Correlation Effects and DMRG

Talk in the seminar
„Condensed Matter Theory“

Augsburg University, 18.11.2003

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Agenda

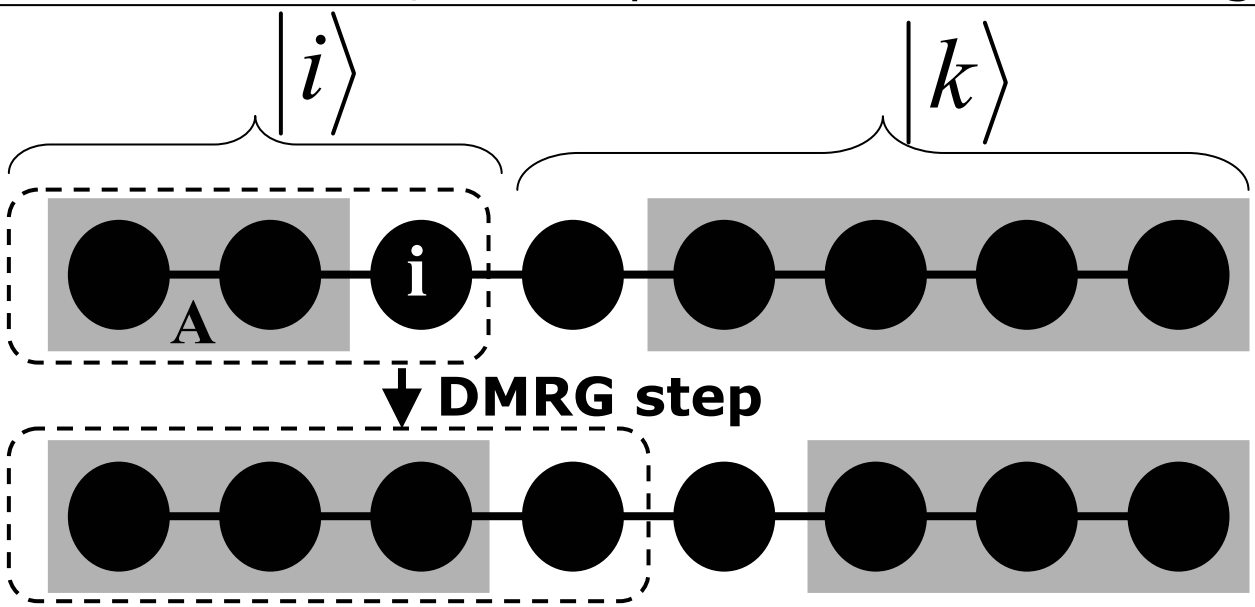
1. The DMRG algorithm
2. Spincluster-Model for NaV_2O_5
3. Dimerized Spinsystems and scaling arguments
4. Hubbard-Ladders
5. Aspects of quantum chemistry with the DMRG
6. Misc / Discussion

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

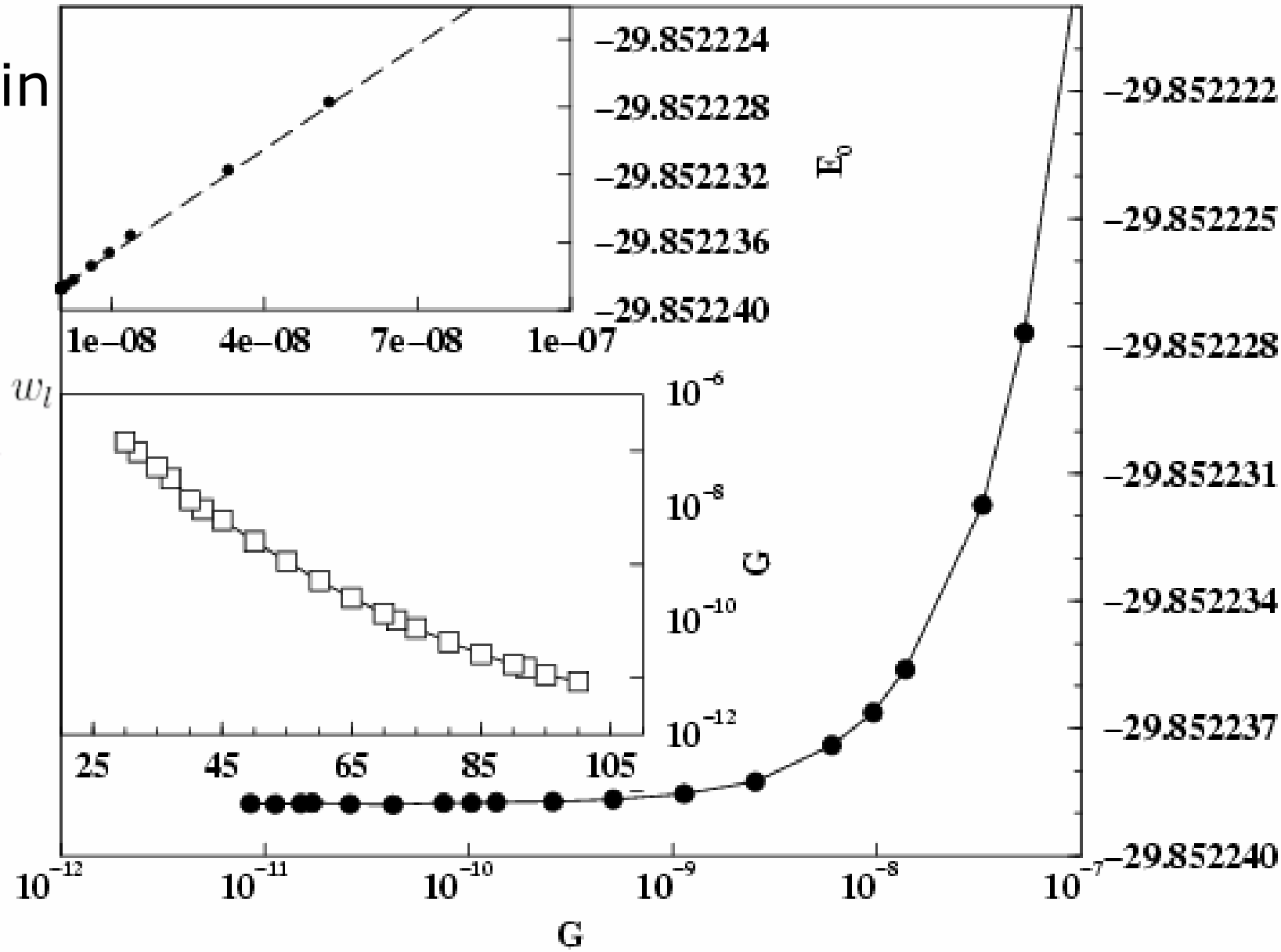


1. Diagonalize H_{total}
2. Build $\rho_{ij} = \sum_k |i,k\rangle\langle k,j|$
3. Diagonalize Density-Matrix ρ, select m „heaviest" eigenstates
4. Build bigger system by
   - transforming operators
   - building $H=H_A+H_i$ for bigger fragment
5. Iterate beginning with 1.

