DISCONTINUOUS QUANTUM AND CLASSICAL MAGNETIC RESPONSE OF THE PENTAKIS DODECAHEDRON

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MOTIVATION

→ Fullerene molecules: 12 pentagons and (n/2) - 10 hexagons.

→ Edge-sharing polygons.

→ Frustration (pentagons)

→ classical magnetization and susceptibility discontinuities.

→ quantum magnetization discontinuities ($I_h$ symmetry).

→ singlets inside the singlet-triplet gap.
MOTIVATION

→ Icosahedron: dual of dodecahedron ($I_h$ symmetry).

→ 12 vertices, 20 edge-sharing triangles → Frustration (triangles)

→ classical magnetization discontinuity.

C. Schroeder, H.-J. Schmidt, J. Schnack, and M. Luban, Phys. Rev. Lett. 94, 207203 (2005)

→ singlets inside the singlet-triplet gap.

→ strong similarities in low-energy spectrum with dodecahedron.

→ consider bigger $I_h$ fullerene duals → quantum discontinuities?

→ next bigger: pentakis dodecahedron.
PENTAKIS DODECAHEDRON

32 vertices

→ 20 6-fold vertices,
   12 5-fold vertices,
   60 edge-sharing triangles.

→ 2 nonequivalent edges (black-red).

Dual of the truncated icosahedron.

$I_h$ spatial symmetry group
→ 120 symmetry operations.
→ 10 irreducible representations.
Antiferromagnetic Heisenberg Model

\[
H = \sum_{ij} s_i \cdot s_j + J \sum_{ij} s_i \cdot s_j - h \sum_i s_i^z , \quad J > 0
\]

\( J=0 \): dodecahedron + uncoupled spins.

\( J \to \infty \): quadrangles linked together.

\([H,S]=0\), \([H,S^z]=0\)

\( I_h \) and spin inversion symmetry characterize states.

FRUSTRATION: \( s_i = 1/2, 1, 3/2, \ldots, \infty \)
CLASSICAL SPINS $S_i \to \infty$

Zero-magnetic-field ground-state energy

Dashed lines: change of the symmetry of the lowest-energy configuration.
CLASSICAL SPINS $s_i \rightarrow \infty$

Zero-magnetic-field ground-state correlations

6-fold spins correlations (black bonds)

6-fold and 5-fold spins correlations (red bonds)
CLASSICAL SPINS $s_i \to \infty$

Zero-magnetic-field ground-state magnetization

black: total magnetization, red: total of six-fold spins, green: total of five-fold spins.
CLASSICAL SPINS \( S_i \to \infty \)

Ground-state magnetization and susceptibility discontinuities in a field

\[ +: \text{magnetization discontinuity, } x: \text{susceptibility discontinuity.} \]
CLASSICAL SPINS $s_i \to \infty$

Ground-state magnetization and susceptibility discontinuities in a field

10 magnetization, 1 susceptibility.

3 magnetization, 8 susceptibility.

+: magnetization discontinuity, $x$: susceptibility discontinuity.
**CLASSICAL SPINS** $s_i \to \infty$

