Exact energy bounds for antiferromagnetic Heisenberg systems

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DPG spring meeting, March 27th 2003

unilogo-m-rot.jpg

Aim and Use

- Confine minimal energies as function of M or S;
- Use topological structure of interactions;
- Result improves bounds by Berezin and Lieb (1) and our first try (2);
- Bounds useful as benchmark for approximations like DMRG or variational methods;
- Bounds may serve as approximation of lowest (rotational) band.

(1) E. H. Lieb, Commun. Math. Phys. **31**, 327 (1973)
F. Berezin, Commun. Math. Phys. **40**, 153 (1975)
(2) H.-J. Schmidt, J. Schnack, and M. Luban, Europhys. Lett. **55**, 105 (2001)

Make use of n-cyclicity for upper bounds

$$\underset{\sim}{H} \quad = \quad -J \sum_{i,j} \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(j)$$

- n-cyclicity: directed graph of interactions can be mapped onto oriented cyclic graph with n vertices; 2-cyclicity is related to bi-partiteness;
- rings – N-cyclic, triangular lattice – 3-cyclic, square lattice – 4-cyclic, cubic lattice – 2-cyclic, kagomé lattice – 3-cyclic, but not 6-cyclic;

Variational state and Bloch transform

- Introduce variational state in $\mathcal{H}(M)$: $|\,\phi\,\rangle = C_M \underset{\sim}{U} \, (\underset{\sim}{S}^-)^{Ns-M} \,|\,\Omega\,\rangle$,
  $|\,\Omega\,\rangle \equiv |\,s, s, s, \dots\,\rangle$ magnon vacuum.

- $\underset{\sim}{U}$ is a generalized "Bloch" operator $\underset{\sim}{U}$, which supplements appropriate phases (1).

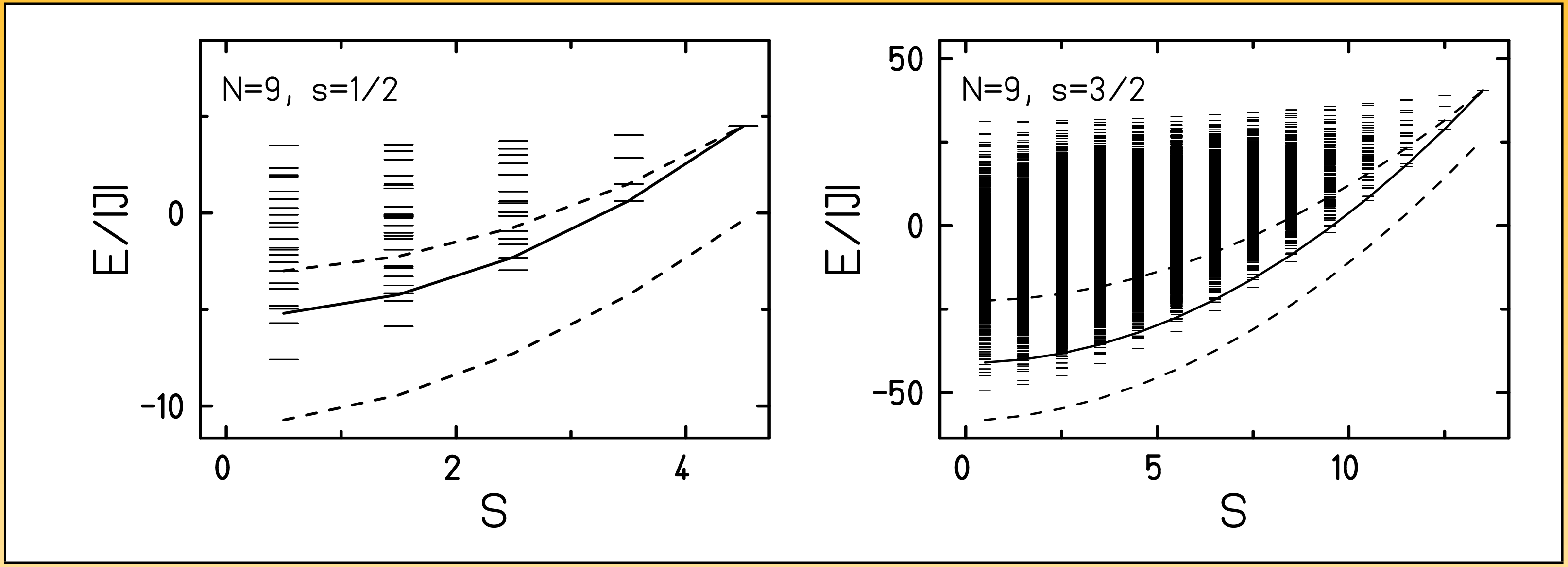
- Transform $\underset{\sim}{H}$ instead of $|\,\Omega\,\rangle$:

$$E_{\text{min}}(M) \quad \leq \quad -Jc\gamma s^2 - J(1-c)\frac{\gamma}{N}\left(Ns^2 - \frac{2s\left((Ns)^2 - M^2\right)}{2Ns-1}\right) \ ,$$