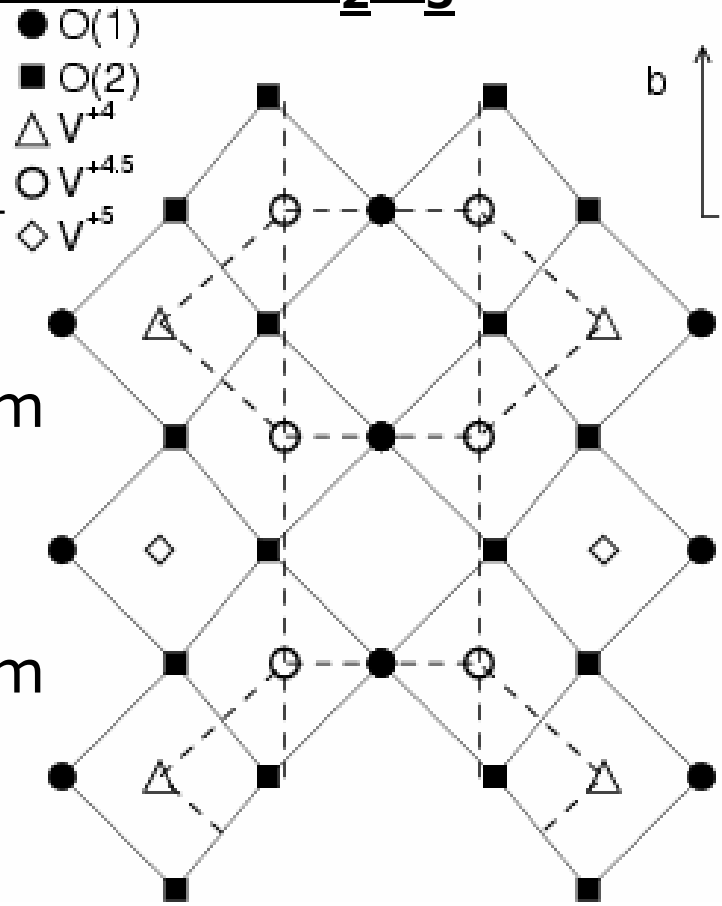
Discarded Weight G is a measure for precision

Spinchain
L=80

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



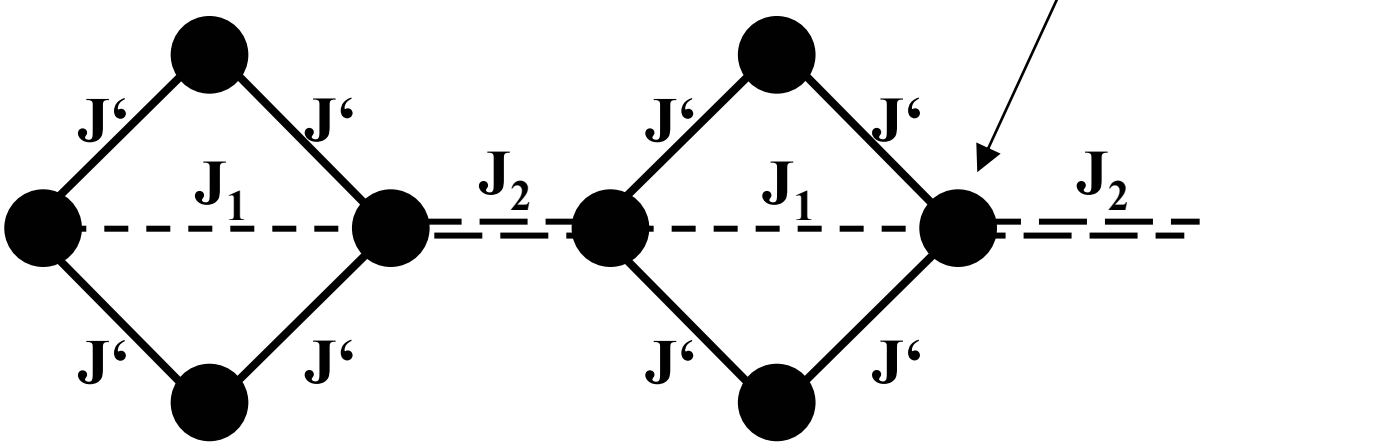
Spincluster-Model for NaV_2O_5



below T_c=34K:

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

Proposed model



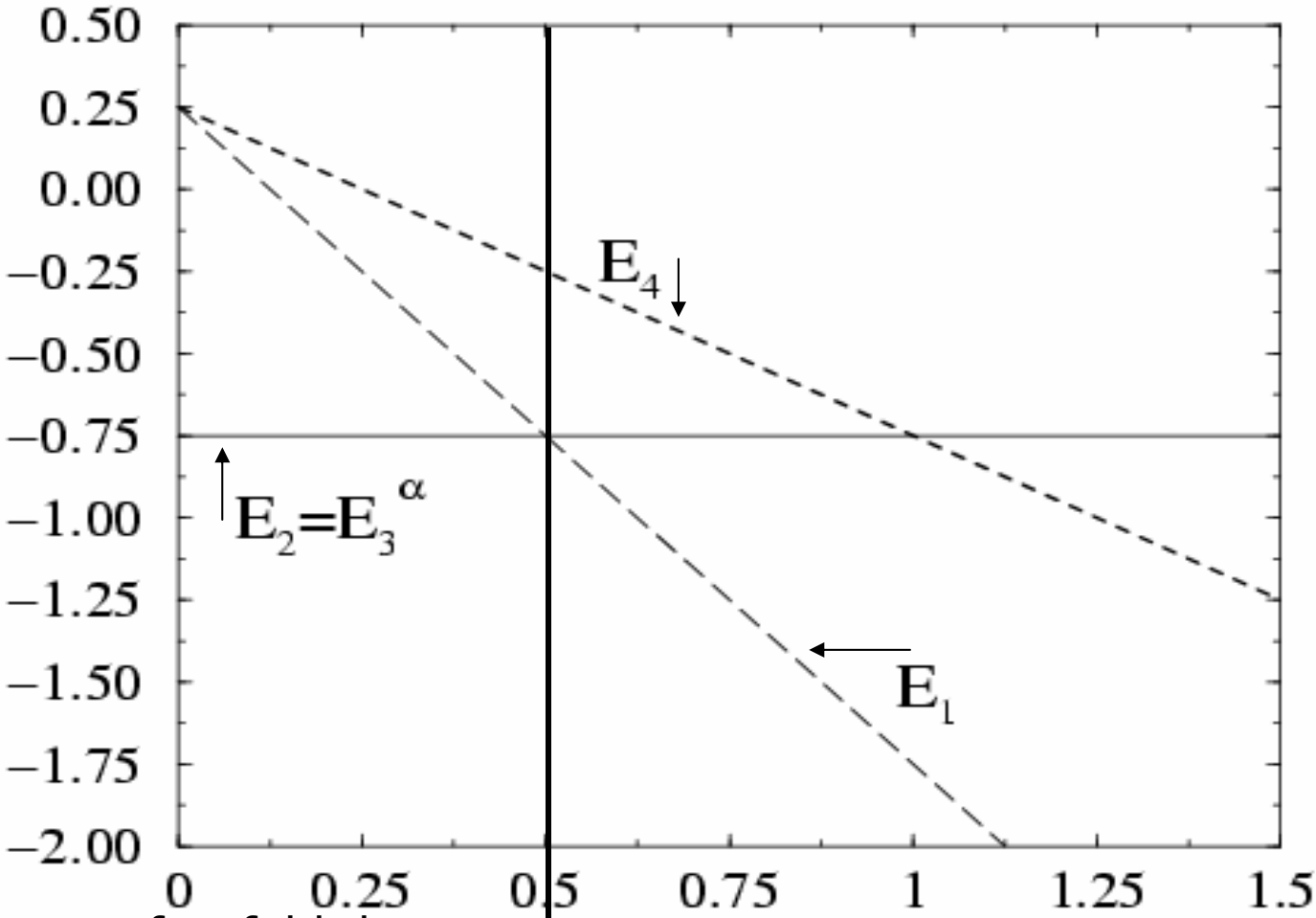
Spin gap not from dimerization

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

Spincluster-Model for NaV_2O_5

Analysis for a single cluster

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



fourfold de-generation (singlet+triplet)

