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)

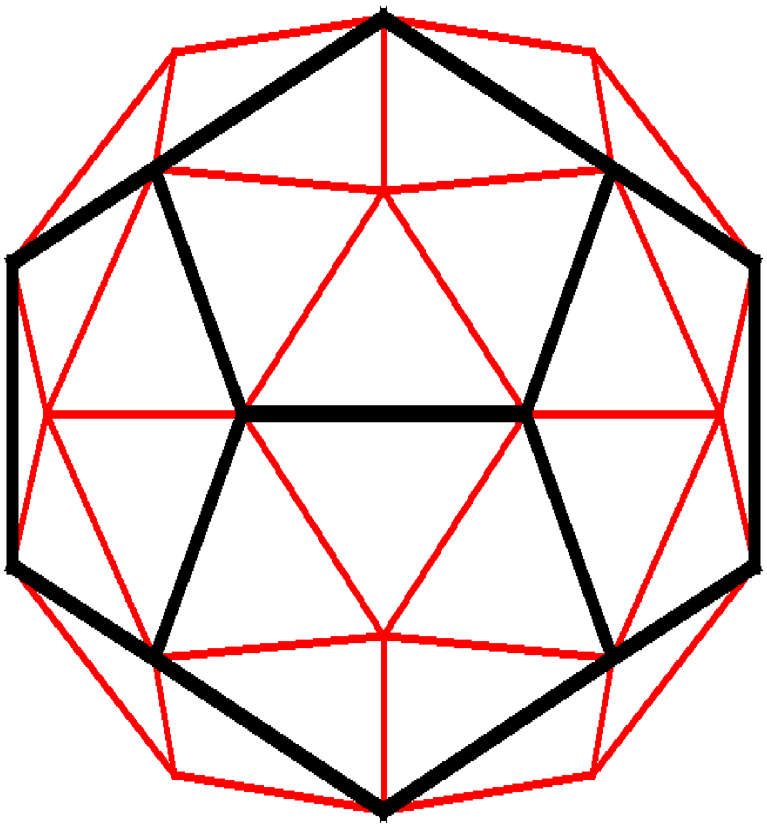
→ singlets inside the singlet-triplet gap.

→ strong similarities in low-energy spectrum with dodecahedron.

→ consider bigger I_h fullerene duals → quantum discontinuities?

→ next bigger: pentakis dodecahedron.

PENTAKIS DODECAHEDRON



32 vertices

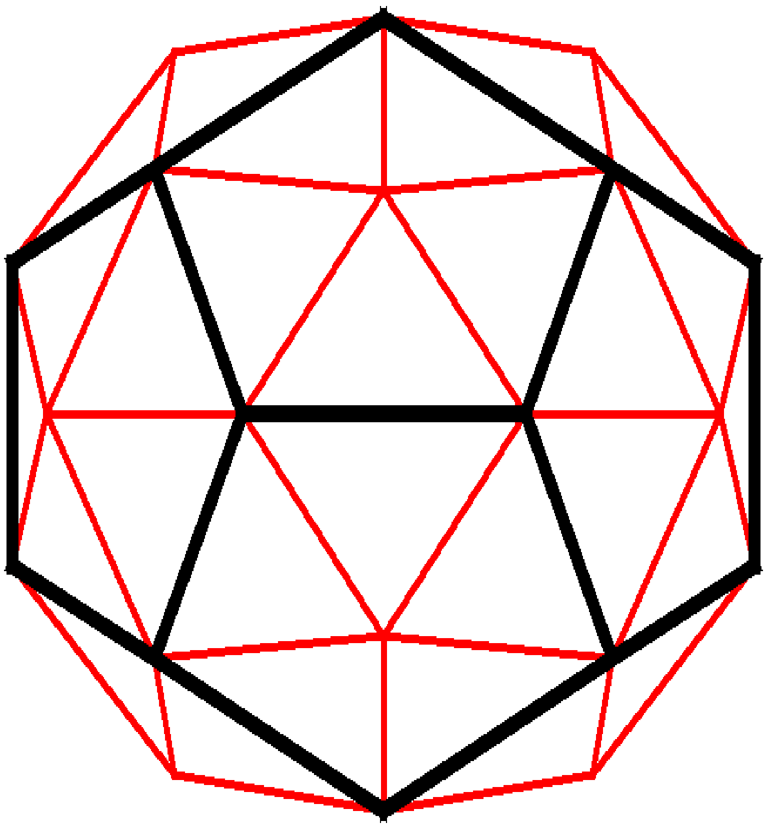
→ 20 6-fold vertices,
12 5-fold vertices,
60 edge-sharing triangles.

→ 2 nonequivalent edges (black-red).

Dual of the truncated icosahedron.

I_h spatial symmetry group
→ 120 symmetry operations.
→ 10 irreducible representations.

PENTAKIS DODECAHEDRON



Antiferromagnetic Heisenberg Model

$H = \sum_{<ij>} \mathbf{s}_i \cdot \mathbf{s}_j + J \sum_{<ij>'} \mathbf{s}_i \cdot \mathbf{s}_j - h \sum_i s_i^z$, $J > 0$

$J=0$: dodecahedron + uncoupled spins.

$J \rightarrow \infty$: quadrangles linked together.

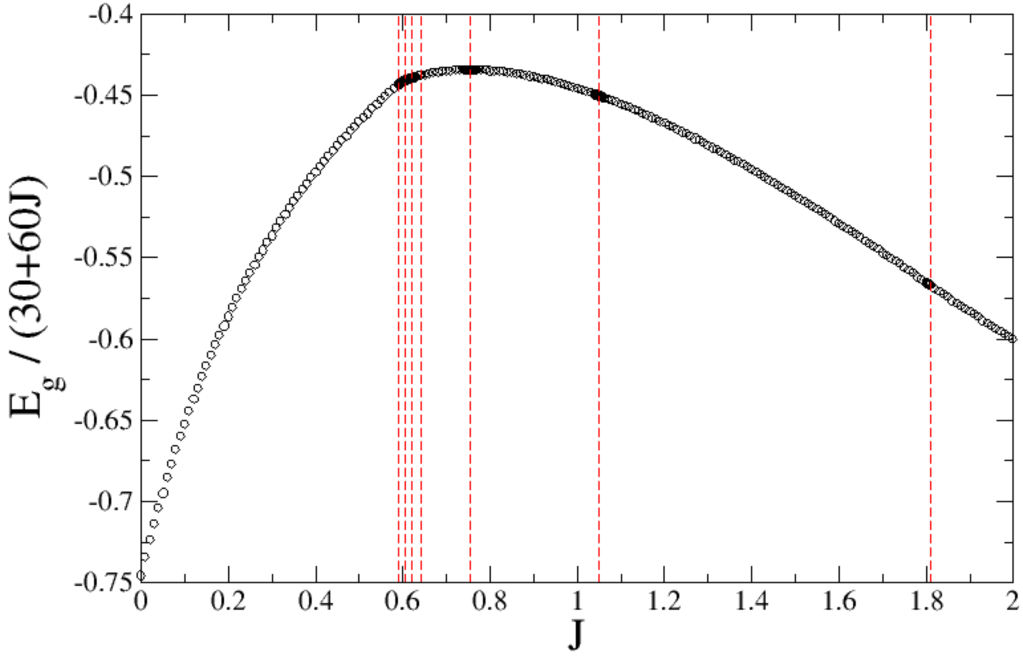
$[H,\mathbf{S}]=0$, $[H,S^z]=0$

→ I_h and spin inversion symmetry characterize states.