Ground-state magnetization and susceptibility discontinuities in a field

| appear | disappear | $J$ | $\frac{\hbar}{k_B}$ | $N_M, N_N$ | appear | disappear | $J$ | $\frac{\hbar}{k_B}$ | $N_M, N_N$ |
|--------|-----------|-----|----------------------|-------------|--------|-----------|-----|----------------------|-------------|
| 1      |           | 0   | 0+                   | 4.0         | 34     |           | -   | 0.75554              | 6.3         |
| 2      |           | 0   | 0.26350              | 4.0         | 35     | 33,11'    | 1.010 | 0.132                | 6.2         |
| 3      |           | 0   | 0.26983              | 4.0         | 36,12' | 4         | 1.012 | 0.597                | 6.3         |
| 4      |           | 0   | 0.73428              | 4.0         | 37     | 3,36      | 1.015 | 0.597                | 5.3         |
| 1', 2' |           | 0   | 0+                   | 4.2         | 38     | 37,12'    | 1.619 | 0.998                | 5.2         |
| 5, 6   |           | 0   | 0.228                | 0.07        | 6,2    | 39,40     | 38   | 1.023                | 6.2         |
| 7, 8   |           | 0   | 0.229                | 0.07        | 8,2    | 41,42     | -    | 1.04939              | 8.2         |
| 9      |           | 0   | 0.281                | 0.0414      | 7,2    | 13'       | 41   | 1.04942              | 7.3         |
| 10     |           | 0   | 0.406                | 0.225       | 5,2    | 14', 13'  | 1.04984 | 0                  | 7.3         |
| 11, 13 | 1'        | 0   | 0.147                | 0.240       | 6,1    | 43        | 34,42 | 1.0497               | 6.3         |
| 12     | 4'        | 0   | 0.4194               | 0.233       | 6.2    | 44        | 35,43 | 1.0509               | 5.3         |
| 13, 15 | 5'        | 0.247 | 0.024               | 6,1         | 50     | 40,48     | 1.06266 | 0.654               | 4.4         |
| 14, 16 | 6'        | 0.503 | 0.024               | 7,1         | 51     | 46,49     | 1.06271 | 0.548               | 3.4         |
| 15, 17 | 12        | 0.512 | 0.0166              | 7,2         | 52     | 51,15'    | 1.0664 | 0.506               | 3.3         |
| 16     | 7'        | 0.526 | 0.0228              | 8,1         | 53     | 45,10'    | 1.0706 | 0.296               | 3.2         |
| 17, 18 |           | 0   | 0.526                | 0.026       | 10,1   | 54        | 53,9'  | 1.0714               | 3.1         |
| 18     | 16, 17    | 0.526 | 0.024               | 9,1         | 55,16' | 52        | 1.07262 | 0.425               | 3.2         |
| 19     | 8'        | 0.527 | 0.01656              | 10,0        | 56,17' | 54        | 1.073852 | 0.371               | 3.3         |
| 20     |           | 0   | 0.532                | 0.0168      | 9,0    | 57,18'    | 56   | 1.073859              | 3.4         |
| 21     | 14, 19    | 0.544 | 0.0171              | 8,0         | -      | 55,17'    | 55   | 1.0738508             | 3.5         |
| 22     | 21, 22    | 0.535 | 0.0164              | 7,0         | 58,50  | 50        | 1.07625 | 0.897               | 2.4         |
| 23     | 24, 25    | 0.355 | 0.053               | 8,0         | 60,19' | 59        | 1.07643 | 0.8991              | 2.5         |
| 26, 9' | 28        | 0.511 | 0.114               | 8,1         | 20', 21' | 19'  | 1.07647 | 0.8996              | 2.6         |
| 10'    | 26        | 0.586 | 0.117               | 7,2         | 61,22', 23' | -   | 1.0788 | 1                  | 3.8         |
| 27, 28 | 24        | 0.588 | 0.0127              | 8,2         | 62     | 60,22'    | 1.07923 | 0.933               | 3.7         |
| 29     | 15, 23    | 0.590 | 0.0021              | 7,2         | 63     | 62,23'    | 1.07959 | 0.937               | 3.6         |
| 30     | 9         | 0.5015500 | 0   | 7,2    | 64     | 61,63     | 1.080146 | 0.9435              | 2.6         |
| 31     | 29, 30    | 0.596 | 0.0007              | 6,2         | -      | 58,20', 21' | 1.085 | 0.9101              | 1.4         |
| 32     | 27, 31    | 0.600 | 0.0004              | 5,2         | -      | 64        | $\frac{1}{2}(5 + \sqrt{5})$ | 1       | 0.4         |
|        | 32        | 0.603929 | 0   | 4,2    | 24', 25' | 11', 16', 17', 18' | $\frac{3}{2}(5 + \sqrt{5})$ | $\frac{1}{3}$ | 0.2        |
| 33     |           | 0.620646 | 0   | 5,2    | -      | 24'      | $\frac{24}{25} \frac{5 + \sqrt{5}}{5}$ | 0       | 0.1        |
| 11'    |           | 0.64075 | 0   | 5,3    |        |         |         |         |            |
CLASSICAL SPINS $s_i \to \infty$

Width of ground-state magnetization discontinuities in a field
CLASSICAL SPINS $s_i \rightarrow \infty$

Lowest-energy configuration unique polar angles

$J=0.3$

red arrows: magnetization discontinuities,

green arrows: susceptibility discontinuities,

$CF_i$: lowest energy configurations.

