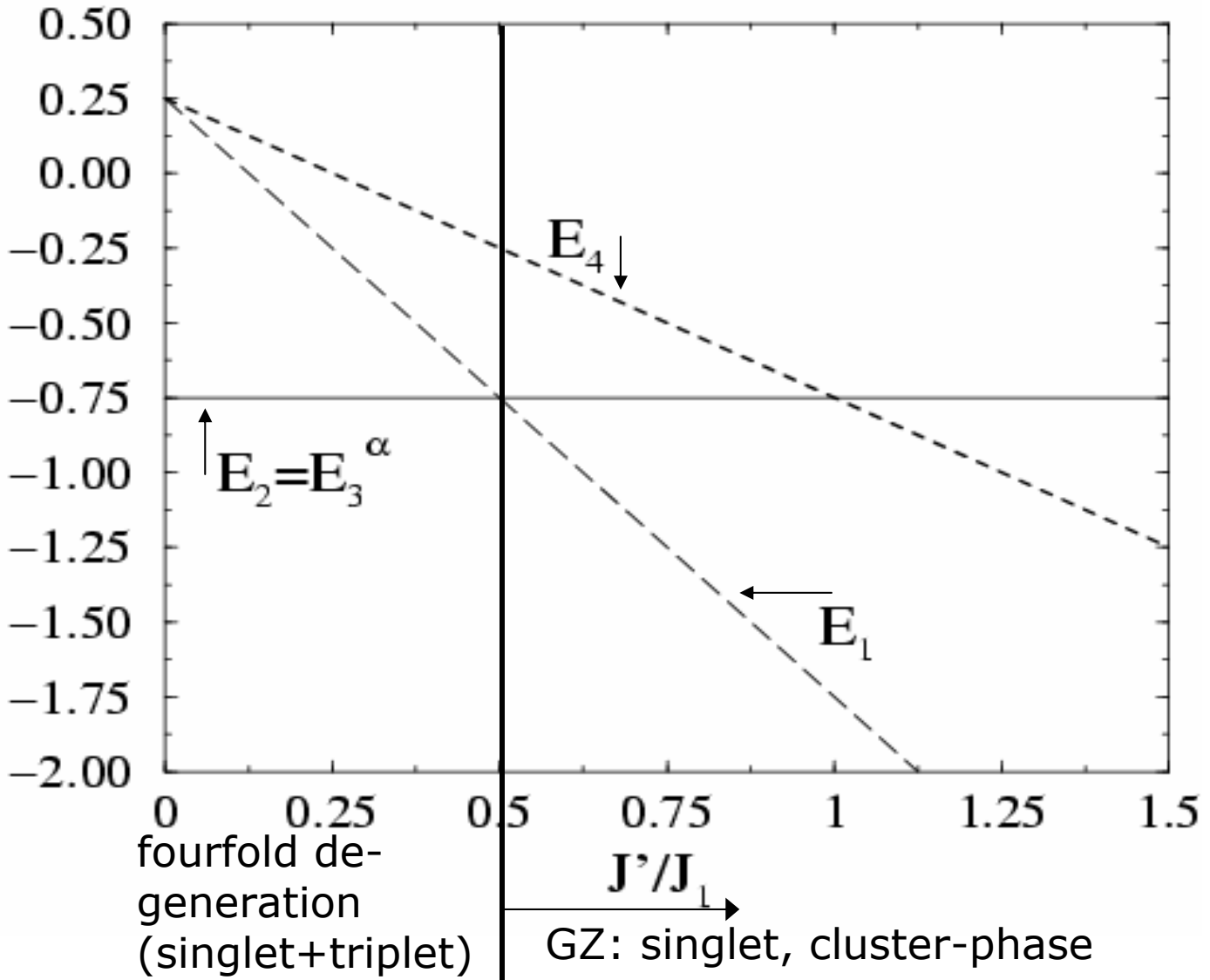
Spin gap not from dimerization

$[J_{1/2} = J \cdot (1 \pm \delta)]$, but gap of clusters

Spincluster-Model for NaV₂O₅

Analysis for a single cluster

s_{ij} , t_{ij} singlet/triplet of spins i, j in cluster



J_2 lowers the energy of the triplet \Rightarrow spin-1-chain
Haldane-phase

$$\psi_2 = s_{12} s_{34}$$

$$\psi_3^\alpha = s_{12} t_{34}^\alpha$$

$$\psi_1 = \frac{1}{\sqrt{3}} \left[t_{12}^0 t_{34}^0 - t_{12}^+ t_{34}^- - t_{12}^- t_{34}^+ \right]$$

Cluster-Operator-Theory

Idea: describe degrees of freedom in a cluster by bosonic d.o.f.

$$\psi_1 \rightarrow s_n^+ \quad \psi_3^\alpha \rightarrow b_{n,3,\alpha}^+ \quad \psi_4^\alpha \rightarrow b_{n,4,\alpha}^+$$

restricting bosonic
Hilbert-space
to physical space

$$s_n^+ s_n + \sum_{\tau,\alpha} b_{n,\tau,\alpha}^+ b_{n,\tau,\alpha} = 1$$

Spin operators (similar for S^x, S^y)

$$S_{n,1/2}^z = \pm \frac{b_{n,3,0}^+ s_n + s_n^+ b_{n,3,0}}{\sqrt{12}} - \frac{b_{n,4,0}^+ s_n + s_n^+ b_{n,4,0}}{\sqrt{6}}$$

