The Osnabrück k-rule for odd antiferromagnetic rings

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Brainstorming Meeting on Anti-Ferromagnetic Rings

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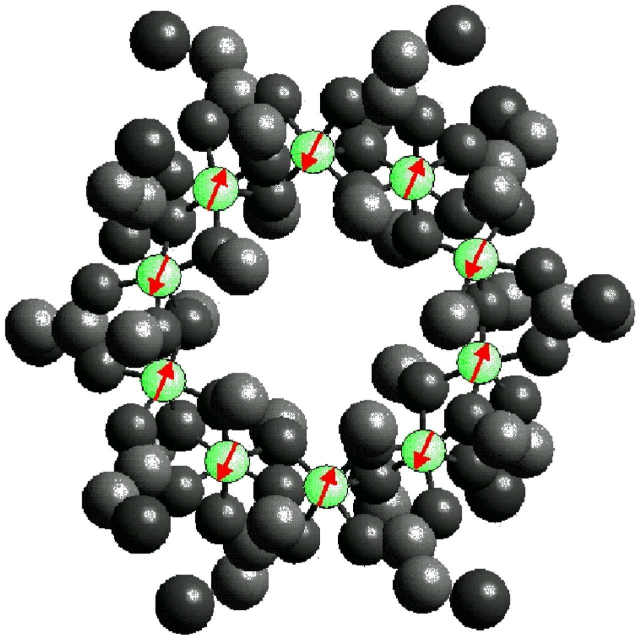
Will be delivered today!

1. Idea behind the gymnastics
2. Heisenberg-Hamiltonian and symmetries for rings
3. Bipartiteness and consequences
4. Surprise for odd rings: the Osnabrück k–rule
5. Generalization of ground state properties
6. Solitons on antiferromagnetic Heisenberg rings?

Idea behind the gymnastics



Fe_{10}

- Numerical limitations in calculating spectra of large spin systems.
- Goal: determine dependence of general properties of the magnetic spectrum on the structure, i.e. topology of spin couplings.
- E. g. quantum numbers like total spin S, total magnetic quantum number M, degeneracy, and momentum k of certain low-lying states.
- Problem solved for bipartite spin systems, e.g. even rings (Marshall, Peierls, Lieb, Schultz, Mattis).
- Findings: It turns out that also for odd-membered af spin rings such relations hold.

Heisenberg Hamiltonian for rings

Hamiltonian

$$\underset{\sim}{H} = -2\,J \sum_i \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(i+1) \qquad + \qquad g\,\mu_B\,B \sum_i^N \underset{\sim}{s}_z(i)$$

Heisenberg — Zeeman

$J < 0$ for af coupling

Product basis

$$|\,\vec{m}\,\rangle = |\,m_1, \dots, m_N\,\rangle \quad \text{with} \quad \underset{\sim}{s}_z(u)\,|\,\dots, m_u, \dots\rangle = m_u\,|\,\dots, m_u, \dots\rangle$$

Symmetries

Total spin $\underset{\sim}{\vec{S}}$ and $\underset{\sim}{S}_z$

$$\left[\underset{\sim}{H}, \underset{\sim}{\vec{S}}^2\right] = 0 \quad \& \quad \left[\underset{\sim}{H}, \underset{\sim}{S}_z\right] = 0 \quad \& \quad \left[\underset{\sim}{\vec{S}}^2, \underset{\sim}{S}_z\right] = 0$$