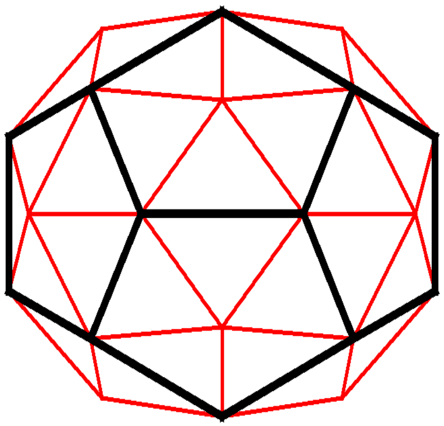
FRUSTRATION: $s_i = 1/2, 1, 3/2, ..., \infty$

CLASSICAL SPINS $s_i \to \infty$

Zero-magnetic-field ground-state energy

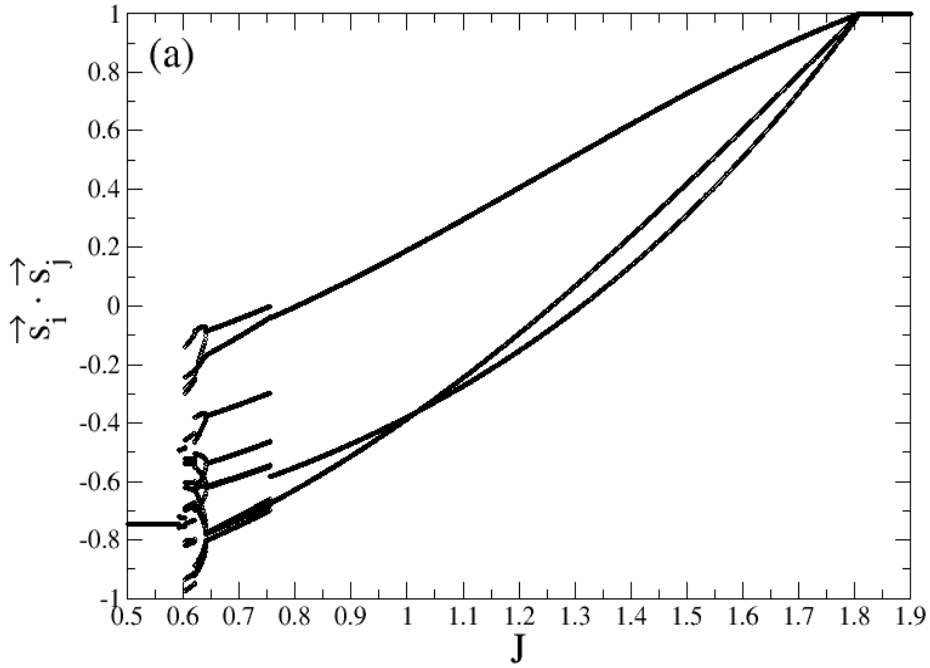


Dashed lines: change of the symmetry of the lowest-energy configuration.

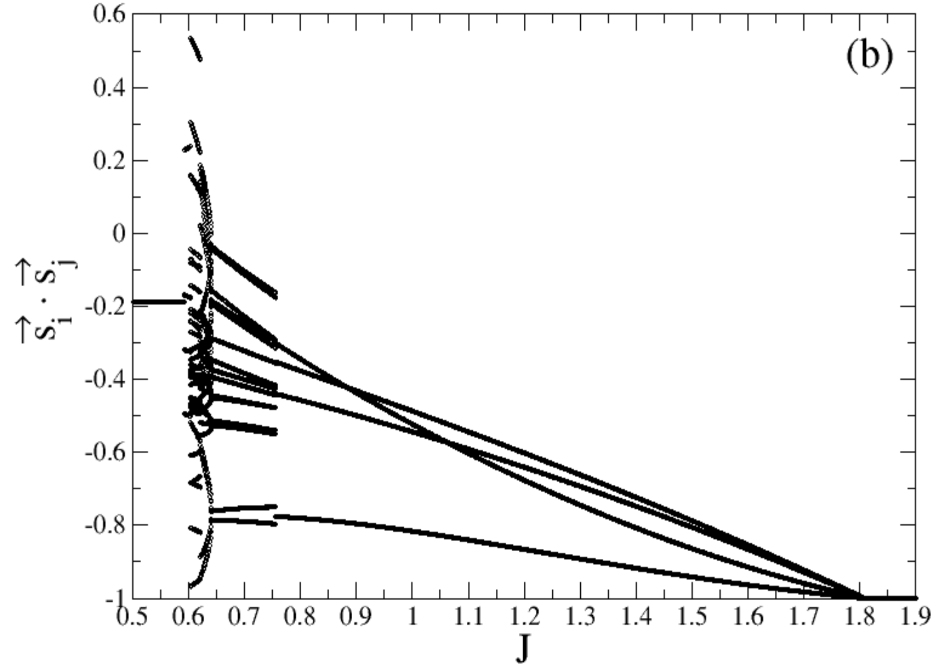


CLASSICAL SPINS $s_i \to \infty$

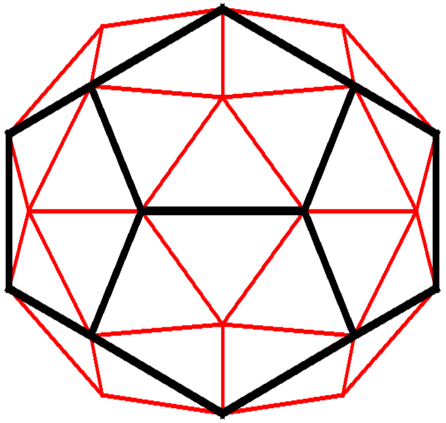
Zero-magnetic-field ground-state correlations



6-fold spins correlations (black bonds)