Linearized Holstein-Primakov approximation

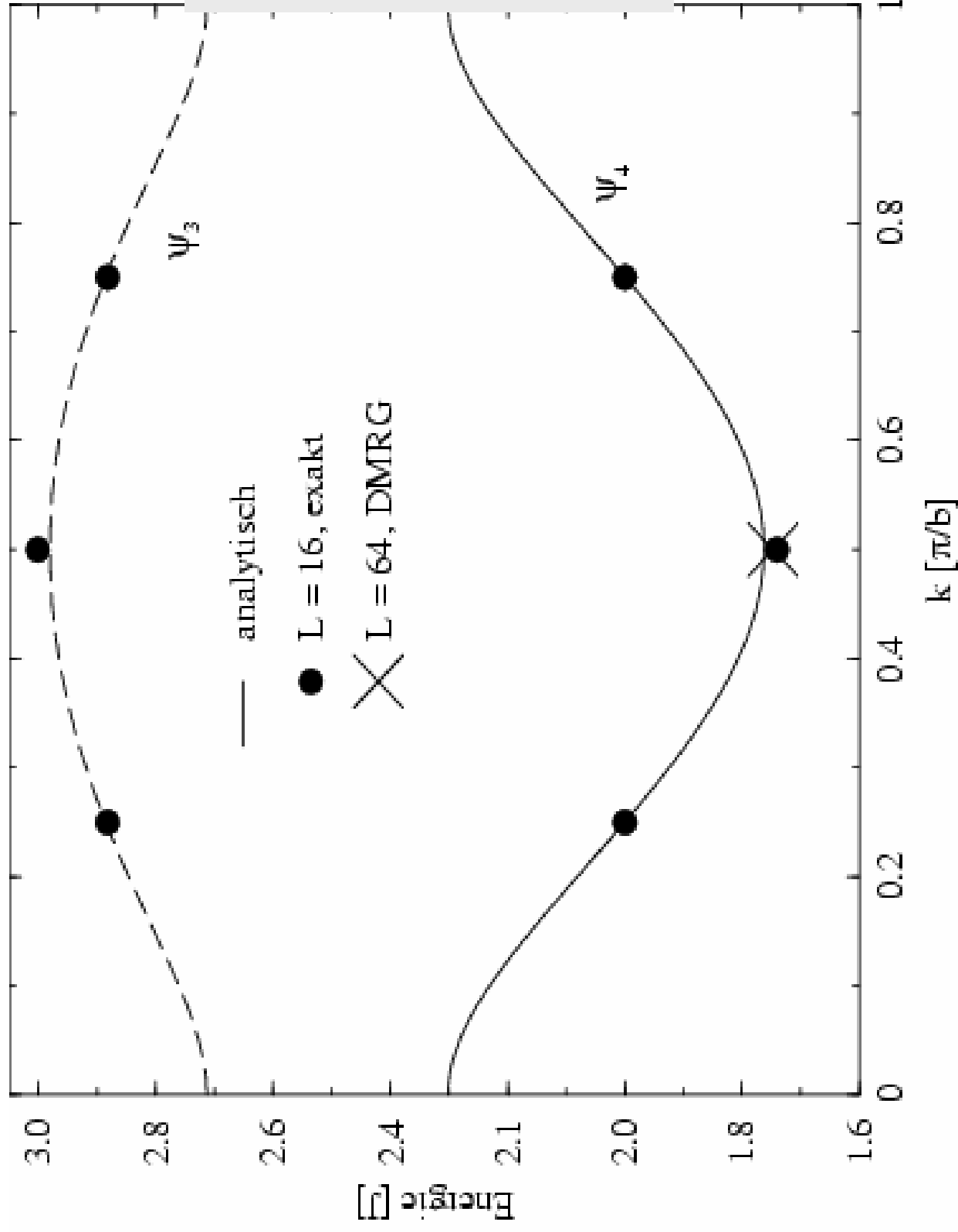
$$s_n^+, s_n \rightarrow 1$$

which gives by straight-forward diagonalization the dispersion

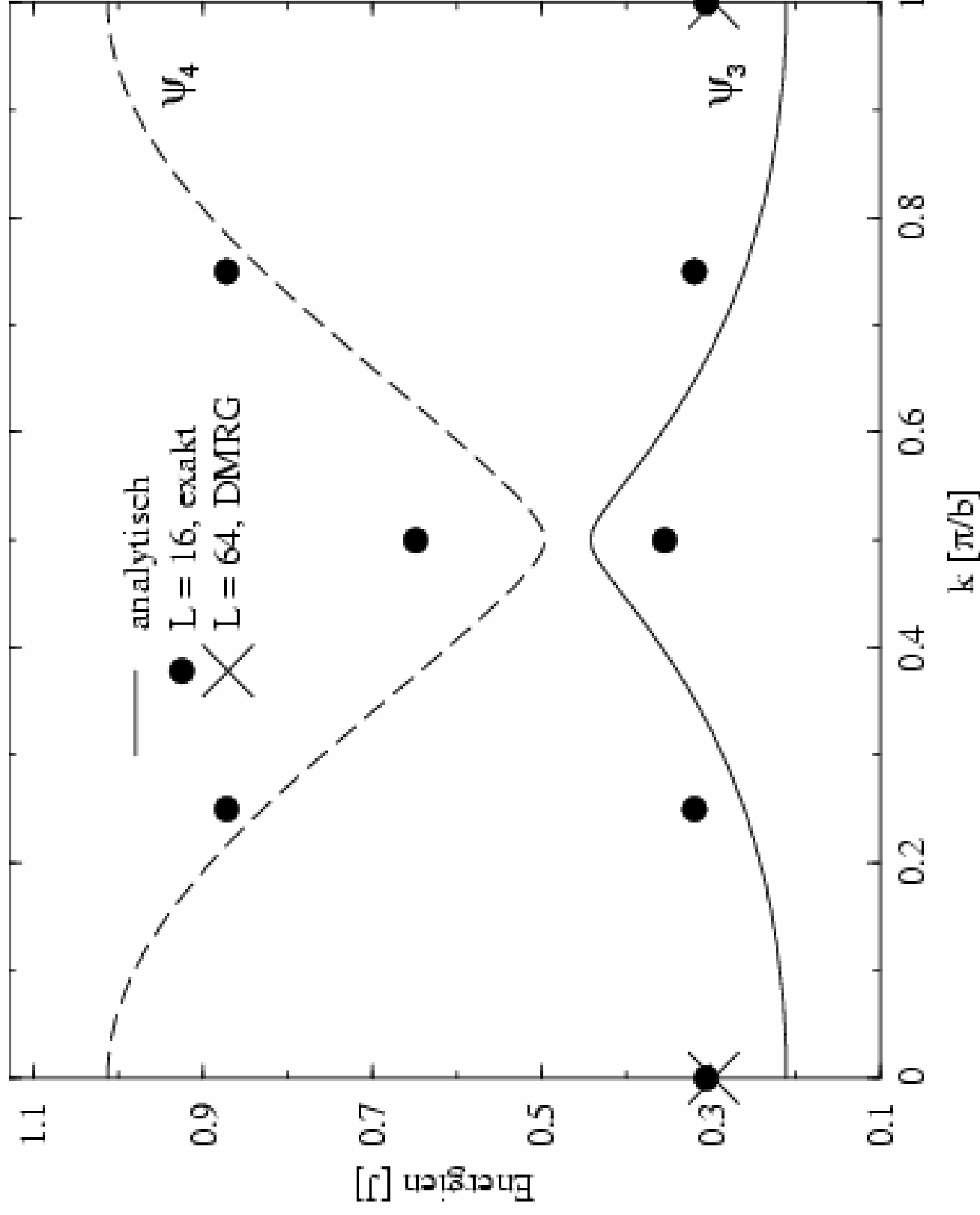
$$\omega_{\pm} = t \pm \sqrt{t^2 - s}$$

With some very complicated expressions for t and s / Skipped for your convenience