GZ: singlet, cluster-phase

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

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

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

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

Cluster-Operator-Theory

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

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

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

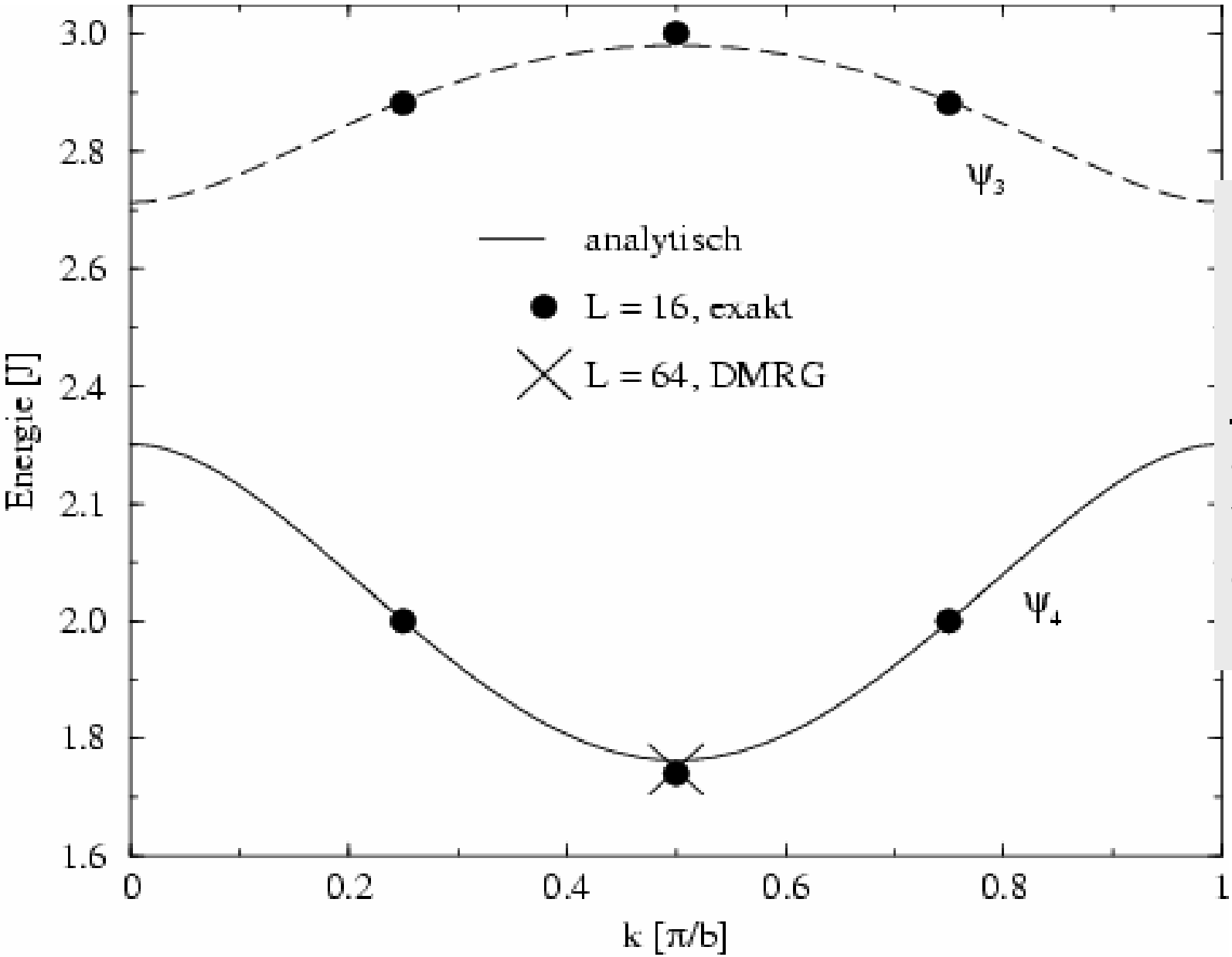
$$s_n^+, s_n \rightarrow 1$$

which gives by straight-forward diagonalization the dispersion

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

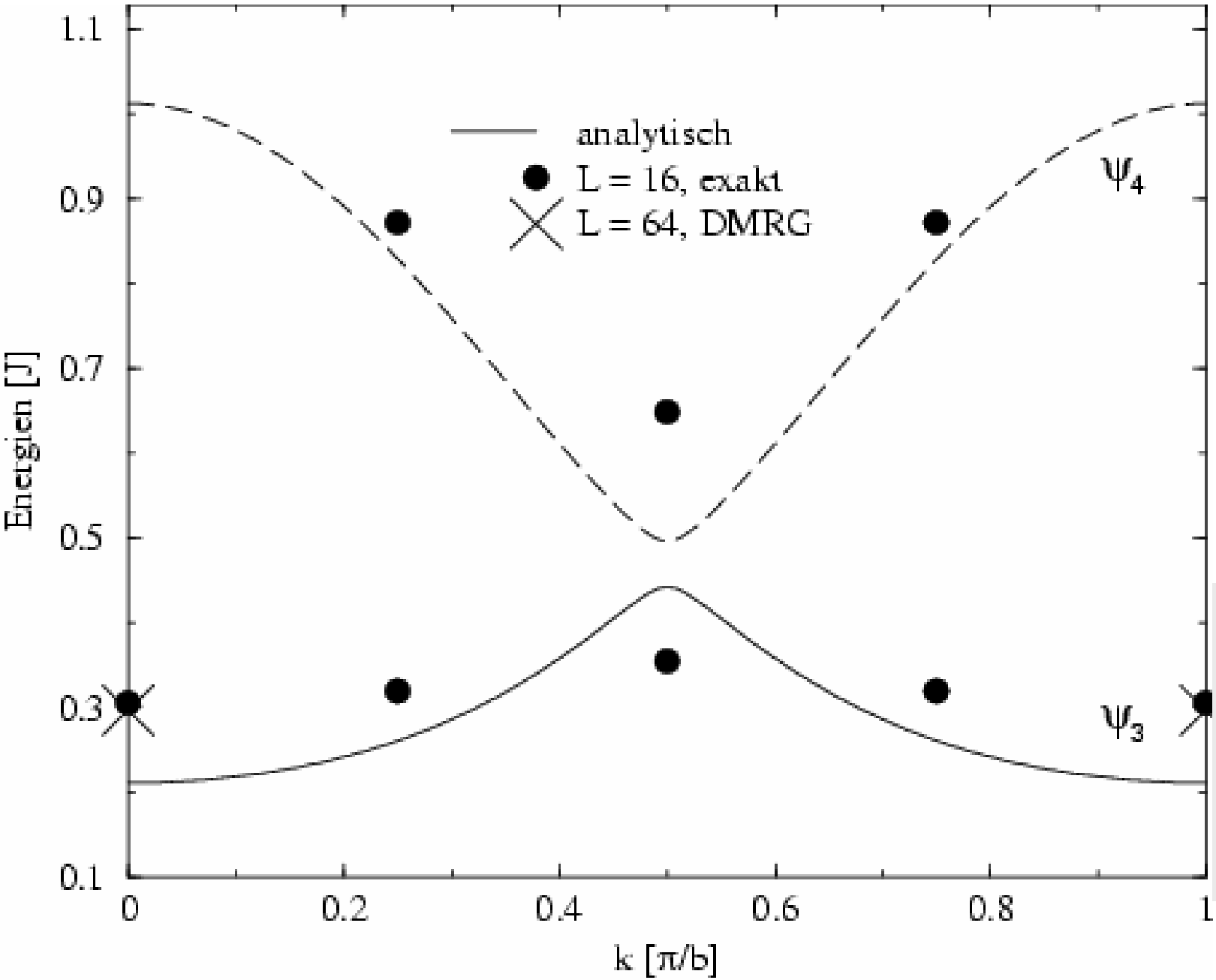
With some very complicated expressions for *t* and *s* / Skipped for your convenience

Results for the Cluster-Phase



location of minima/ maxima **not** in agreement with experiment

Results for the Haldane-Phase



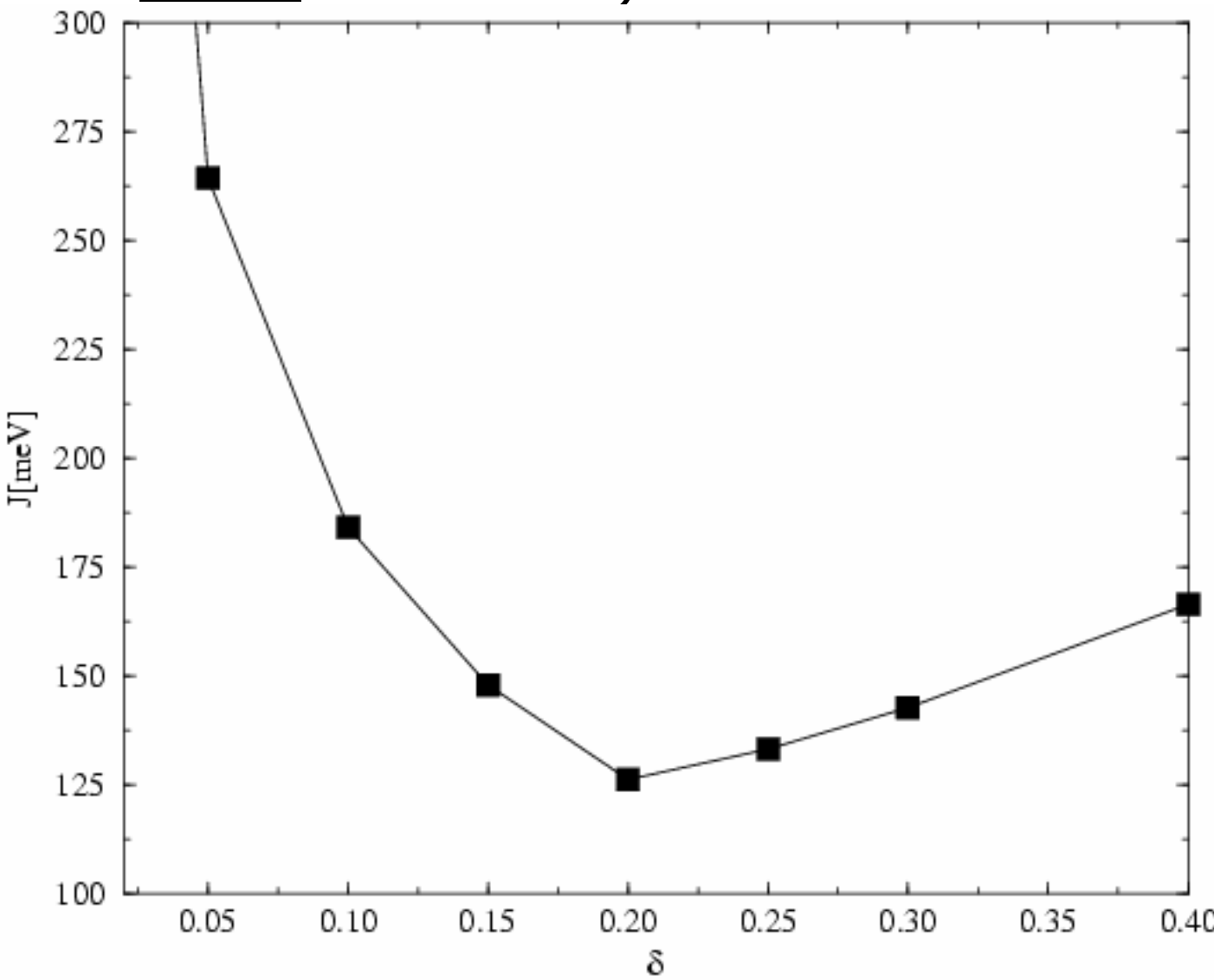
location of minima/ maxima **in** agreement with experiment