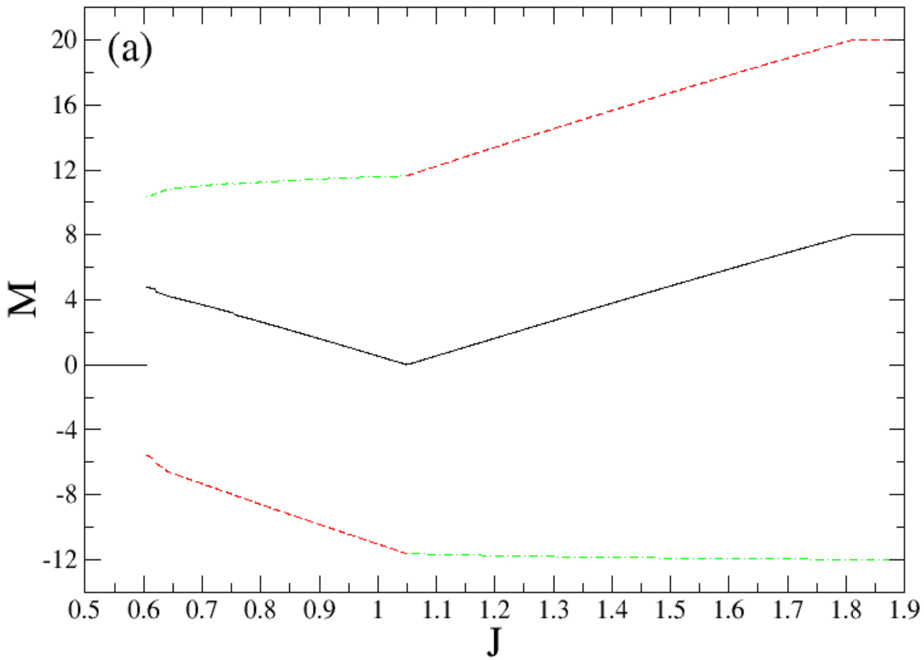


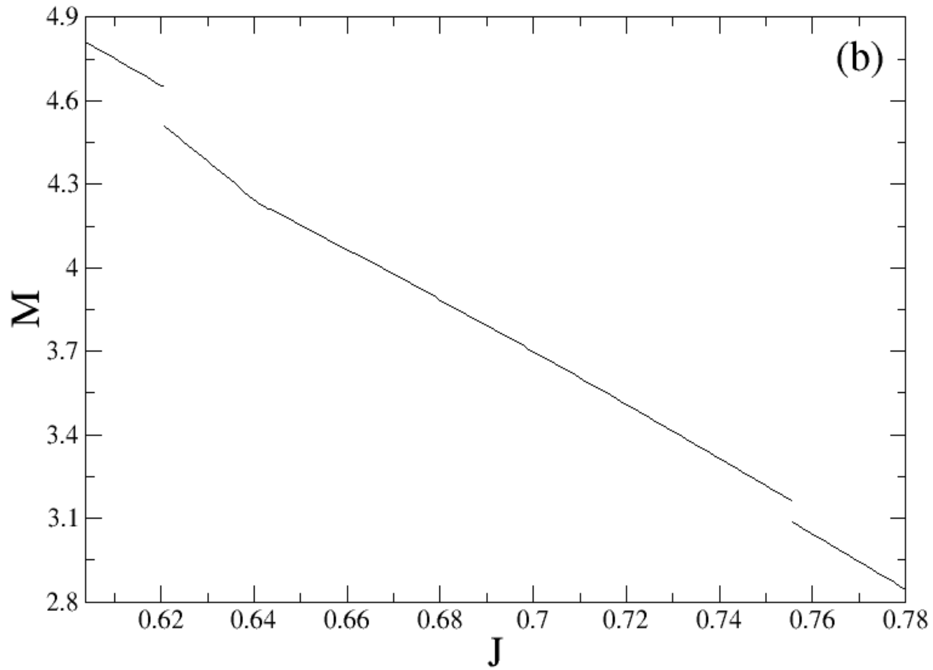
6-fold and 5-fold spins correlations (red bonds)



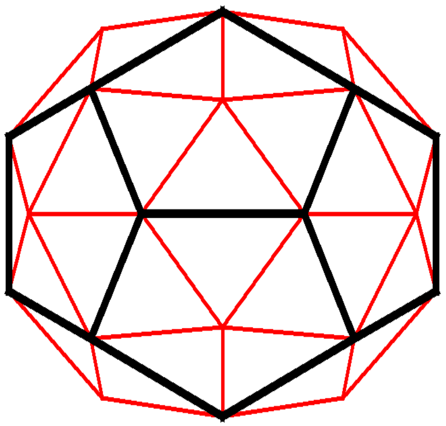
CLASSICAL SPINS $s_i \rightarrow \infty$

Zero-magnetic-field ground-state magnetization



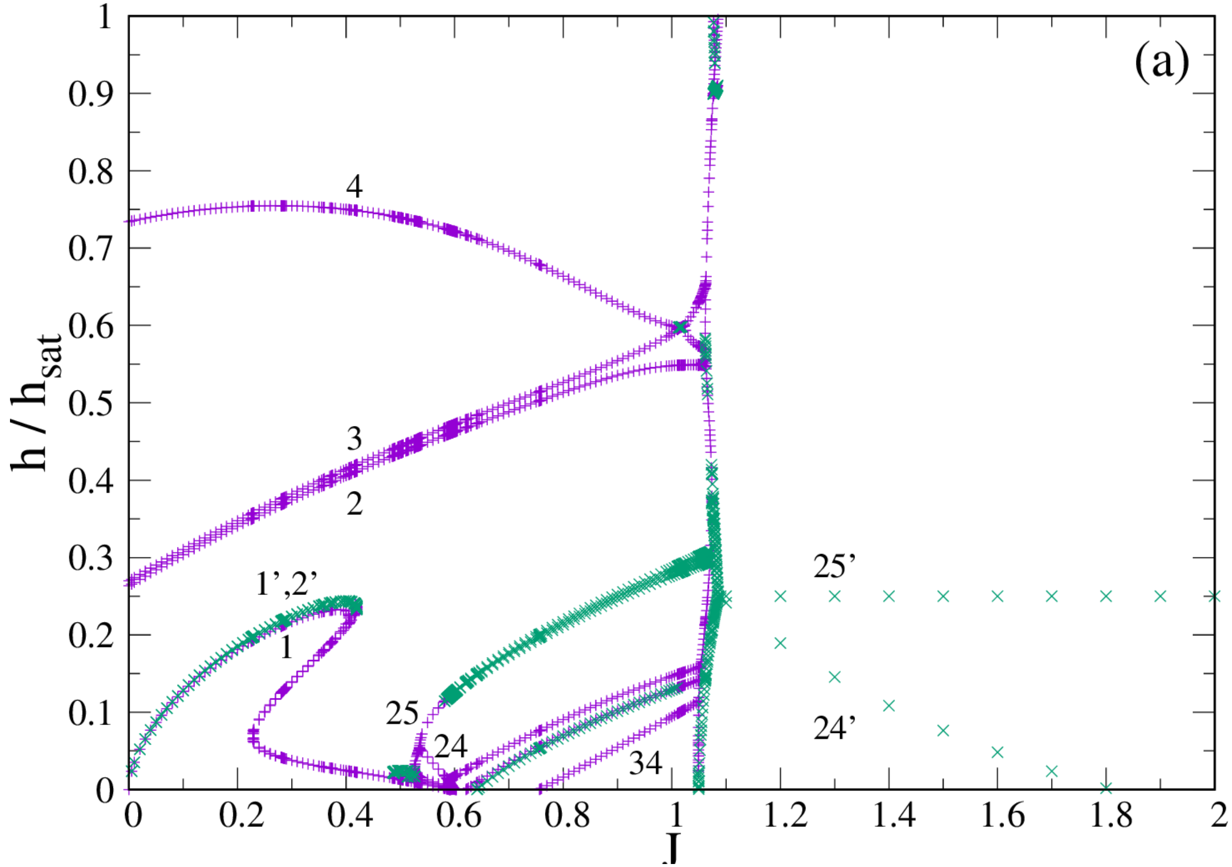


black: total magnetization, red: total of six-fold spins, green: total of five-fold spins.