Results for the Cluster-Phase



Results for the Haldane-Phase



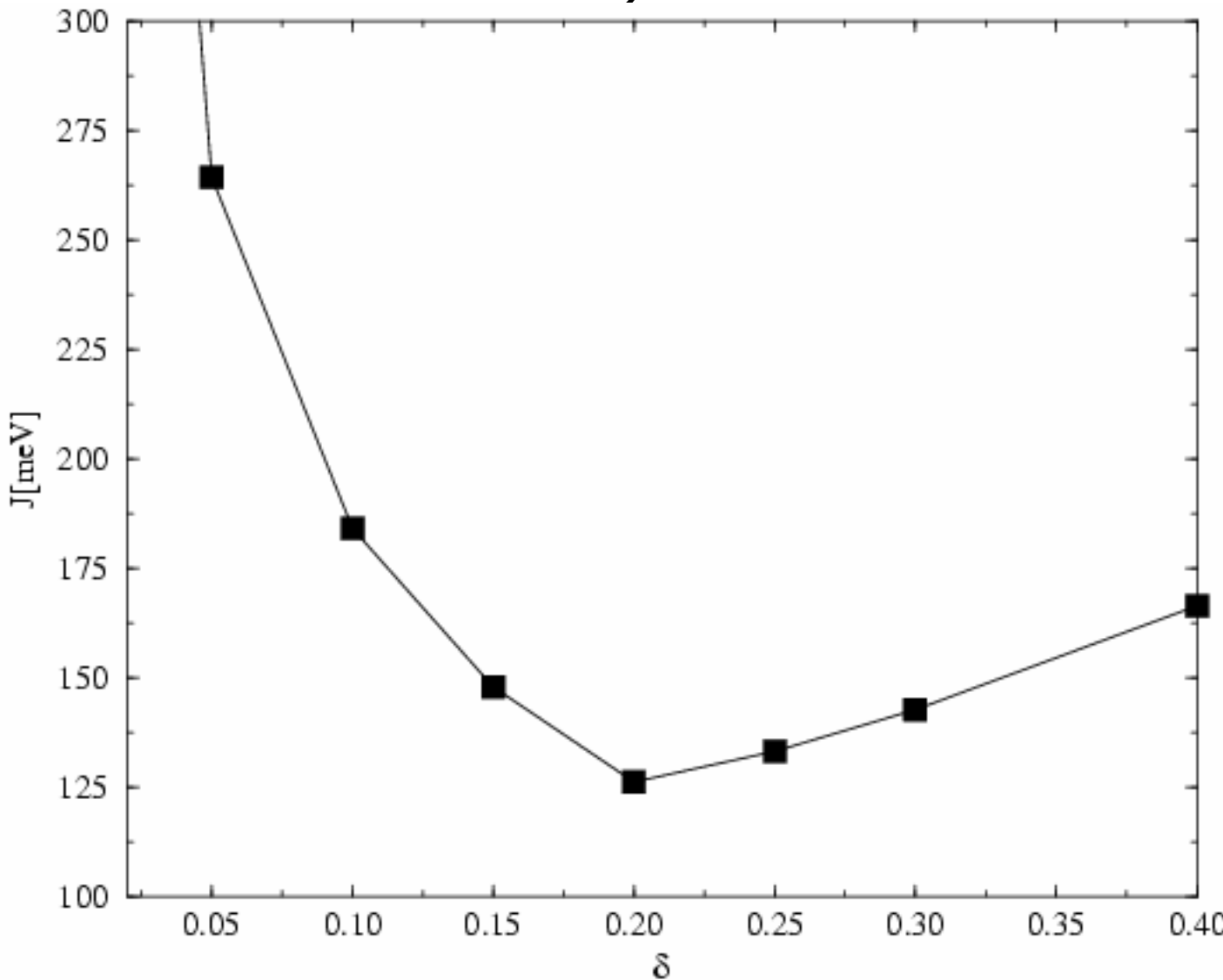
location of
minima/
maxima
in
agreement
with
experiment

ATTENTION:
cluster-
operator-
theory
overestimates
the magnon
dispersion

Haldane-Phase

Q: What interaction strength J is needed to mimic the experimental findings?