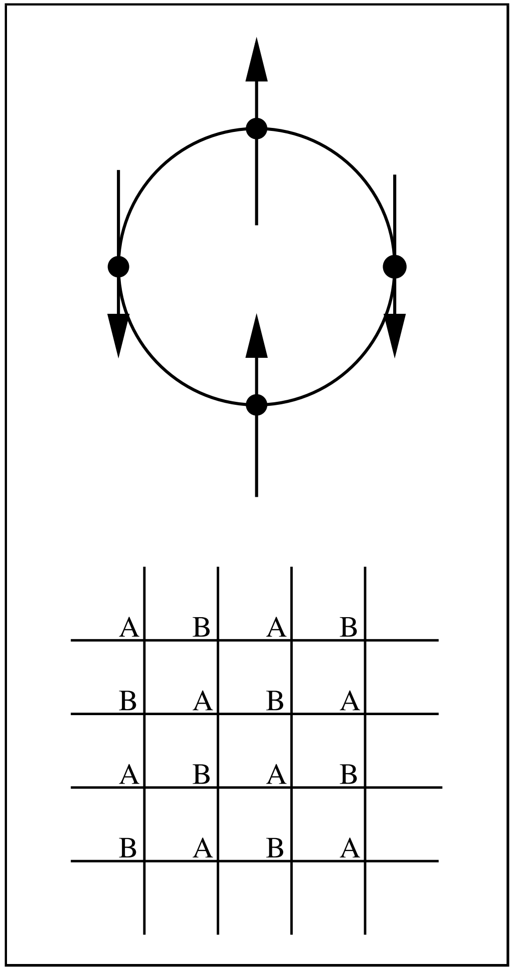
Cyclic shift operator $\underset{\sim}{T}$ and shift quantum number k

$$\underset{\sim}{T} \mid m_1, \dots, m_{N-1}, m_N \rangle = \mid m_N, m_1, \dots, m_{N-1} \rangle$$

eigenvalues: $z = \exp\left\{-i\frac{2\pi k}{N}\right\} \quad , \quad k = 0, 1, \dots, N-1$

$$\left[\underset{\sim}{H}, \underset{\sim}{T}\right] = \left[\underset{\sim}{\vec{S}}^2, \underset{\sim}{T}\right] = \left[\underset{\sim}{S}_z, \underset{\sim}{T}\right] = 0$$

Bipartiteness and consequences

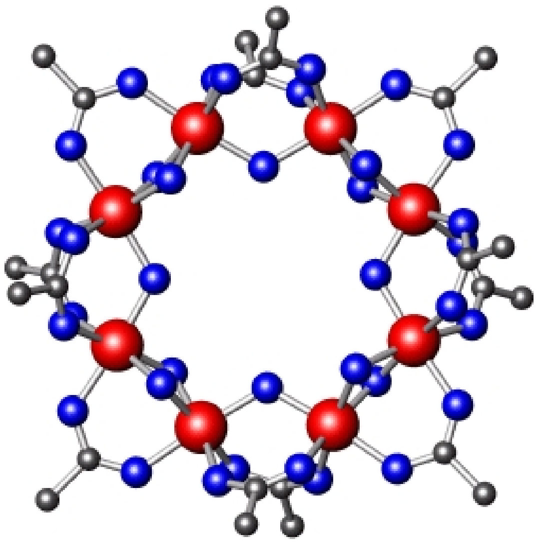


- Very general statements about the ground states of the subspaces $\mathcal{H}(M)$ can be made for **bipartite** spin systems (1 & 2).
- An antiferromagnetic spin system is bipartite, if it can be decomposed into two sublattices A and B such that:

$$J(x_A, y_B) \leq g^2 \, , J(x_A, y_A) \geq g^2 \, , J(x_B, y_B) \geq g^2 .$$

(1) E.H. Lieb, T.D. Schultz, and D.C. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961)
(2) E.H. Lieb and D.C. Mattis, J. Math. Phys. **3**, 749 (1962)

Lieb, Schultz, and Mattis for even rings



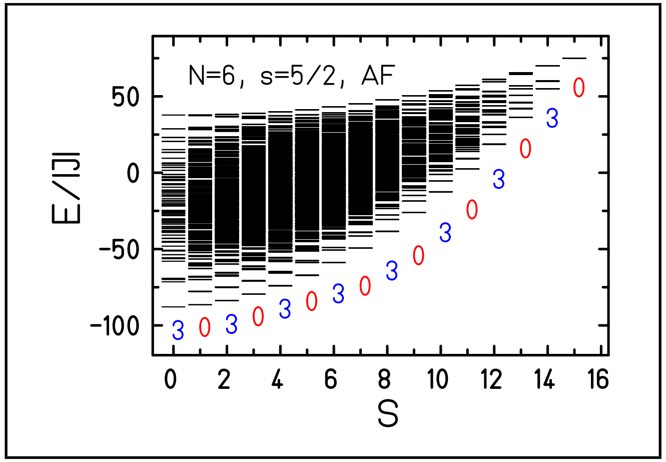
Cr_8

Statements of (1) and (2):