CLASSICAL SPINS $s_i \to \infty$

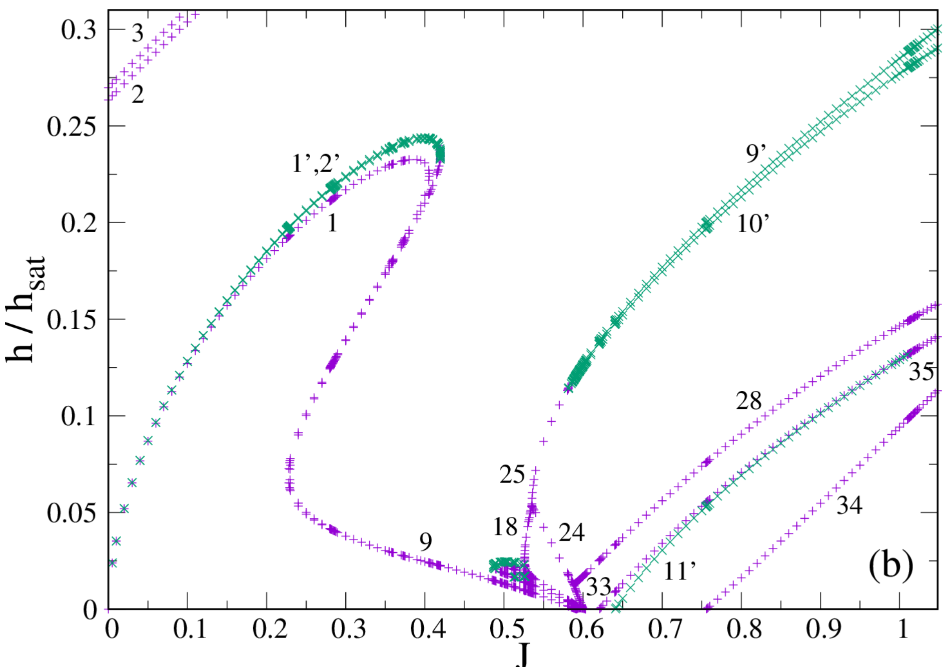
Ground-state magnetization and susceptibility discontinuities in a field

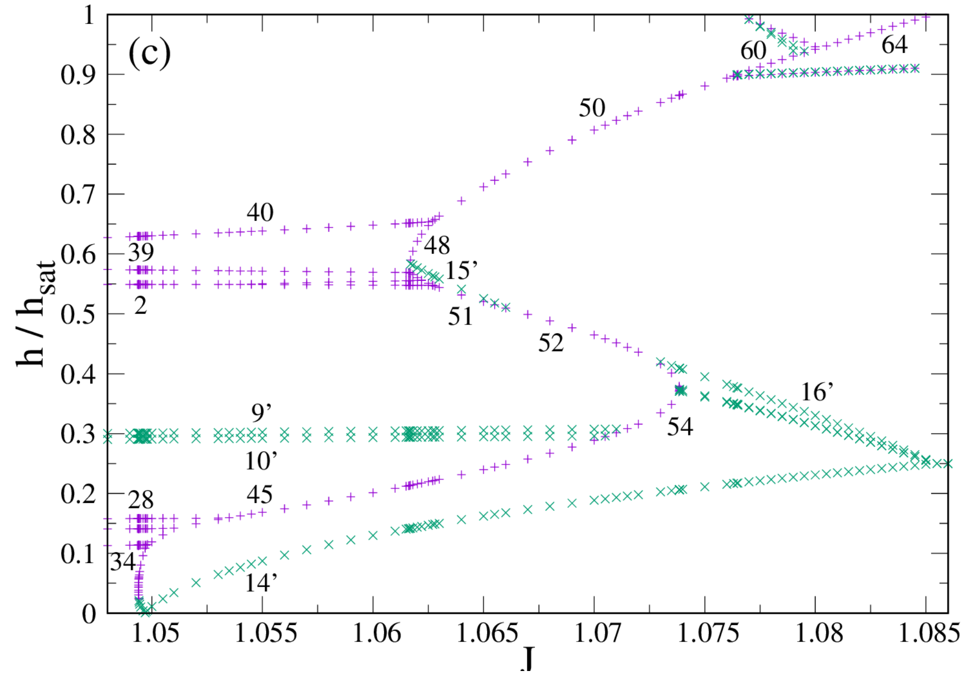


+: magnetization discontinuity, x: susceptibility discontinuity.

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.