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)



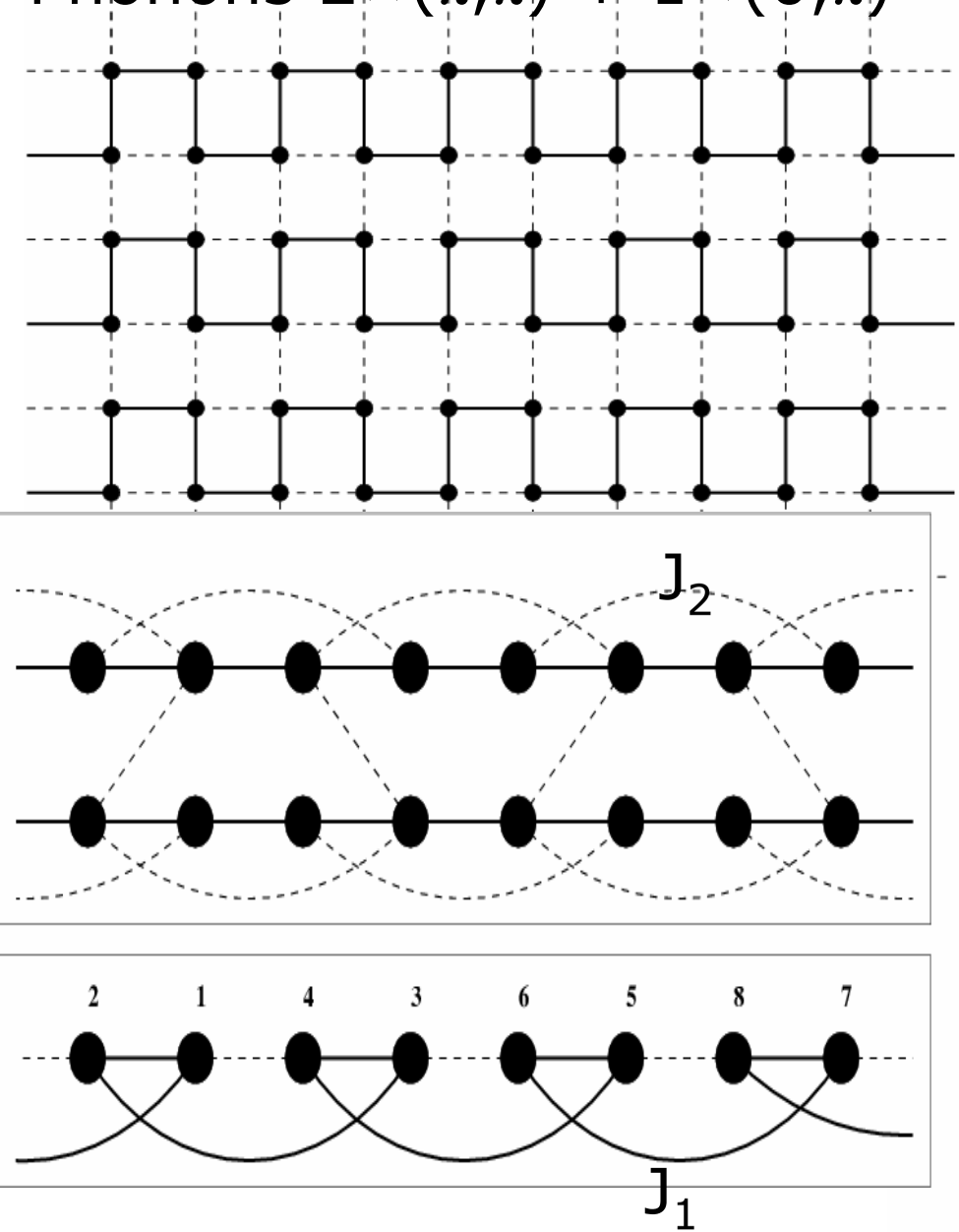
So, we need at least J≈125meV, but experiment gives 38 meV

Model is at least factor 3 off!