- Each Hilbert subspace $\mathcal{H}(M)$ contains a non-degenerate ground state.
- This ground state has $S = |M|$ with ground state energy E_S.
- If all $s_i = s$ then $E_S < E_{S+1}$ and thus the total ground state has $S = 0$.

(1) E.H. Lieb, T.D. Schultz, and D.C. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961)
(2) E.H. Lieb and D.C. Mattis, J. Math. Phys. **3**, 749 (1962)

Marshall-Peierls sign rule for even rings



- Expanding the ground state in $\mathcal{H}(M)$ in the product basis yields a sign rule for the coefficients

$$| \Psi_0 \rangle = \sum_{\vec{m}} c(\vec{m}) \, | \vec{m} \rangle \qquad \text{with } \sum_{i=1}^{N} m_i = M$$

$$c(\vec{m}) = (-1)^{\left(\frac{Ns}{2} - \sum_{i=1}^{N/2} m_{2i} \right)} a(\vec{m})$$

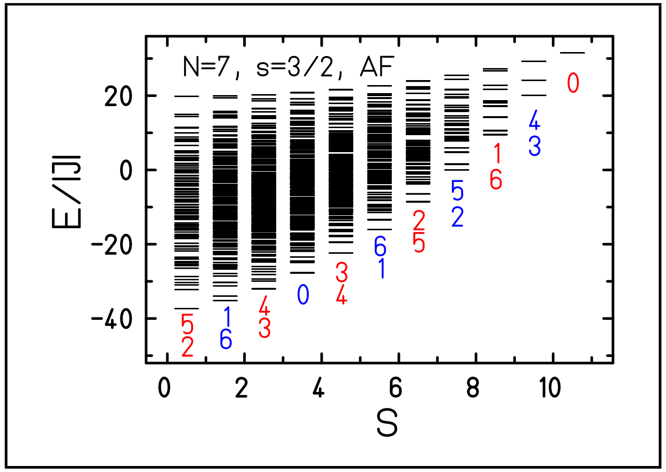
All $a(\mathbf{m})$ are non-zero, real, and of equal sign.

- Yields for the shift quantum number: $k \equiv a \frac{N}{2} \mod N \,, \quad a = Ns - M$

(1) W. Marshall, Proc. Royal. Soc. A (London) **232**, 48 (1955)

Anything alike for odd rings?

Numerical findings for odd rings



- For odd N and half integer s, i.e. $s = 1/2, 3/2, 5/2, \ldots$ we find that (1)
  - the ground state has total spin $S = 1/2$;
  - the ground state energy is **fourfold** degenerate.

- Reason: In addition to the (trivial) degeneracy due to $M = \pm 1/2$, a degeneracy with respect to k appears (2):
  $k = \lfloor \frac{N+1}{4} \rfloor$ and $k = N - \lfloor \frac{N+1}{4} \rfloor$

- For the first excited state similar rules could be numerically established (3).