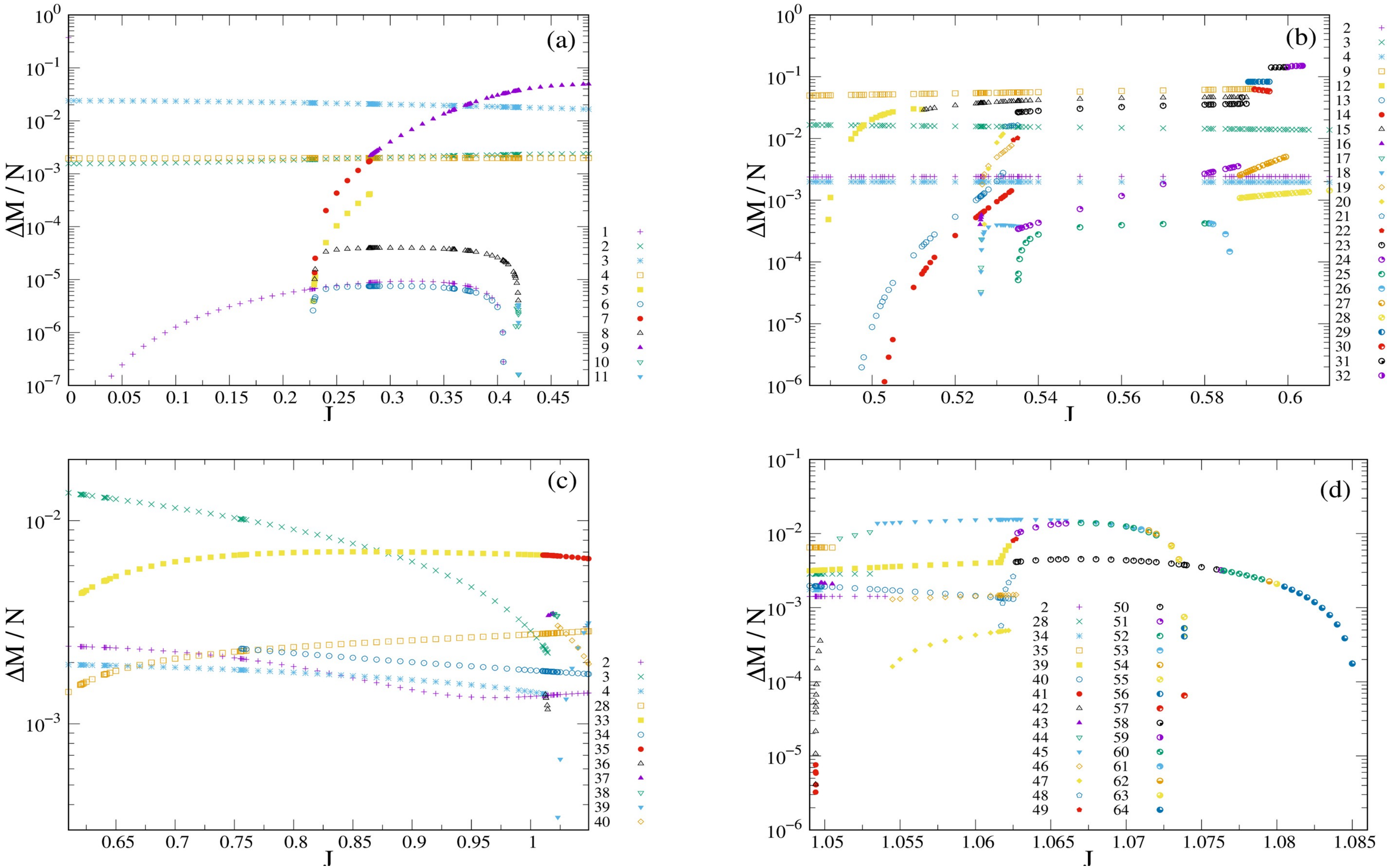
CLASSICAL SPINS $s_i \to \infty$

Ground-state magnetization and susceptibility discontinuities in a field

appear	disappear	J	$\frac{h}{h_{sat}}$	N_M, N_χ	appear	disappear	J	$\frac{h}{h_{sat}}$	N_M, N_χ
1	-	0	0+	4,0	34	-	0.755654	0	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	$37,12'$	1.019	0.598	5,2
5,6	-	0.228	0.07	6,2	39,40	38	1.023	0.600	6,2
7,8	-	0.229	0.07	8,2	41,42	-	1.04939	0.04	8,2
9	5,7	0.281	0.0414	7,2	$13'$	41	1.04942	0.02	7,3
-	1,6	0.406	0.225	5,2	$14'$	$13'$	1.049684	0	7,3
10	$1'$	0.417	0.240	6,1	43	34,42	1.0497	0.11	6,3
$11,3'$	8	0.4194	0.233	6,2	44	35,43	1.0509	0.142	5,3
-	10,11	0.41971	0.235	4,2	45	28,44	1.0534	0.159	4,3
-	$2', 3'$	0.41979	0.235	4,0	46,47	2	1.0542	0.549	5,3
$4', 5'$	-	0.486	0.022	4,2	$48,15'$	-	1.06168	0.58	6,4
12	$4'$	0.489	0.021	5,1	49	39,47	1.0622	0.556	5,4
$13,6'$	$5'$	0.497	0.024	6,1	50	40,48	1.06266	0.654	4,4
$14,7'$	$6'$	0.503	0.024	7,1	51	46,49	1.06271	0.548	3,4
$15,8'$	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	-	0.526	0.026	10,1	54	$53,9'$	1.0714	0.308	3,1
19	16,17	0.526	0.024	9,1	$55,16'$	52	1.07262	0.425	3,2
20	$8'$	0.527	0.01696	10,0	$56,17'$	54	1.073852	0.371	3,3
21	13,20	0.532	0.0168	9,0	$57,18'$	56	1.073859	0.374	3,4
22	14,19	0.534	0.0171	8,0	-	55,57	1.07385998	0.375	1,4
23	21,22	0.535	0.0164	7,0	58,59	50	1.07625	0.897	2,4
24,25	18	0.535	0.053	8,0	$60,19'$	59	1.07643	0.8991	2,5
$26,9'$	25	0.581	0.114	8,1	$20', 21'$	$19'$	1.07647	0.8996	2,6
$10'$	26	0.586	0.117	7,2	$61,22', 23'$	-	1.0768	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	0.591550	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	$\frac{3}{20}(5+\sqrt{5})$	1	0,4
-	32	0.603929	0	4,2	$24', 25'$	$14', 16', 17', 18'$	$\frac{3}{20}(5+\sqrt{5})$	$\frac{1}{4}$	0,2
33	-	0.620646	0	5,2	-	$24'$	$\frac{5+\sqrt{5}}{4}$	0	0,1
$11'$	-	0.64075	0	5,3					

CLASSICAL SPINS $s_i \to \infty$

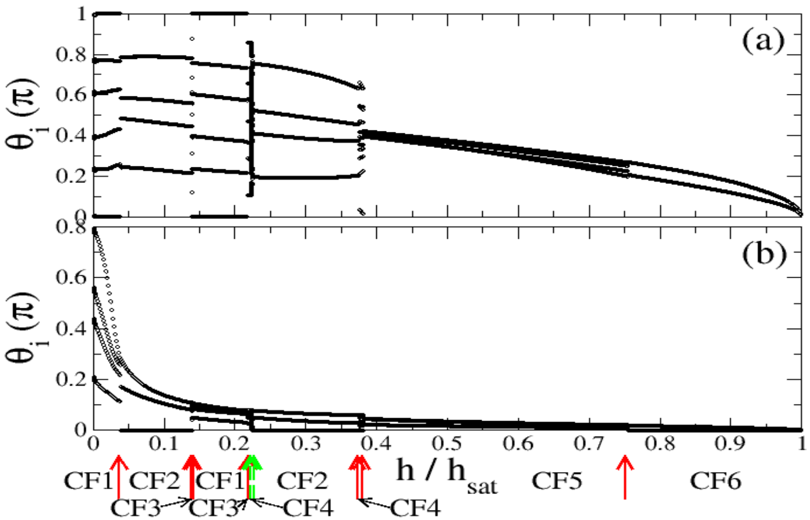
Width of ground-state magnetization discontinuities in a field



CLASSICAL SPINS $s_i \rightarrow \infty$

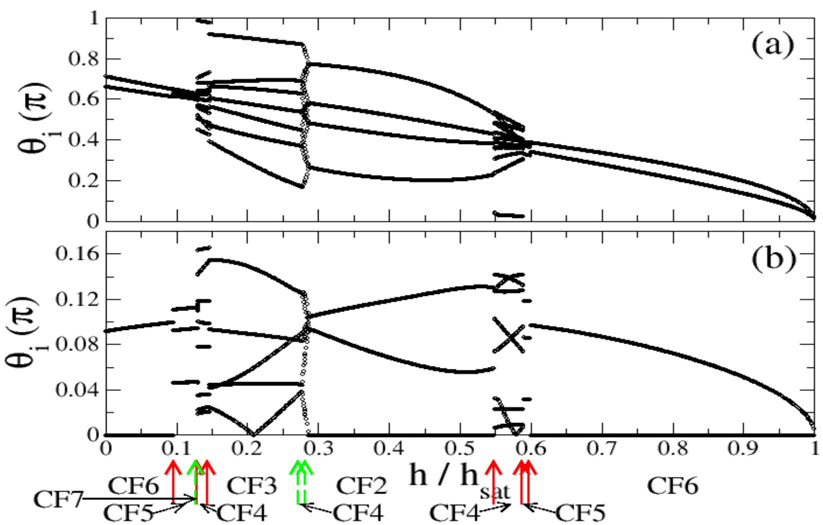
Lowest-energy configuration unique polar angles

J=0.3

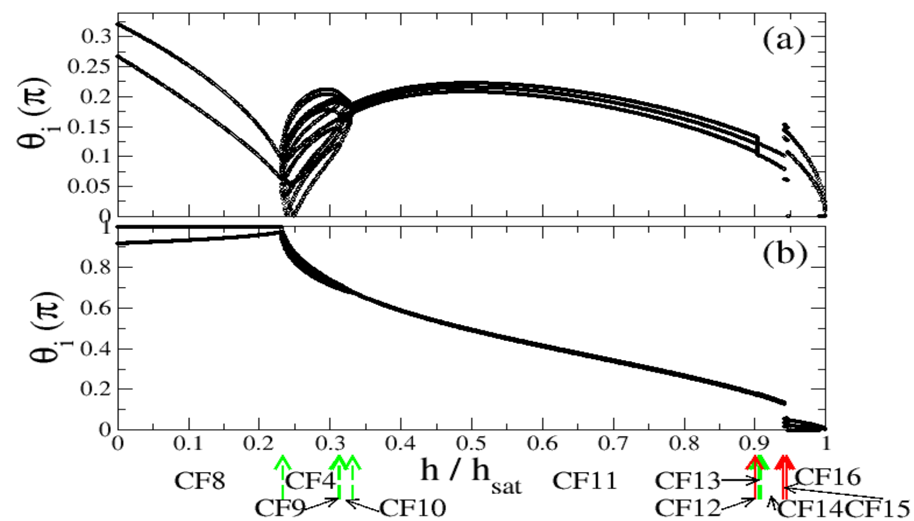


red arrows: magnetization discontinuities,
green arrows: susceptibility discontinuities,
CF_i: lowest energy configurations.