A: spin cluster operator theory
(overestimates dispersion, therefore underestimates J)

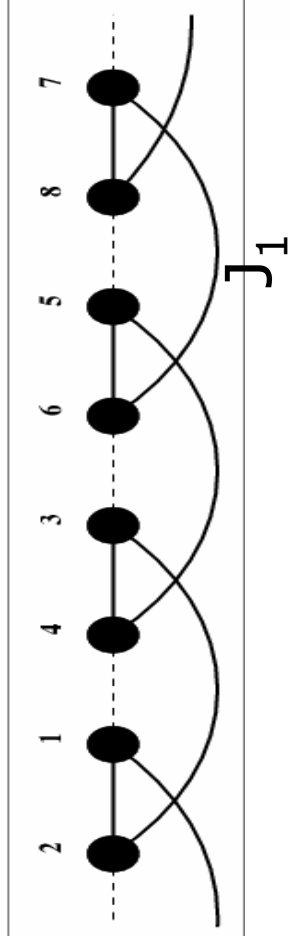
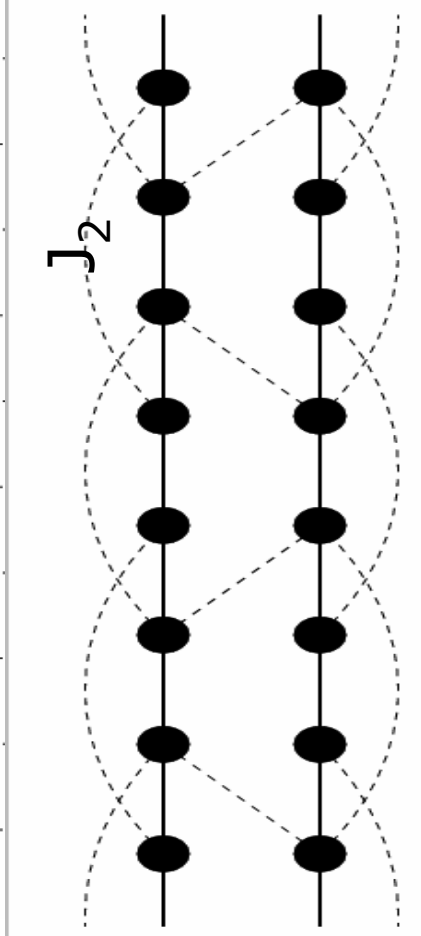
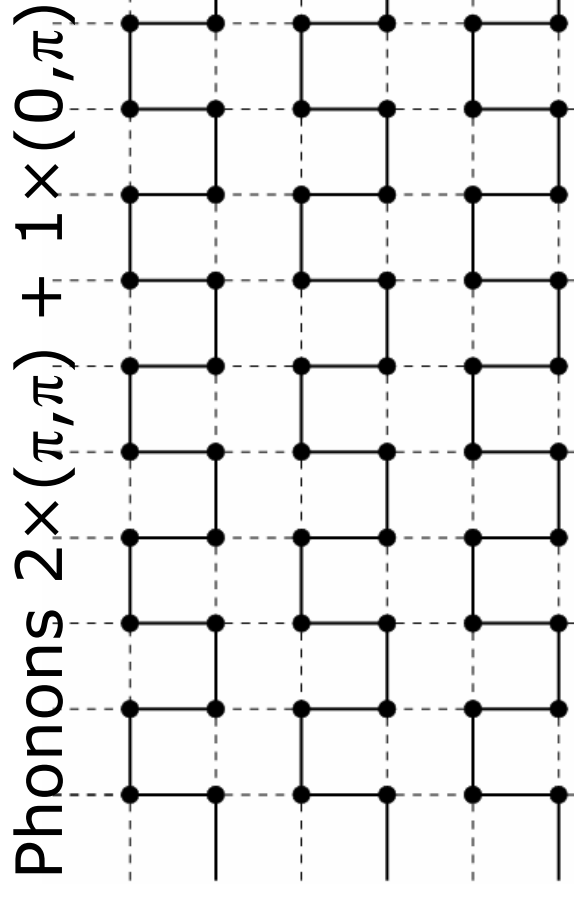