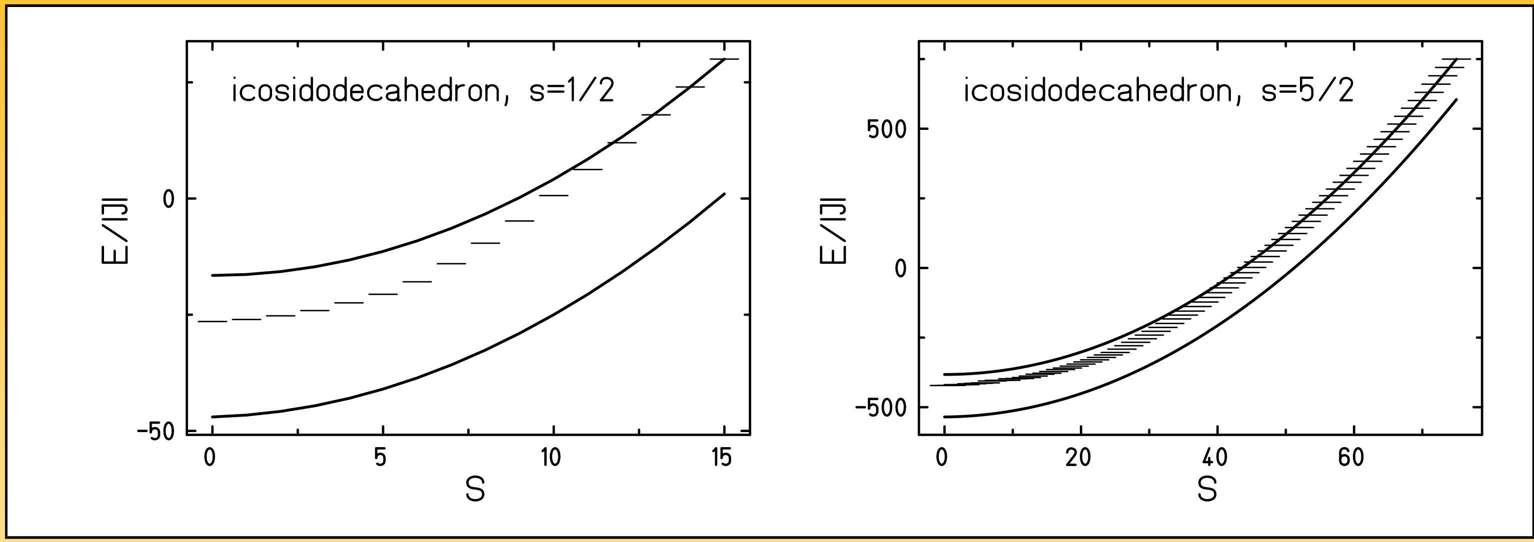
where $c=-1$ in the case of even n (bipartite) and $c = -\cos\frac{\pi}{n}$ for odd n, γ is the number of interacting pairs.

(1) I. Affleck, E. H. Lieb, Lett. Math. Phys. **12** (1986) 57

Spin ring with $N = 9$



Bounds for the icosidodecahedron



- Minimal energies for the icosidodecahedron: $s = 1/2$ from J. Richter (2), $s = 5/2$ DMRG (3).

- Upper bound rather close to true minimal energies, the better the larger s.