J=1



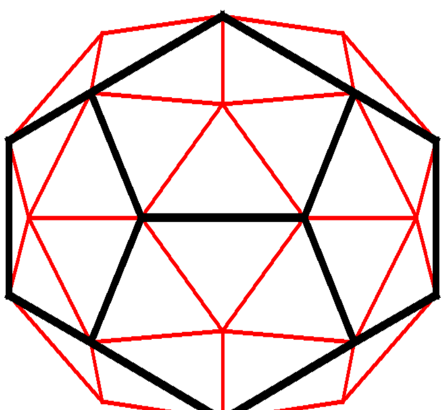
J=1.08



QUANTUM SPINS $s_i = 1/2$

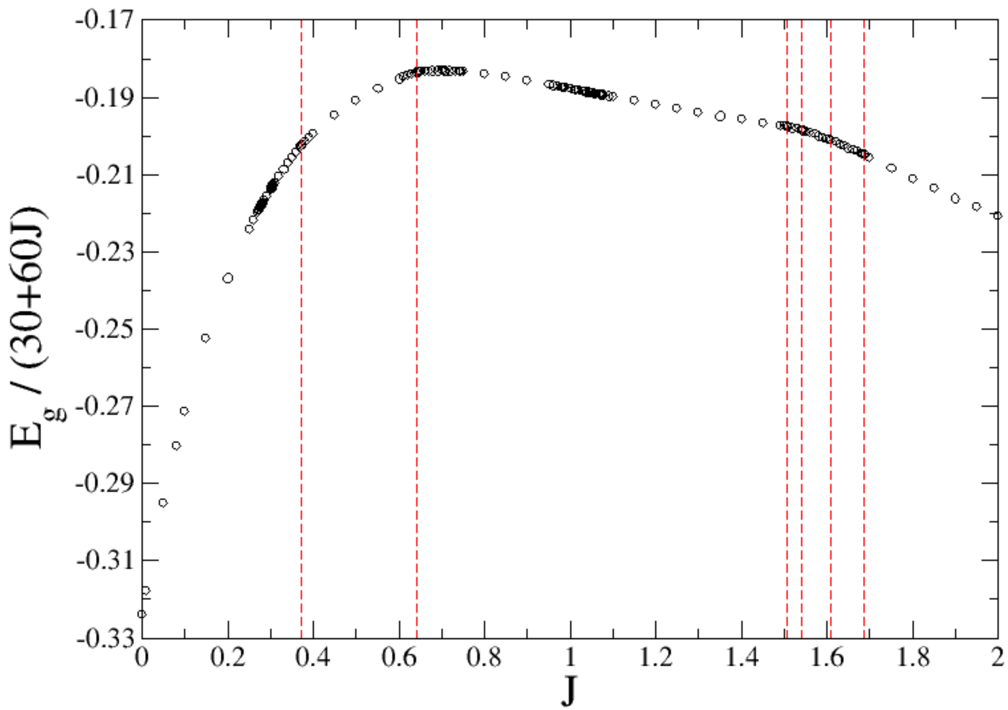
Block-diagonalization with symmetries

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.



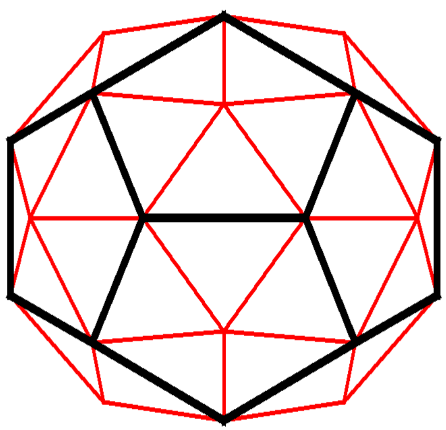
QUANTUM SPINS $s_i = 1/2$

Zero-magnetic-field ground-state energy



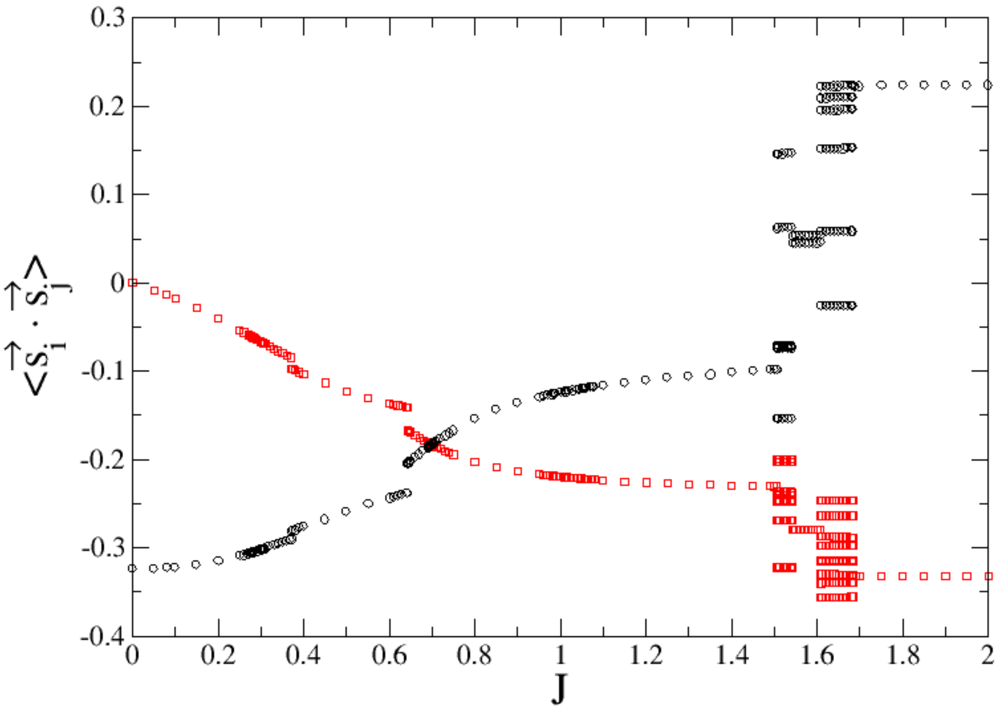
Dashed lines: change of the total spin S and the symmetry of the lowest-energy configuration.

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

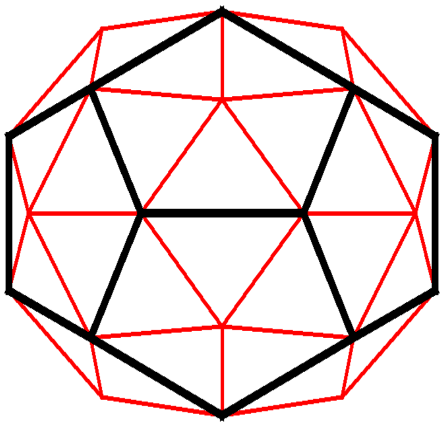


QUANTUM SPINS $s_i = 1/2$

Zero-magnetic-field ground-state correlations



Black circles: 6-fold spins correlations.
Red squares: 6-fold and 5-fold spins correlations.