So, we need at least $J \approx 125 \text{ meV}$, but experiment gives 38 meV

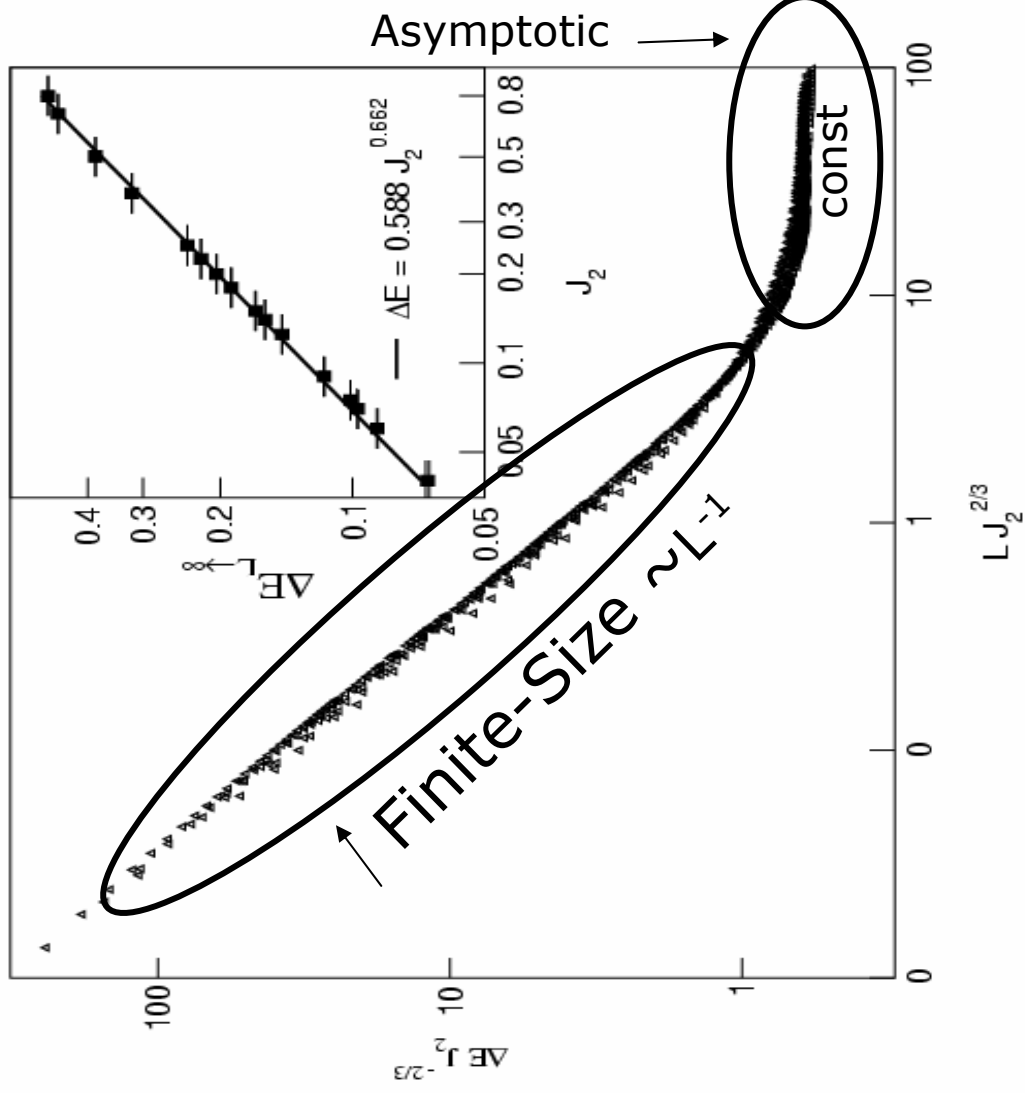
Model is at least factor 3 off!

2D dimerized spinsystems (z.B. CaV_4O_9) – scaling arguments

Sirker, Klümper, Hamacher,
PRB 65(2002), 134409

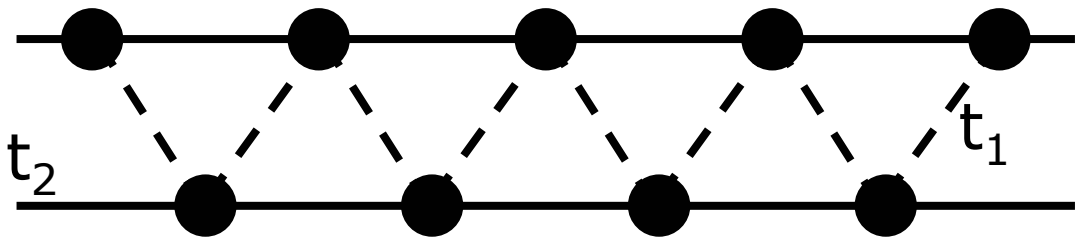


RG: $\Delta E \sim J_2^{2/3}$



Hubbard ladders

(e.g. SrCuO₂ or LiV₂O₅, half-filling)



$$H = -t_1 \sum_{i=1, \sigma}^L \{c_{i\sigma}^+ c_{i+1\sigma} + h.c.\} \\ - t_2 \sum_{i=1, \sigma}^L \{c_{i\sigma}^+ c_{i+2\sigma} + h.c.\} \\ + U \sum_{i=1}^L n_{i\uparrow} n_{i\downarrow}$$