Gros, Valenti, Alvarez, Hamacher, Wenzel, *PRB* 62(2000)R14617

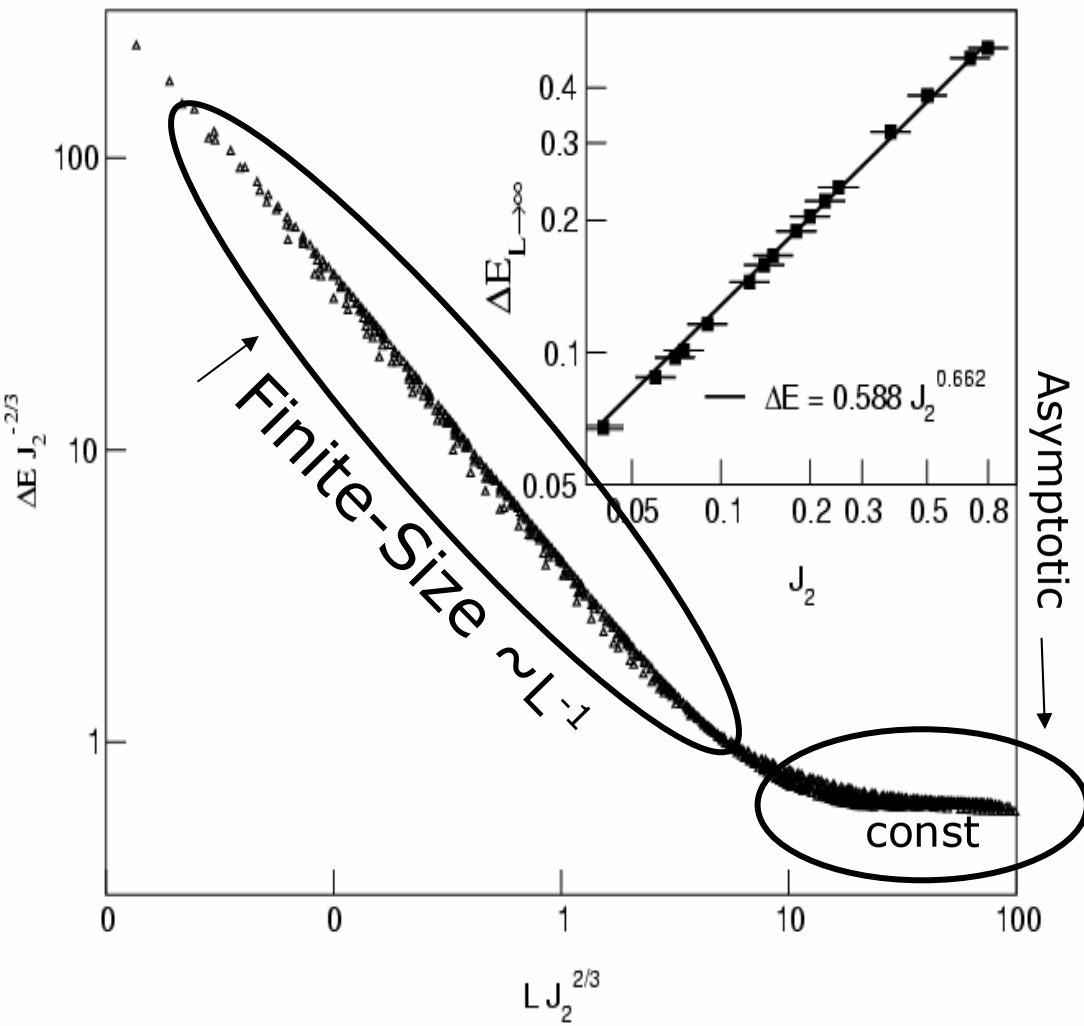
2D dimerized spinsystems (z.B. CaV_4O_9) – scaling arguments

Phonons 2×(π,π) + 1×(0,π)



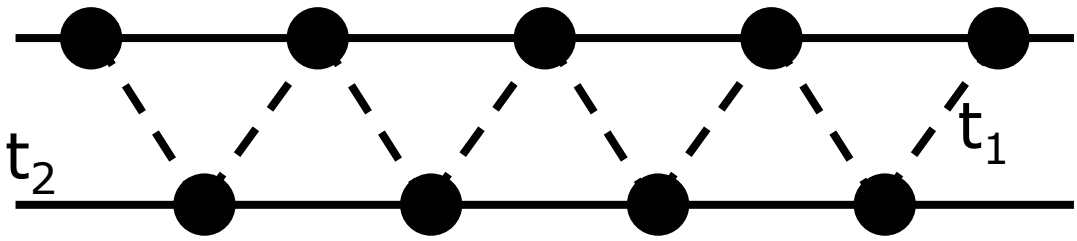
Sirker, Klümper, Hamacher,
PRB 65(2002), 134409

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



Hubbard ladders

(e.g. $SrCuO_2$ or LiV_2O_5, half-filling)



$$H = -t_1 \sum_{i=1,\sigma}^{L} \left\{ c^{+}_{i\sigma}\, c_{i+1\sigma} + h.c. \right\}$$

$$- t_2 \sum_{i=1,\sigma}^{L} \left\{ c^{+}_{i\sigma}\, c_{i+2\sigma} + h.c. \right\}$$

$$+ U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow}$$

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

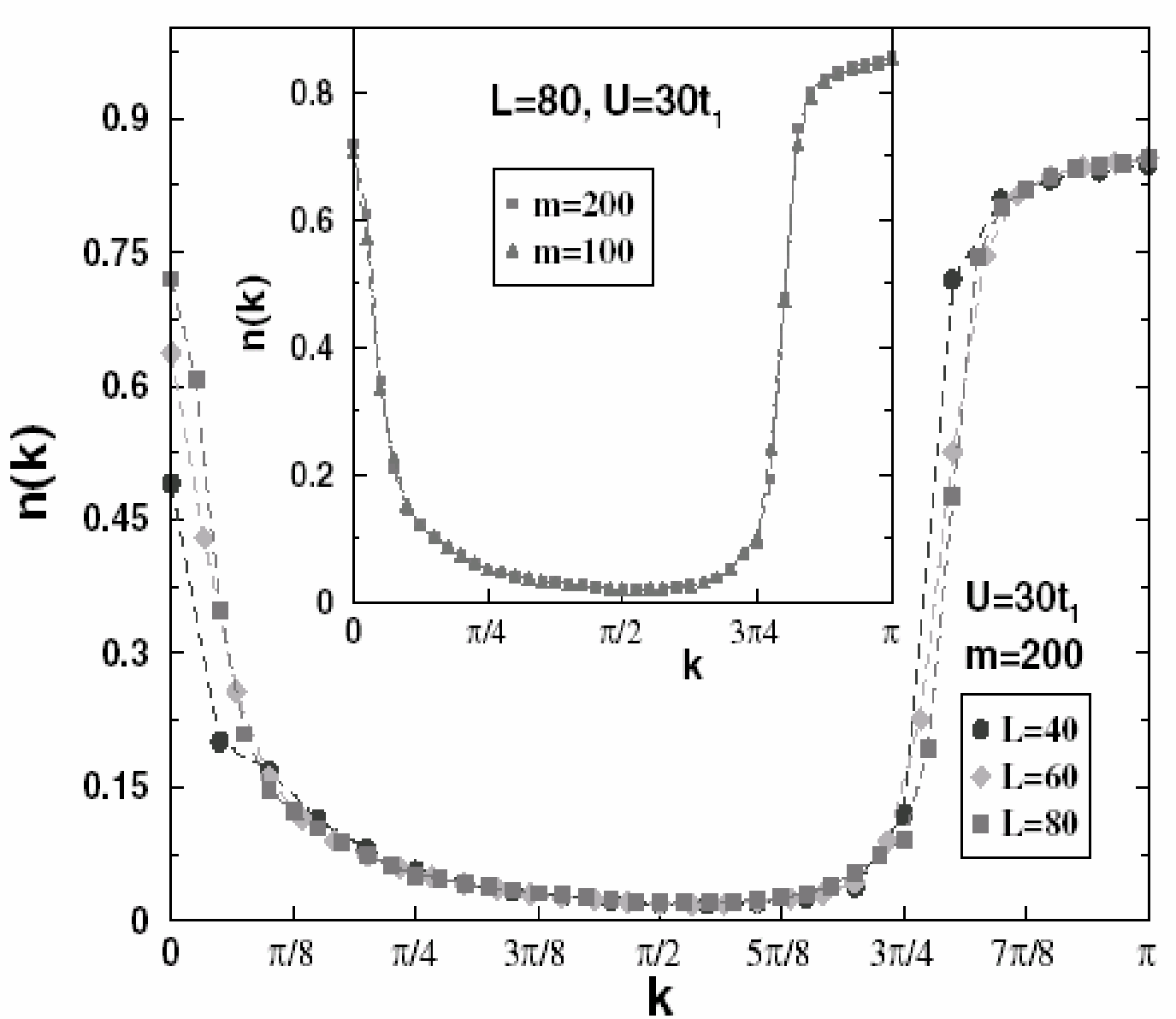
DMRG-computations for PBC and quarter-filling, $t_2/t_1=-3$ (convergence)