(1) K. Bärwinkel, H.-J. Schmidt, J. Schnack, J. Magn. Magn. Mater. **220**, 227 (2000)
(2) $\lfloor \cdot \rfloor$ largest integer, smaller or equal
(3) J. Schnack, Phys. Rev. B **62**, 14855 (2000)

The Osnabrück k-rule for odd rings

- An extended k-rule can be inferred from our numerical investigations which yields the k quantum number for relative ground states of subspaces $\mathcal{H}(M)$ for even as well as odd spin rings, i.e. for all rings (1)

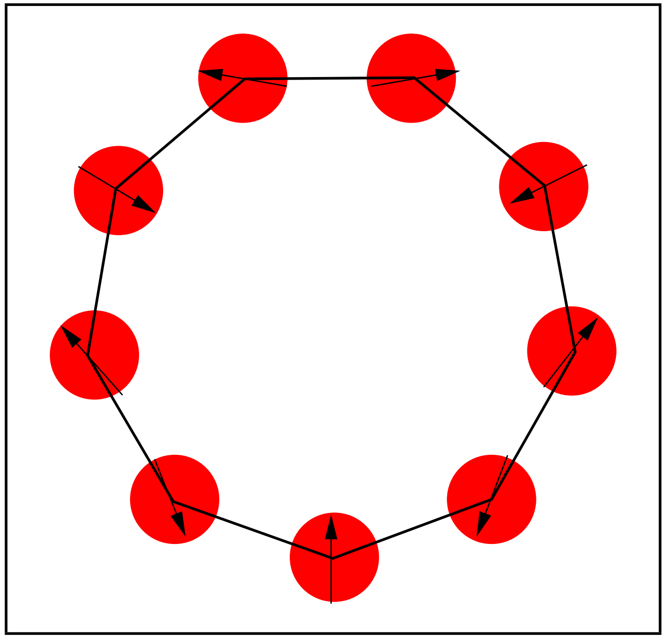
$$\text{If } N \neq 3 \quad \text{then} \quad k \equiv \pm a \left\lceil \frac{N}{2} \right\rceil \mod N \,, \quad a = Ns - M$$

The degeneracy is minimal.

N	s	a: 0	1	2	3	4	5	6	7	8	9
7	1/2	0	4	$8 \equiv 1$	$12 \equiv 5$	-	-	-	-	-	-
8	1/2	0	4	$8 \equiv 0$	$12 \equiv 4$	$16 \equiv 0$	-	-	-	-	-
9	1/2	0	$5 \equiv 4$	$10 \equiv 1$	$15 \equiv 3$	$20 \equiv 2$	-	-	-	-	-
9	1	0	$5 \equiv 4$	$10 \equiv 1$	$15 \equiv 3$	$20 \equiv 2$	$25 \equiv 2$	$30 \equiv 3$	$35 \equiv 1$	$40 \equiv 4$	$45 \equiv 0$
10	1/2	0	5	$10 \equiv 0$	$15 \equiv 5$	$20 \equiv 0$	$25 \equiv 5$	-	-	-	-

(1) K. Bärwinkel, P. Hage, H.-J. Schmidt, and J. Schnack, Phys. Rev. B **68**, 054422 (2003)

Examples for odd rings



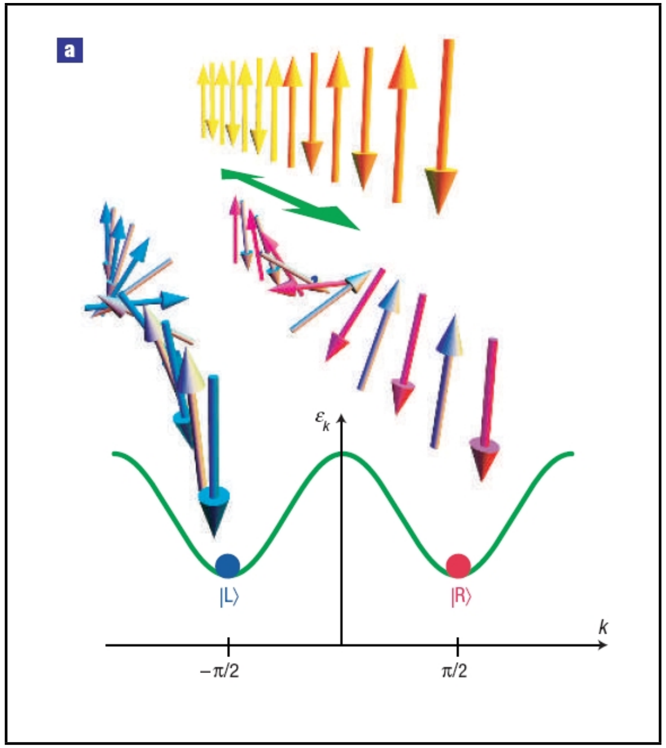
- Fe_9 with $s = 5/2$ (1)
  - the ground state has total spin $S = 1/2$;
  - the ground state has $k = 2$ and $k = 7$;
  - the ground state energy is **fourfold** degenerate.
- In the real compound the symmetry is reduced, which may or may not lift the degeneracy (1).
- Rings with integer spin have a non-degenerate $S = 0$ ground state.
- Very little can be proven for odd af rings (2)!