RG treatment $\Delta k_{F1/2} \sim U^2$

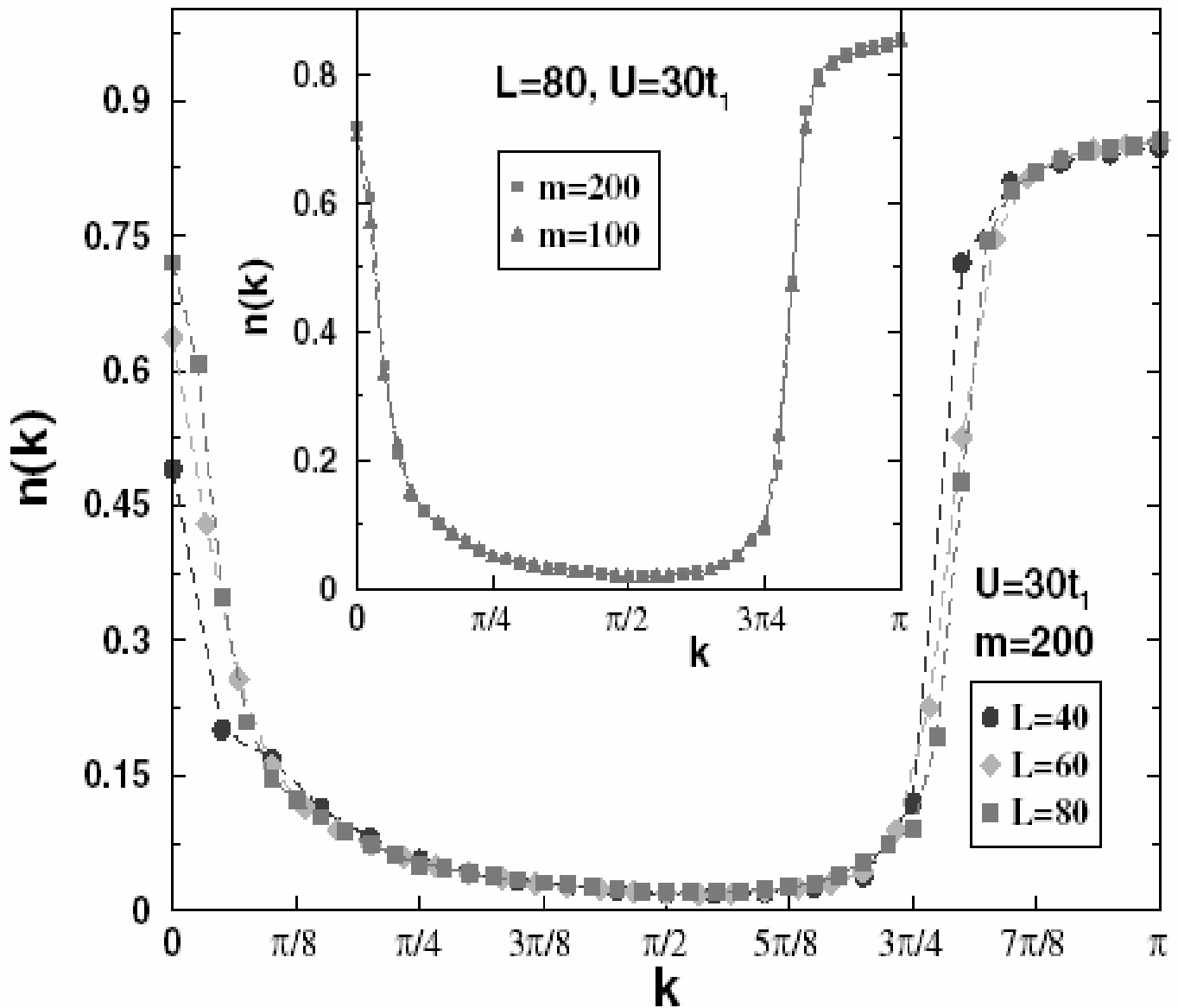
DMRG-computations for PBC and quarter-filling, $t_2/t_1 = -3$ (convergence)

Computing Correlation Functions is a difficult job

$$n_{\sigma}(k) = \frac{2}{L} \sum_{n, n'=1}^L \cos[k(n-n')] \langle c_{n, \sigma}^+ c_{n', \sigma} \rangle$$

$2L^2$ operators to store!

Checking precision of DMRG



Consistent with high-precision-calculations for OBC ✓

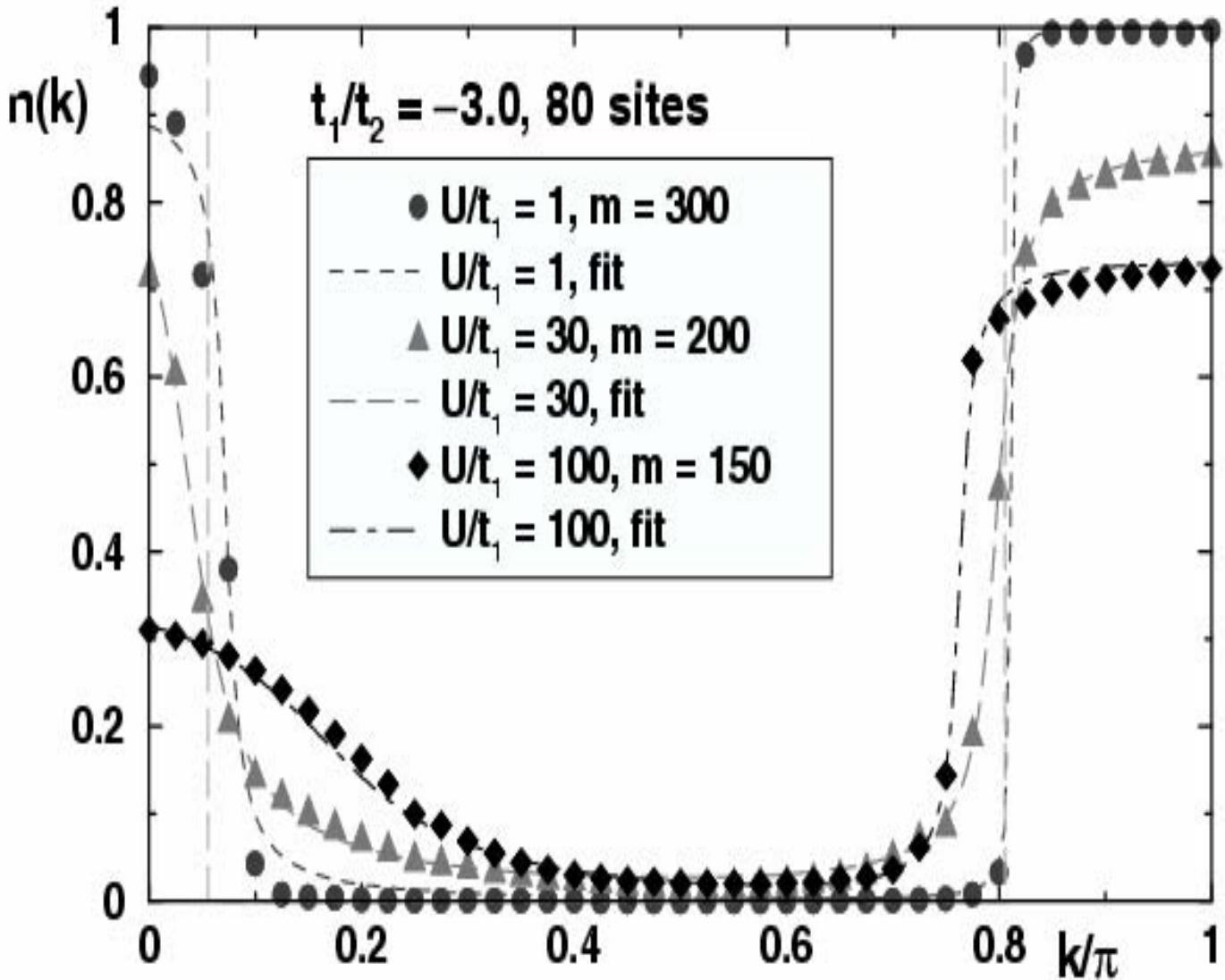
No instability spin gap (ferromagnetism)