Computing Correlation Functions is a difficult job

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

$2L^2$ operators to store!

Checking precision of DMRG



Consistent with high-precision-calculations for OBC ✓

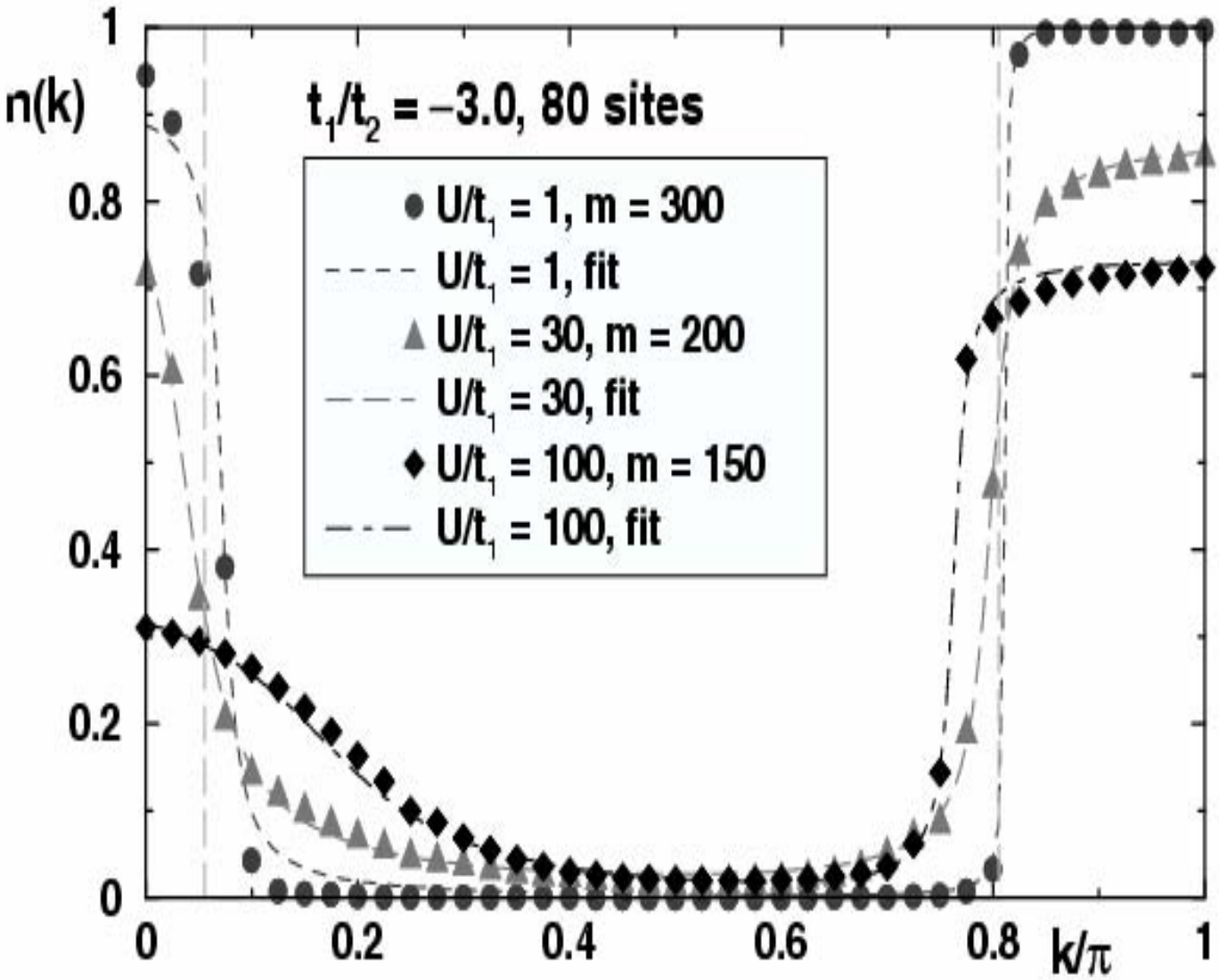
No instability spin gap (ferromagnetism)

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

No instability charge gap (phase separation)

