"Heisenberg Model"

We are going to build on problem you did on addition of two spin 1/2 particles to discuss one of the fundamental models of magnetic order in CM physics — the "Heisenberg Model"

$$\hat{H} = \frac{J}{\hbar^2} \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

"Exchange energy" (More on this later)

spin operators on sites i, j

usually spin-1/2

Simplest example: 2 sites

$$\hbar^2 \hat{H} = J \vec{S}_1 \cdot \vec{S}_2$$

$$= J\left(S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z\right)$$

$$= \frac{J}{2}\left(S_1^+ S_2^- + S_1^- S_2^+\right) + J S_1^z S_2^z$$

H2

$$\overset{S_1^z}{\swarrow} \quad \overset{S_2^z}{\swarrow}$$

Basis $|++\rangle$

$|+-\rangle$

$|-+\rangle$

$|--\rangle$

$$S_1^2 |++\rangle = \hbar^2\left(\tfrac{1}{2}\right)\left(\tfrac{1}{2}+1\right)|++\rangle$$
$$= 3/4\,\hbar^2 |++\rangle$$

$$S_1^z |++\rangle = \tfrac{\hbar}{2}|++\rangle \quad \text{etc}$$

$$\hat{H}|++\rangle = J/4\,|++\rangle$$

$$\hat{H}|+-\rangle = -J/4\,|+-\rangle + J/2\,|-+\rangle$$

$$\hat{H}|-+\rangle = -J/4\,|-+\rangle + J/2\,|+-\rangle$$

$$\hat{H}|--\rangle = +J/4\,|--\rangle$$

matrix for $\hat{H}$ is $\dfrac{J}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

Eigenvalues $+J/4 \quad (\times 2)$

$$(-1-\lambda)^2 - 2^2 = 0 \qquad \lambda+1 = \pm 2$$
$$\lambda = 1, -3$$

$$J/4,\ -3J/4$$

"singlet" $-3J/4 \qquad \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$

H3

"Triplet"
$|++\rangle$
$|--\rangle$ $+J/4$
$\frac{1}{\sqrt{2}}\left(|+-\rangle+|-+\rangle\right)$

Another sol'n $J\,\vec{S}_1\cdot\vec{S}_2 = \frac{J}{2}\left[(S_1+S_2)^2 - S_1^2 - S_2^2\right]$

$S_1+S_2 = 0$ $\quad (S_1+S_2)^2 = 0(0+1)$
$\qquad\quad 1 \qquad\qquad 1(1+1)$

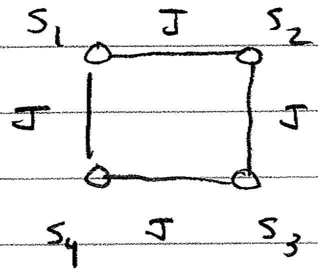
$S_1+S_2=0$ $\quad \frac{J}{2}\left[0-3/4-3/4\right] = -3J/4 \leftarrow \times 1$

$S_1+S_2=1$ $\quad \frac{J}{2}\left[2-3/4-3/4\right] = +J/4 \leftarrow \times 3$

H4

4 site Heisenberg model

$$\hat{H} = J(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_4 + \vec{S}_4 \cdot \vec{S}_1)$$



"Straight forward" approach

$$\hbar^2 \hat{H} = \frac{J}{2}\left(S_1^+ S_2^- + S_1^- S_2^+ + S_2^+ S_3^- + S_2^- S_3^+ + S_3^+ S_4^- + S_4^+ S_3^- + S_4^+ S_1^- + S_4^- S_1^+\right)$$

$$+ J\left(S_1^z S_2^z + S_2^z S_3^z + S_3^z S_4^z + S_4^z S_1^z\right)$$

Q: Dim of Hilbert space A: 16

$$\hat{H}|{+}{+}{+}{+}\rangle = J\left(\tfrac{1}{2}\cdot\tfrac{1}{2} + \tfrac{1}{2}\cdot\tfrac{1}{2} + \ldots\right)|{+}{+}{+}{+}\rangle = J|{+}{+}{+}{+}\rangle$$

$$\hat{H}|{+}{+}{+}{-}\rangle = J\left[\tfrac{1}{2}\tfrac{1}{2} + \tfrac{1}{2}\cdot\tfrac{1}{2} + \tfrac{1}{2}\left(-\tfrac{1}{2}\right) + \left(-\tfrac{1}{2}\right)\left(\tfrac{1}{2}\right)\right]|{+}{+}{+}{-}\rangle$$

$$+ J/2\,|{+}{+}{-}{+}\rangle + J/2\,|{-}{+}{+}{+}\rangle$$

4×4 MATRIX

$$\frac{J}{2}\begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

See pages TD1-5 for general theory of tridiagonal matrices.

$$\lambda_k = J/2\left[0 - 2\cos k\right] \qquad k = \frac{2\pi}{4}\{1,2,3,4\}$$

$$= 0, J, 0, -J$$

Hardest subspace is $S^z_{TOT} = 0$ $|++--\rangle$

Q: what dimension? A: 6

You will continue brute force approach in HW.