$$\Delta E_F = E(N_\uparrow + 1, N_\downarrow - 1) - E(N_\uparrow, N_\downarrow) \quad \checkmark$$

No instability charge gap (phase separation)

$$\Delta E_{Ph} = E(N_\uparrow + 1, N_\downarrow + 1) + E(N_\uparrow - 1, N_\downarrow - 1) - 2E(N_\uparrow, N_\downarrow) \quad \checkmark$$

Interaction induces Collapse of a Section of the Fermi Sea



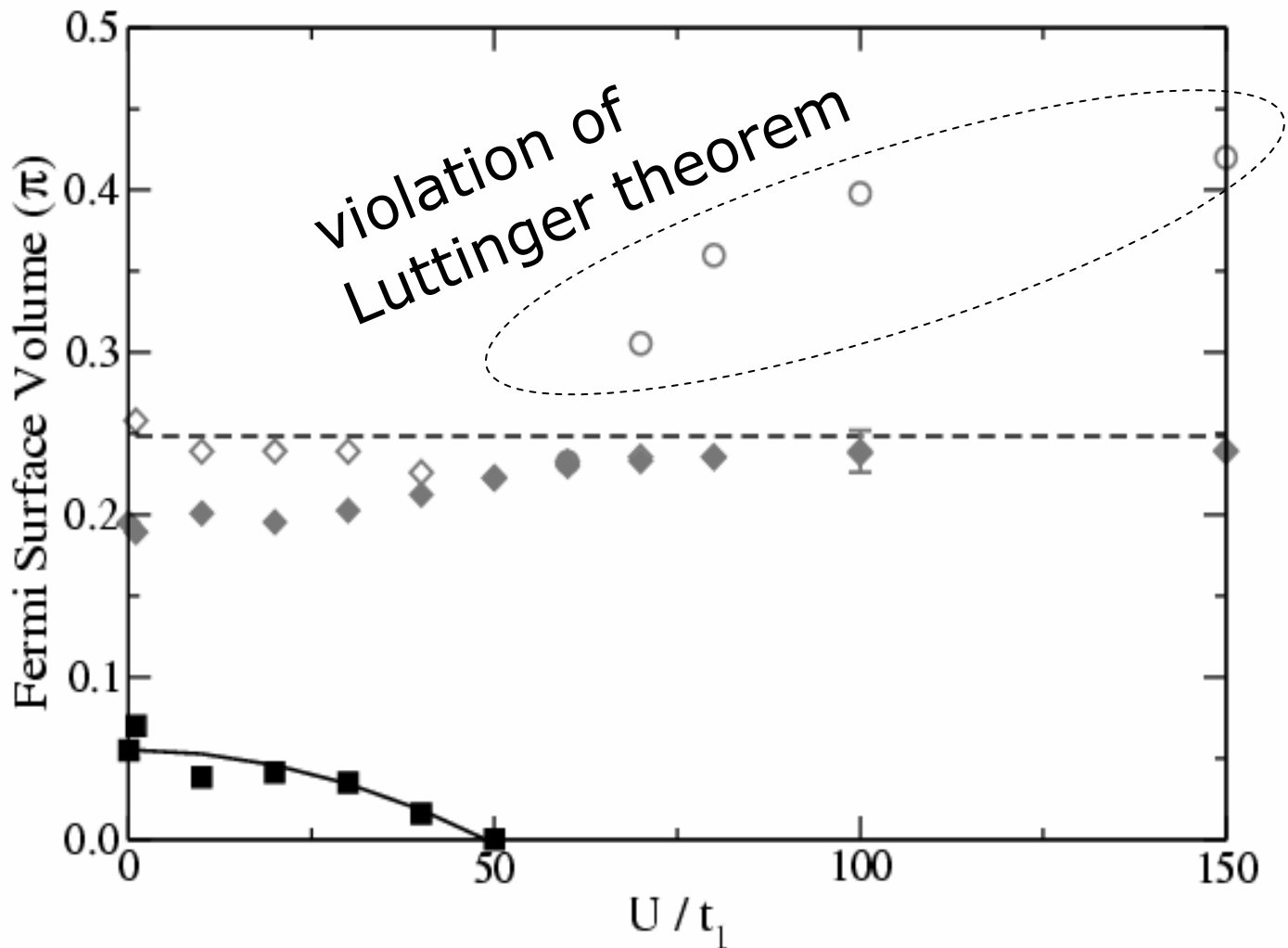
Linearization around the Fermi-Point gives $E_{1/2} \sim v_{F,1/2} k$

but $v_1 = 0.658t_1$ and $v_2 = 6.620t_1$

resulting in more/less creation of particle-hole-excitations and therefore different „speed“ of emptiness