QUANTUM SPINS $s_i = 1/2$

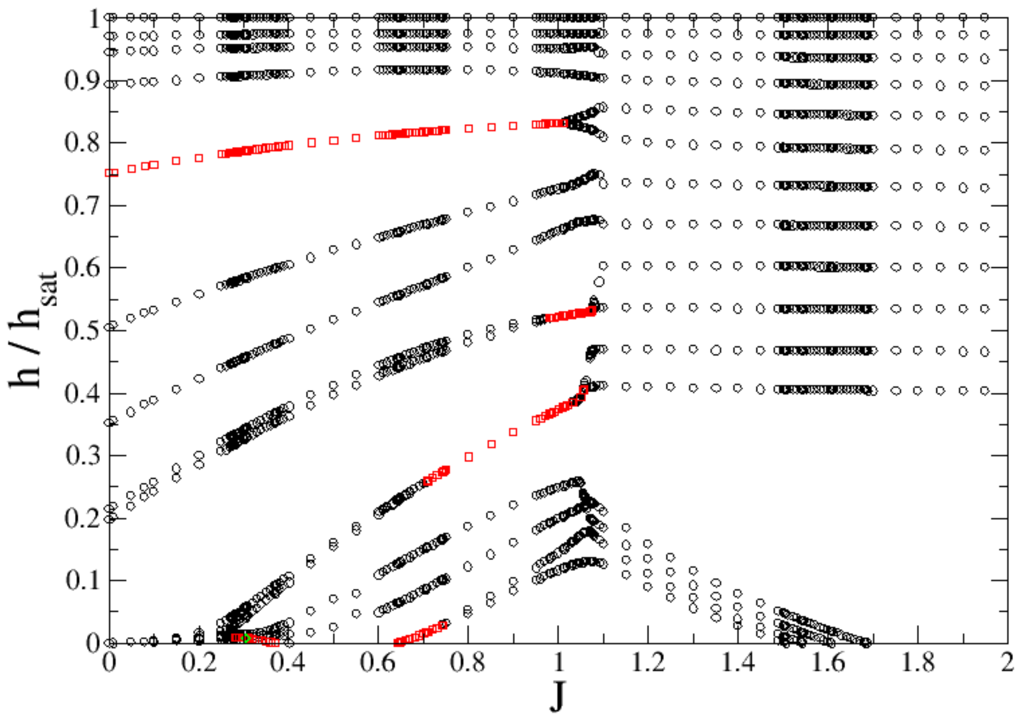
Low-energy spectrum

$\frac{E}{30+60J}$	S	irrep.	mult.	$\frac{E}{30+60J}$	S	irrep.	mult.	$\frac{E}{30+60J}$	S	irrep.	mult.	$\frac{E}{30+60J}$	S	irrep.	mult.	$\frac{E}{30+60J}$	S	irrep.	mult.
$J = 0$				$J = 0.2$				$J = 0.3$				$J = 0.4$				$J = 0.5$			
-0.32407	0	A_u	1	-0.23675	0	A_u	1	-0.21384	0	A_u	1	-0.19929	2	A_g	5	-0.19068	2	A_g	5
-0.31355	0	H_g	5	-0.23643	1	T_{2g}	9	-0.21332	1	T_{2g}	9	-0.19891	0	A_u	1	-0.18985	2	F_g	20
-0.31175	0	A_g	1	-0.23636	1	T_{1g}	9	-0.21323	1	T_{1g}	9	-0.19875	0	A_g	1	-0.18976	0	A_g	1
-0.30695	1	T_{2g}	9	-0.23619	1	T_{2u}	9	-0.21298	1	T_{2u}	9	-0.19866	1	T_{1u}	9	-0.18950	1	T_{1u}	9
-0.30622	1	F_u	12	-0.23618	0	H_u	5	-0.21288	0	A_g	1	-0.19859	2	F_g	20	-0.18950	2	H_u	25
-0.30435	1	T_{2u}	9	-0.23617	0	F_u	4	-0.21286	0	F_u	4	-0.19849	3	F_g	28	-0.18941	0	A_u	1
-0.29904	1	T_{1g}	9	-0.23613	0	A_u	1	-0.21280	1	H_u	15	-0.19845	2	H_u	25	-0.18932	3	F_g	28
-0.29599	0	H_u	5	-0.23610	0	A_g	1	-0.21276	0	H_g	5	-0.19844	1	T_{1g}	9	-0.18927	1	T_{2u}	9
-0.28983	1	T_{2u}	9	-0.23609	1	H_u	15	-0.21276	0	A_u	1	-0.19844	1	T_{2u}	9	-0.18906	2	H_g	25
-0.28981	1	H_u	15	-0.23608	1	F_u	12	-0.21275	0	H_u	5	-0.19841	0	H_g	5	-0.18905	0	H_g	5
-0.28886	1	T_{1u}	9	-0.23607	0	H_u	5	-0.21272	1	F_u	12	-0.19837	1	T_{2g}	9	-0.18901	1	F_u	12
-0.28834	2	F_g	20	-0.23603	2	H_u	25	-0.21270	2	A_g	5	-0.19820	3	T_{1u}	21	-0.18900	1	T_{2g}	9
$J = 0.6$				$J = 0.7$				$J = 0.8$				$J = 0.9$				$J = 1$			
-0.18517	2	A_g	5	-0.18307	0	A_u	1	-0.18390	0	A_u	1	-0.18566	0	A_u	1	-0.18774	0	A_u	1
-0.18436	0	A_u	1	-0.18216	1	T_{2g}	9	-0.18157	1	T_{2g}	9	-0.18243	0	F_g	4	-0.18458	0	F_g	4
-0.18423	2	F_g	20	-0.18168	1	T_{1u}	9	-0.18101	1	T_{1u}	9	-0.18193	0	A_g	1	-0.18383	0	A_g	1
-0.18421	1	T_{2g}	9	-0.18152	2	A_g	5	-0.18075	0	A_g	1	-0.18172	1	T_{2g}	9	-0.18282	0	H_g	5
-0.18415	0	A_g	1	-0.18127	0	A_g	1	-0.18075	0	F_g	4	-0.18111	1	T_{1u}	9	-0.18231	1	T_{2g}	9
-0.18392	1	T_{1u}	9	-0.18118	1	T_{2u}	9	-0.18041	1	T_{2u}	9	-0.18096	0	H_u	5	-0.18225	0	H_u	5
-0.18379	2	H_u	25	-0.18095	1	F_g	12	-0.18040	0	H_u	5	-0.18082	0	H_g	5	-0.18196	0	H_g	5
-0.18356	1	F_g	12	-0.18095	0	H_u	5	-0.18008	1	F_g	12	-0.18046	1	T_{2u}	9	-0.18165	1	T_{1u}	9
-0.18355	1	T_{2u}	9	-0.18055	2	F_g	20	-0.17990	0	H_g	5	-0.18044	0	H_g	5	-0.18160	1	A_u	3
-0.18349	1	T_{1u}	9	-0.18054	1	F_u	12	-0.17948	1	F_u	12	-0.18016	1	F_g	12	-0.18106	1	F_g	12
-0.18340	1	F_u	12	-0.18051	0	H_g	5	-0.17947	0	H_g	5	-0.17941	1	A_u	3	-0.18105	0	F_u	4
-0.18339	1	T_{2u}	9	-0.18043	0	F_g	4	-0.17925	1	T_{1g}	9	-0.17940	1	F_u	12	-0.18091	1	T_{2u}	9
$J = 1.1$				$J = 1.2$				$J = 1.3$				$J = 1.4$				$J = 1.5$			
-0.18985	0	A_u	1	-0.19190	0	A_u	1	-0.19385	0	A_u	1	-0.19568	0	A_u	1	-0.19739	0	A_u	1
-0.18680	0	F_g	4	-0.18895	0	F_g	4	-0.19116	1	T_{1u}	9	-0.19437	1	T_{1u}	9	-0.19732	1	T_{1u}	9
-0.18595	0	A_g	1	-0.18807	0	A_g	1	-0.19100	0	F_g	4	-0.19408	1	T_{2g}	9	-0.19702	1	T_{2g}	9
-0.18504	0	H_g	5	-0.18767	1	T_{1u}	9	-0.19089	1	T_{2g}	9	-0.19292	0	F_g	4	-0.19679	2	H_g	25
-0.18405	0	H_u	5	-0.18745	1	T_{2g}	9	-0.19014	0	A_g	1	-0.19264	1	F_u	12	-0.19649	2	A_g	5
-0.18403	1	T_{2g}	9	-0.18725	0	H_g	5	-0.18936	1	F_u	12	-0.19246	2	H_g	25	-0.19574	2	H_u	25
-0.18397	1	T_{1u}	9	-0.18611	0	H_g	5	-0.18936	0	H_g	5	-0.19220	0	A_g	1	-0.19566	1	F_u	12
-0.18395	0	H_g	5	-0.18610	0	H_u	5	-0.18860	1	F_g	12	-0.19214	2	A_g	5	-0.19538	3	T_{2u}	21
-0.18375	1	A_u	3	-0.18582	1	F_u	12	-0.18831	0	H_g	5	-0.19181	1	F_g	12	-0.19481	1	F_g	12
-0.18343	0	F_u	4	-0.18578	1	A_u	3	-0.18822	0	H_u	5	-0.19145	1	T_{2u}	9	-0.19472	0	F_g	4
-0.18305	0	T_{2u}	3	-0.18571	0	F_u	4	-0.18814	1	T_{2u}	9	-0.19139	2	H_u	25	-0.19452	1	T_{2u}	9
-0.18294	1	F_g	12	-0.18541	1	F_g	12	-0.18785	0	F_u	4	-0.19135	0	H_g	5	-0.19442	0	A_g	1
$J = 1.6$				$J = 1.7$				$J = 1.8$				$J = 2$				$J \to \infty$			
-0.20073	2	H_g	25	-0.20558	4	A_g	9	-0.21106	4	A_g	9	-0.22074	4	A_g	9	-0.33288	4	A_g	9
-0.20062	3	T_{2u}	21	-0.20540	3	T_{2u}	21	-0.20977	3	T_{2u}	21	-0.21749	3	T_{2u}	21	-0.31975	3	T_{1u}	21
-0.20045	2	A_g	5	-0.20433	2	H_g	25	-0.20819	3	F_g	28	-0.21599	3	F_g	28	-0.30980	3	H_g	35
-0.20003	1	T_{1u}	9	-0.20407	2	A_g	5	-0.20764	2	H_g	25	-0.21371	3	T_{1u}	21	-0.30756	3	T_{2u}	21
-0.19973	1	T_{2g}	9	-0.20377	3	F_g	28	-0.20738	2	A_g	5	-0.21350	2	H_g	25	-0.30708	2	H_g	25
-0.19970	2	H_u	25	-0.20333	2	H_u	25	-0.20666	2	H_u	25	-0.21325	2	A_g	5	-0.30681	3	F_g	28
-0.19958	4	A_g	9	-0.20253	1	T_{1u}	9	-0.20485	1	T_{1u}	9	-0.21255	2	H_u	25	-0.30656	5	A_g	11
-0.19900	0	A_u	1	-0.20222	1	T_{2g}	9	-0.20462	3	T_{1u}	21	-0.21098	2	H_g	25	-0.30604	3	F_u	28
-0.19895	3	F_g	28	-0.20107	2	F_g	20	-0.20451	1	T_{2g}	9	-0.21045	2	F_g	20	-0.30356	2	A_g	5
-0.19843	1	F_u	12	-0.20099	1	F_u	12	-0.20445	2	F_g	20	-0.20994	2	F_u	20	-0.29817	4	T_{1u}	27
-0.19756	1	F_g	12	-0.20051	0	A_u	1	-0.20379	2	H_g	25	-0.20951	3	H_g	35	-0.29802	2	T_{2u}	15
-0.19738	2	F_u	20	-0.20032	2	F_u	20	-0.20376	2	F_u	20	-0.20926	3	F_u	28	-0.29726	2	H_u	25