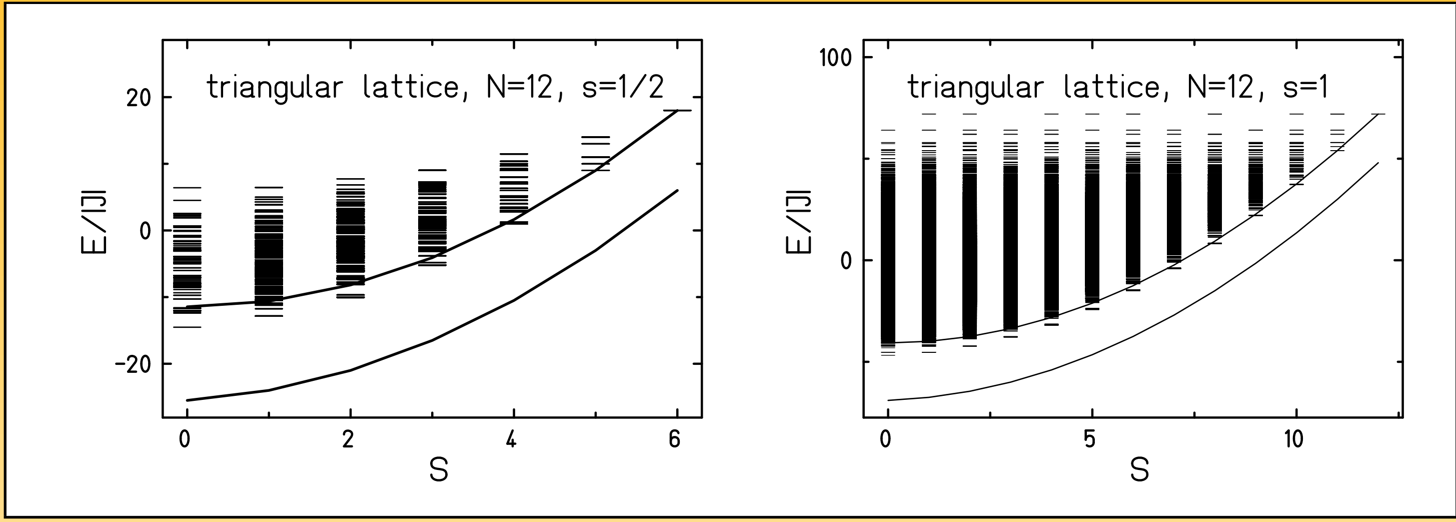
(1) K. Bärwinkel, H.-J. Schmidt, and J. Schnack, Eur. Phys. J. B (2002) submitted, cond-mat/0210458
(2) J. Schnack, H.-J. Schmidt, J. Richter, J. Schulenburg, Eur. Phys. J. B **24** (2001) 475
(3) M. Exler, J. Schnack, Phys. Rev. B (2002), accepted, cond-mat/0205068

Lower bounds for n-homogeneous systems

$$\underset{\sim}{H} = \sum_{\mu\nu} J_{\mu\nu} \underset{\sim}{\vec{s}}_\mu \cdot \underset{\sim}{\vec{s}}_\nu \ , \qquad \sum_{b \in \mathcal{A}_\mu} J_{ab} = \begin{cases} j^{\text{in}} & \text{if} \quad a \in \mathcal{A}_\mu \\ j^{\text{ex}} & \text{if} \quad a \notin \mathcal{A}_\mu \end{cases}$$

- Matrix $\mathbb{J} \equiv (J_{\mu\nu})$ be symmetric and have constant row sums j;
- n-homogeneous: set of spin sites be divided into n disjoint subsets of equal size m, $\{1, \dots, N\} = \bigcup_{\nu=1}^n \mathcal{A}_\nu$;
  within each $\mathcal{A}_\nu$: $J_{\mu\nu} \leq 0$, but ≥ 0 between $\mathcal{A}_\nu$ and $\mathcal{A}_\mu$ for $\nu \neq \mu$;
- smallest eigenvalue j_{min} at least $(n-1)$-times degenerate because of n-homogeneity, j_2 is the remaining smallest eigenvalue;
- construction of a coupling matrix $\widetilde{\mathbb{J}}$ with eigenvalues j (1), j_{min} $(n-1)$, j_2 $(N-n)$;
- $\mathbb{J} \geq \widetilde{\mathbb{J}} \quad \Rightarrow \quad \underset{\sim}{H} \geq \frac{j - j_{\text{min}}}{N} S(S+1) + N j_{\text{min}} s(s+1) + (N-n)(j_2 - j_{\text{min}}) s \quad .$

Bounds for the triangular lattice



$$9S_c^2 - 3s^2 - 3s \leq \lim_{N\to\infty} \frac{E_{\text{min}}(S)}{N} \leq 9S_c^2 - 3s^2 \ ,$$

where $S_c = S/N$ running from 0 to s.

K. Bärwinkel, H.-J. Schmidt, and J. Schnack, Eur. Phys. J. B (2002) submitted, cond-mat/0210458

Thank you very much for your attention.

Collaboration

- Prof. K. Bärwinkel, Prof. H.-J. Schmidt, M. Brüger, D. Mentrup, M. Exler, P. Hage, F. Hesmer, P. Shechelokovskyy (Uni Osnabrück);
- Prof. M. Luban, Prof. R. Modler, Dr. P. Kögerler, Dr. Chr. Schröder (Ames Lab, Iowa, USA);
- Prof. S. Blügel (FZ Jülich);
- Prof. J. Richter, J. Schulenburg (Uni Magdeburg);
- Dr. A. Honecker (Uni Braunschweig).