Interaction induces Collapse of a Section of the Fermi Sea

1. Fit $n_{L=80}(k)$ on combination of washed-out step-functions $N(k)$
2. Determine point k_m of maximal slope of $N(k)$
3. Interpret k_m to be Fermi point



Remarks

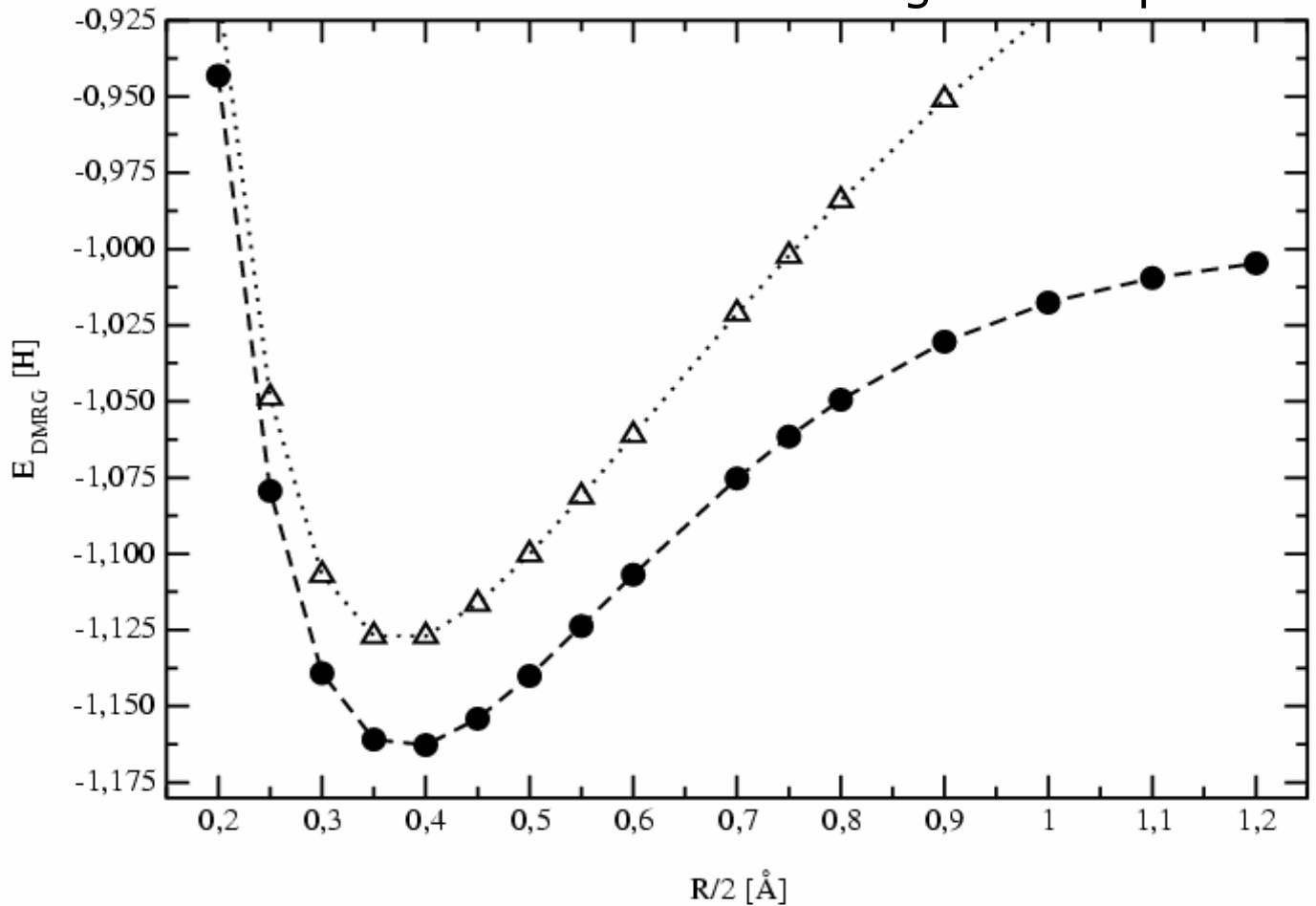
- DMRG-convergence for half-filling worse
- U_c drastically reduced near half-filling (*Louis et al.*)
- Coulomb is long-ranged and therefore more Coulomb-contribution than from simple U

Quantum Chemistry

$$H = - \sum_{ij\sigma} \langle i|h|j \rangle c_{i\sigma}^+ c_{j\sigma} + \frac{1}{2} \sum_{ijkl\sigma\sigma'} \langle ij|V|kl \rangle c_{i\sigma}^+ c_{j\sigma'}^+ c_{l\sigma'} c_{k\sigma}$$

generalized density-operators, long-range interaction
Therefore every operator to be stored in every step!

$\Delta_{FCI/DMRG} \approx 10^{-7} \text{ H}$ $m=30$, cc-pVDZ => 10 „sites“
=> avg. 1560 operators



Approximation $\sum |k\rangle\langle k| \approx 1$

saves some 50% of operators, because of excitations from HF-determinant but increases CPU-time

Further Steps

- Computations for other Transition Metal Compounds (coupling e.g. from SCF-calculations)
- Further studies on Hubbard-models
- Quantum chemistry: approximation to reduce no. of operators, spectrum of models to work on (Hückel, PPP, INDO, ab-initio) for chain-like molecules

Collaborations

W. Wenzel (FZ Karlsruhe)

C. Gros (U Saarbrücken)

J. Stolze (U Dortmund)

A. Klümper (U Wuppertal)

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... and now to your questions ...

or visit <http://www.kay-hamacher.de>