no more time option

(1) H.C. Yao, J.J. Wang, Y.S. Ma, O. Waldmann,W.X. Du, Y. Song, Y.Z. Li, L.M. Zheng, S. Decurtins, X.Q. Xin, Chem. Commun., 1745 (2006)
(2) K. Bärwinkel, P. Hage, H.-J. Schmidt, and J. Schnack, Phys. Rev. B **68**, 054422 (2003)

Solitons on antiferromagnetic Heisenberg rings?

Solitons I



- Solitons are usually discussed in rather unisotropic spin systems (1)

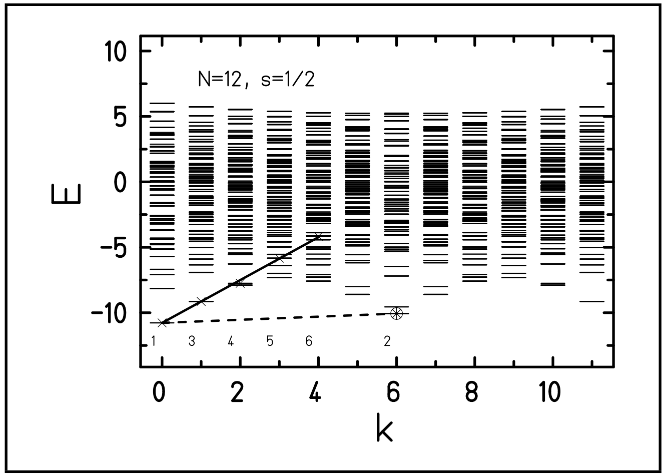
$$\underset{\sim}{H} = -2\,J \sum_i \, \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(i+1) + D \sum_i \, \underset{\sim}{s}_z^2(i)$$

- Approximate equations of motion can be obtained which describe
  - classical discrete spins;
  - or a classical spin density.

- These differential equations, e.g. non-linear Schrödiger equation, have soliton solutions (2).

(1) H.-B. Braun, J. Kulda, B. Roessli, D. Visser, K.W. Krämer, H.-U. Güdel, P. Böni, Nat. Phys. **1**, 159 (2005)
(2) A vast literature exists on solitons in 1-d magnetic systems.

Solitons II



- Do solitons exist in simple af Heisenberg rings?

- Possible definition: for a certain time τ the time evolution equals the shift by one site (1), i.e. dispersion free motion

$$\underset{\sim}{U}(\tau) \mid \Psi_s \rangle = e^{-i\Phi_0} \underset{\sim}{T}^{\pm 1} \mid \Psi_s \rangle$$