Now we will do trick similar to 2 site problem.

H6

$$\hbar^2 \hat{H} = \frac{J}{2}\left[(S_1+S_2+S_3+S_4)^2 - (S_1+S_3)^2 - (S_2+S_4)^2\right]$$

S_1+S_3	S_2+S_4	$S_1+S_2+S_3+S_4$	Counting
0	0	0	1
0	1	1	3
1	0	1	3
1	1	0	1
		1	3
		2	5
			16 states ✓✓

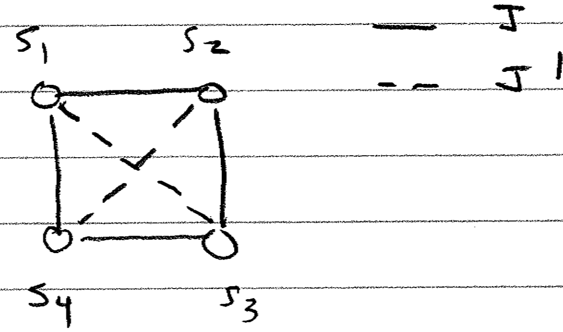
S_1+S_3	S_2+S_4	$S_1+S_2+S_3+S_4$		
1	1	2	5 eigenvalues	$\frac{J}{2}\left[2(3) - 1(2) - 1(2)\right] = +J$
1	1	1	3 eigenvalues	$\frac{J}{2}\left[1(2) - 1(2) - 1(2)\right] = -J$
1	1	0	1 "	$\frac{J}{2}\left[0(1) - 1(2) - 1(2)\right] = -2J$
1	0	1	3 "	$= 0$
0	1	1	3 "	$= 0$
0	0	0	1 "	$= 0$

We had already found J

$0, J, 0, -J$

all of which are on this list. ✓✓

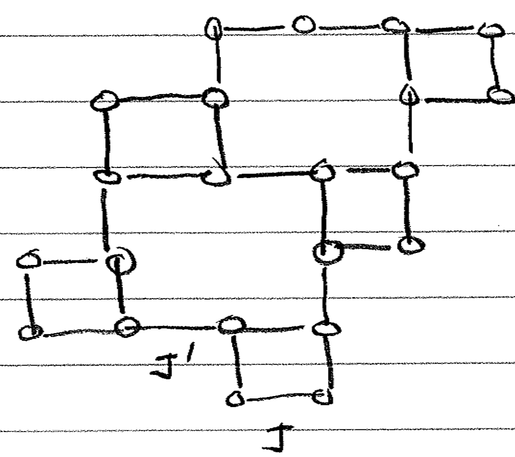
Your HW



$$\hbar^2 \hat{H} = J(S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_4 + S_4 \cdot S_1) + J'(S_1 \cdot S_3 + S_2 \cdot S_4)$$

We will discuss this further as a very simple example of a "quantum phase transition"

CaV_4O_9
magnetism
(Singh)

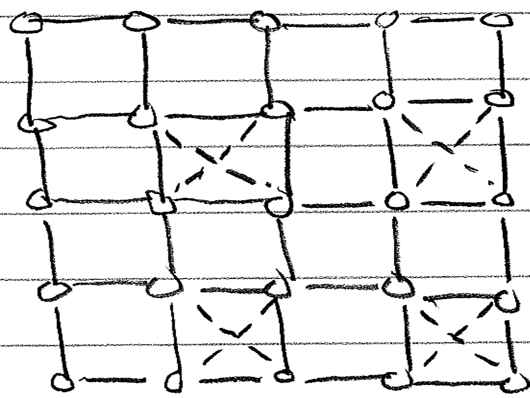


Current Research project!

limits $J' = 0$ 4 site Heisenberg

$J = 0$ 2 site Heisenberg

Another research project of last few years:



"plaquette Heisenberg model"

Numerical questions (HW)

(1) Could you write a computer program to generate matrix elements of $\hat{H}$ and then call a numerical diagonalizer? What would be its ingredients/structure?

(2) How large a system could you solve?

What limits a computer program?

Memory?

cpu time?