$J=1$

$J=1.08$
QUANTUM SPINS $s_i = 1/2$

Block-diagonalization with symmetries

Hilbert space: $2^{32} = 4,294,967,296$ states.

Biggest $S^z$ subsector: $S^z=0$ with $601,080,390$ states.

Biggest symmetry subsector: $H_g$ of $S^z=1$ with $23,585,037$ states.
QUANTUM SPINS $s_i = 1/2$

Zero-magnetic-field ground-state energy

Dashed lines: change of the total spin $S$ and the symmetry of the lowest-energy configuration.

| $J$-range       | $S$ | Irreducible representation | Degeneracy | Spin inversion |
|-----------------|-----|----------------------------|------------|---------------|
| $0 \leq J < 0.371$ | 0   | $A_u$                      | 1          | s             |
| $0.371 \leq J \leq 0.642$ | 2   | $A_g$                      | 5          | s             |
| $0.642 < J \leq 1.506$ | 0   | $A_u$                      | 1          | s             |
| $1.506 < J \leq 1.542$ | 1   | $T_{1u}$                   | 9          | a             |
| $1.542 < J < 1.609$ | 2   | $H_g$                      | 25         | s             |
| $1.609 \leq J < 1.685$ | 3   | $T_{2u}$                   | 21         | a             |
| $1.685 \leq J$     | 4   | $A_g$                      | 9          | s             |
QUANTUM SPINS $s_i = 1/2$

Zero-magnetic-field ground-state correlations

Black circles: 6-fold spins correlations.
Red squares: 6-fold and 5-fold spins correlations.
J=0.9, 1.1, and 1.2: singlets inside the singlet-triplet gap.
QUANTUM SPINS \( s_i = 1/2 \)

Ground-state magnetization discontinuities in a field

Black circles: \( \Delta S^z = 1 \)
Red squares: \( \Delta S^z = 2 \)
Green diamonds: \( \Delta S^z = 3 \)

Higher J: weaker frustration, equidistant jumps
QUANTUM SPINS $s_i = 1/2$

Ground-state magnetization discontinuities in a field

- Black circles: $\Delta S^z = 1$
- Red squares: $\Delta S^z = 2$
- Green diamonds: $\Delta S^z = 3$
QUANTUM SPINS $s_i = 1/2$

Ground-state magnetization discontinuities in a field

| $J$-range       | $S^z_{\text{below}}$ | $S^z_{\text{above}}$ | Irrep. below | Irrep. above |
|-----------------|----------------------|-----------------------|--------------|--------------|
| $0 \leq J \leq 1.012$ | 10                   | 12                    | $A_g$        | $A_u$        |
| $0.279 < J < 0.302$ | 1                    | 3                     | $T_{2g}$     | $F_g$        |
| $0.302 < J < 0.307$ | 0                    | 3                     | $A_u$        | $F_g$        |
| $0.307 \leq J \leq 0.371$ | 0                    | 2                     | $A_u$        | $A_g$        |
| $0.642 < J < 0.743$ | 0                    | 2                     | $A_u$        | $A_g$        |
| $0.707 < J \leq 1.032$ | 4                    | 6                     | $A_g$        | $A_u$        |
| $0.980 \leq J \leq 1.071$ | 6                    | 8                     | $A_u$        | $A_g$        |
| $1.050 \leq J \leq 1.056$ | 4                    | 6                     | $A_g$        | $A_u$        |
| $1.074 < J \leq 1.075$ | 6                    | 8                     | $A_g$        | $A_g$        |

Three discontinuities

$\rightarrow 0.707 < J < 0.743$

$\rightarrow 0.980 \leq J \leq 1.012$

Can have degenerate irreducible representations on either side of a jump
CONCLUSIONS

→ Antiferromagnetic Heisenberg model on the pentakis dodecahedron.

→ Frustration results in nontrivial magnetic properties
  → classical magnetization and susceptibility discontinuities.
  → quantum magnetization discontinuities ($I_h$ symmetry) as big as $\Delta S^z = 3$.
→ singlets inside the singlet-triplet gap.