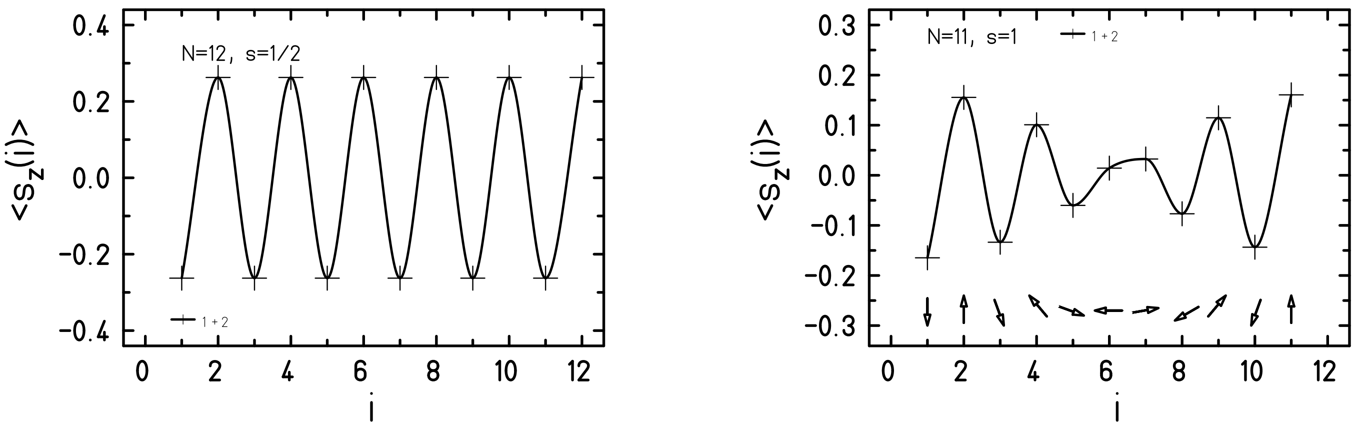
- This is equivalent to

$$\frac{E_\mu \tau}{\hbar} = \pm \frac{2\pi k_\mu}{N} + 2\pi m_\mu + \Phi_0 \quad \text{with } m_\mu \in \mathbb{Z},$$

  i.e. those eigenstates, for which a linear relationship between E_μ and k_μ holds, can be superimposed to form a solitary wave.

(1) J. Schnack, P. Shchelokovskyy, J. Magn. Magn. Mater. (2006) in print.

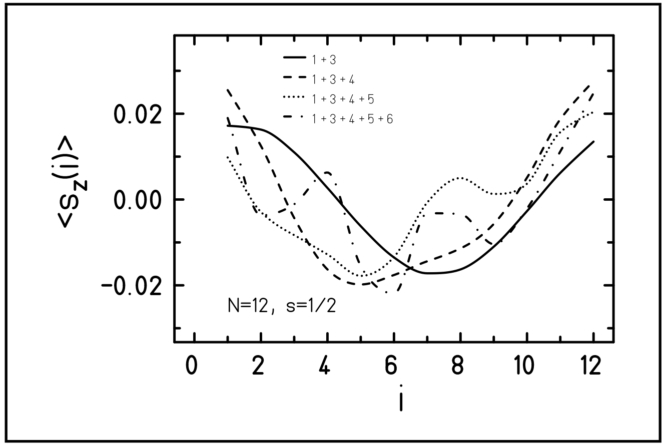
Solitons III



- Two eigenstates of $\underset{\sim}{H}$ always form a (trivial) soliton!
- L.h.s.: Solitary wave for $N = 12$ and $s = 1/2$ consisting of ground state and first excited state with $M = 0$.
- R.h.s.: Solitary wave for $N = 11$ and $s = 1$ consisting of ground state ($k = 0$) and first excited state ($k = 5$) with $M = 0$. The local magnetization distribution is the quantum expression of a topological solitary wave, where the Néel up-down sequence is broken and continued with a displacement of one site.

(1) J. Schnack, P. Shchelokovskyy, J. Magn. Magn. Mater. (2006) in print.

Solitons IV



- Non-trivial solitons are broad due to smallness of the system.
- Fig.: Several solitary waves depending on contributing eigenstates of $\underset{\sim}{H}$ and $\underset{\sim}{T}$ with $M = 0$. All states contribute with the same weight in this presentation. All states with more than two components disperse slowly due to imperfect linearity.
- How to excite? How to measure?

(1) J. Schnack, P. Shchelokovskyy, J. Magn. Magn. Mater. (2006) in print.

Thank you very much for your attention.

The worldwide Ames group

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