J=0.9, 1, 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: $\Delta S^z = 1$

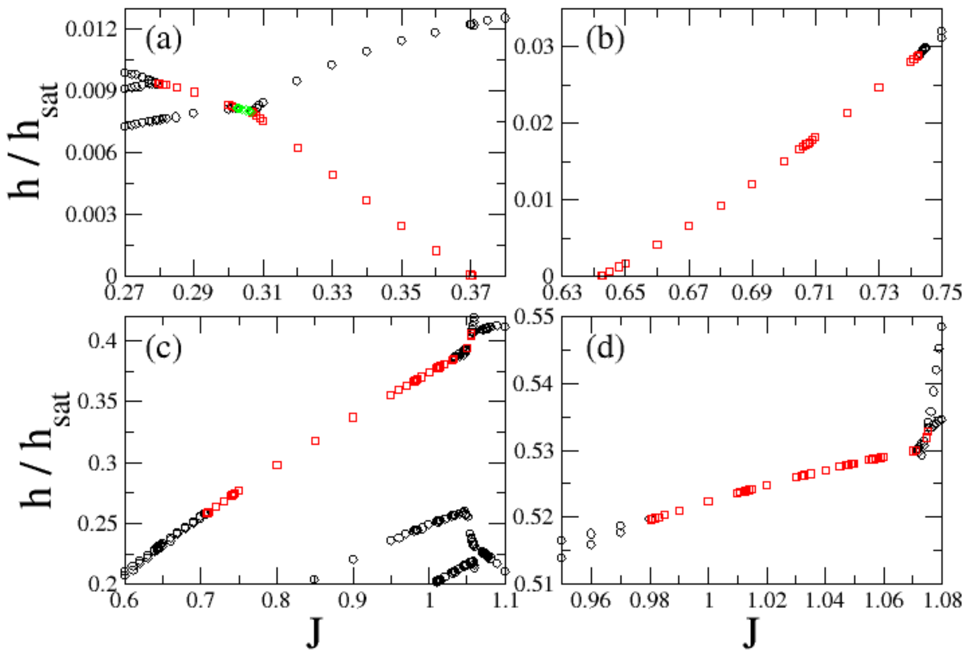
Red squares: $\Delta S^z = 2$

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: $\Delta S^z = 1$

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Green diamonds: $\Delta S^z = 3$

QUANTUM SPINS $s_i = 1/2$

Ground-state magnetization discontinuities in a field

J-range	S^z_{below}	S^z_{above}	Irrep. below	Irrep. above
$0 \leq J \leq 1.012$	10	12	A_g	A_u
$0.279 < J \leq 0.302$	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

→ $0.707 < J < 0.743$

→ $0.980 \leq J \leq 1.012$

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.