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

Interaction induces Collapse of a Section of the Fermi Sea



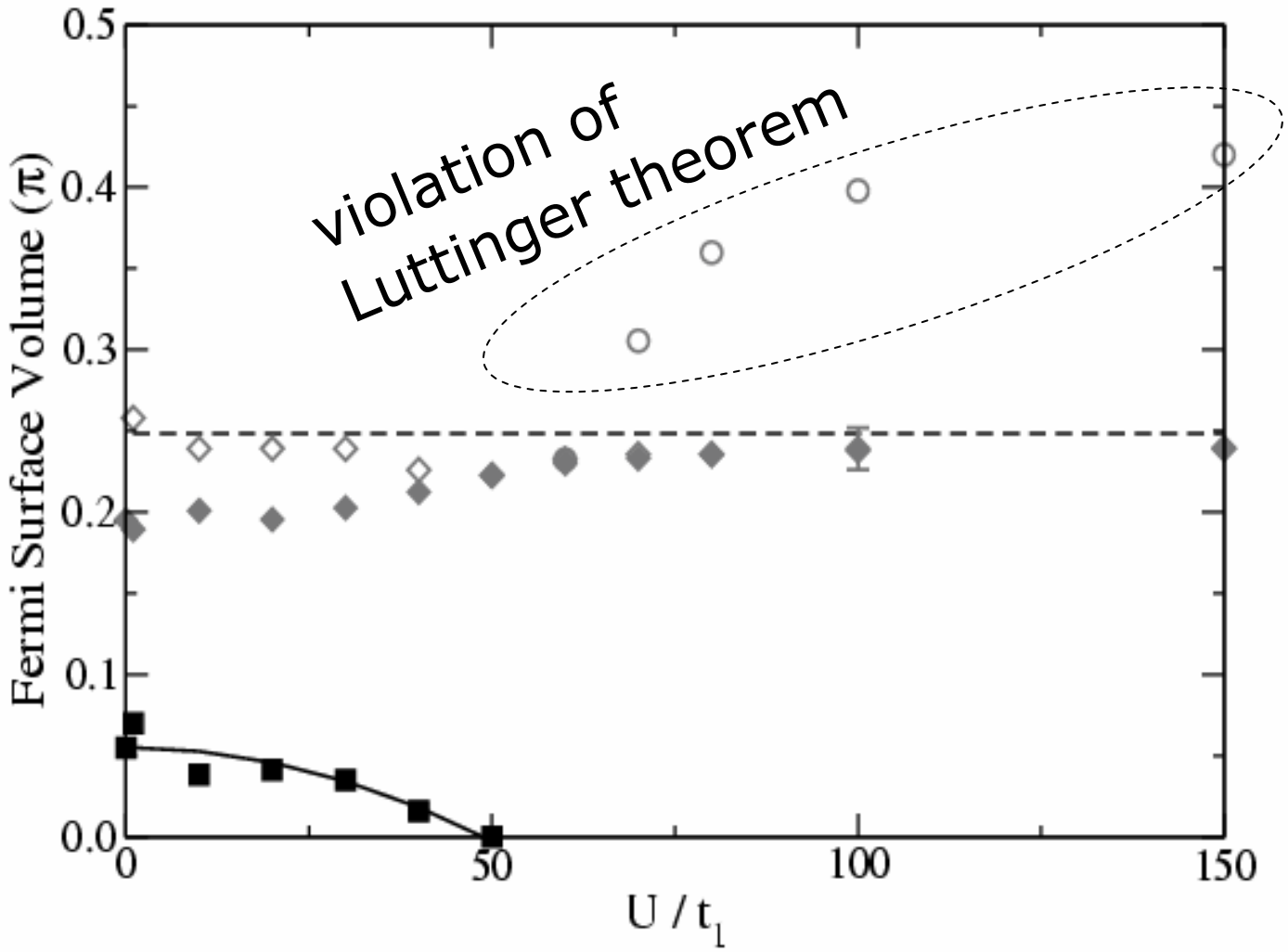
Linearization around the Fermi-Point gives $E_{1/2} \sim v_{F,1/2} k$

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

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

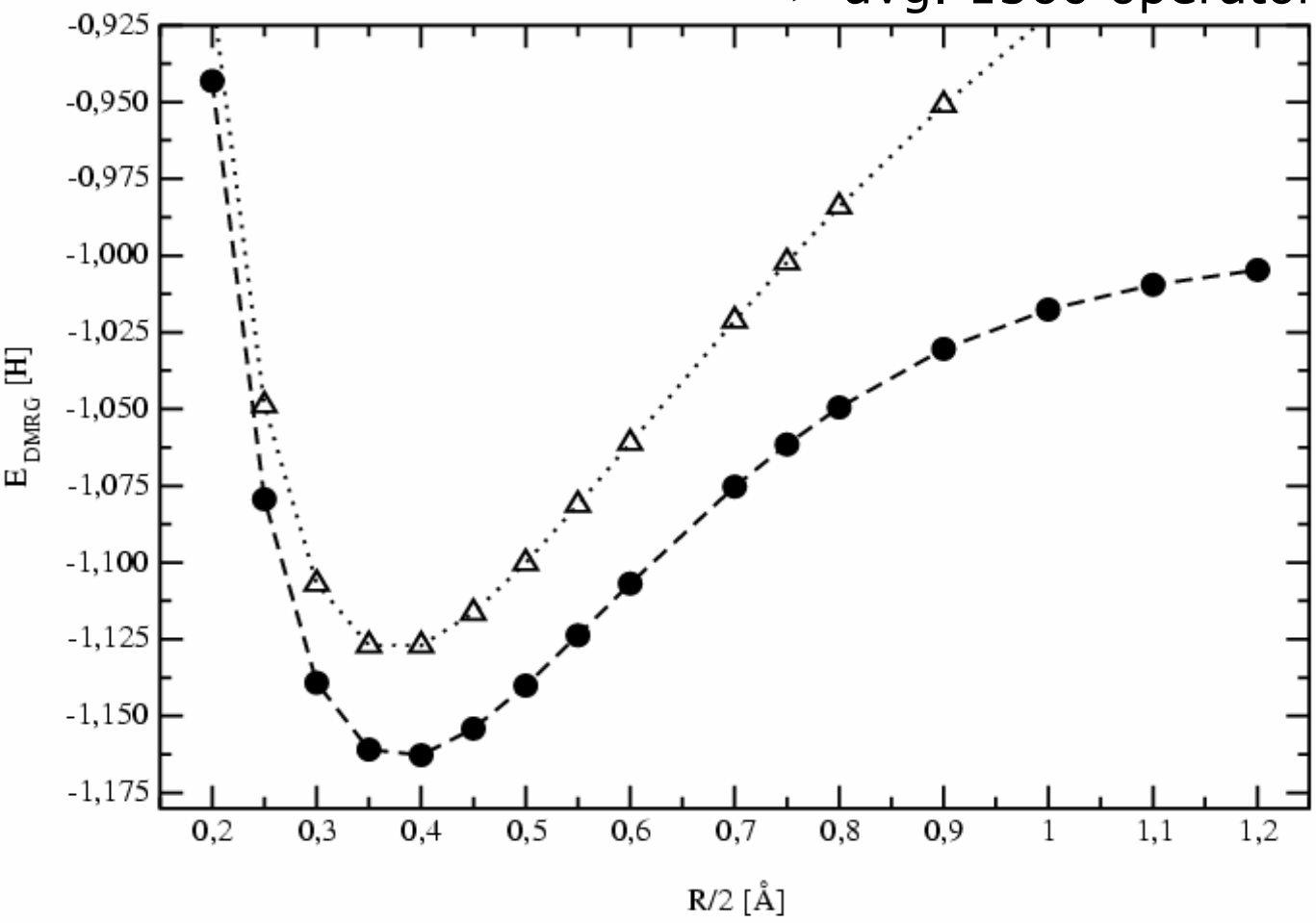
Hamacher, Gros, Wenzel *PRL* 88(2002)217203

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!

$\Delta_{FCI/DMRG} \approx 10^{-7}\,\mathrm{H}$ 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