

The first two problems review some of Physics 215A.

[1.] Consider a system whose state space, which is three dimensional, is spanned by the orthonormal basis $|u_1\rangle, |u_2\rangle, |u_3\rangle$. In this basis, the Hamiltonian H and the observable M are given by,

$$\hat{H} = E \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \hat{M} = F \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix}$$

Here E and F are real numbers. The initial state is

$$|\Psi(t=0)\rangle = \frac{3}{5}|u_2\rangle + \frac{4}{5}|u_3\rangle.$$

What is the expectation value of the energy, $\langle \hat{H} \rangle$ at $t=0$?

What are the possible values of a measurement of \hat{M} ?

What is the expectation value $\langle \hat{M} \rangle(t)$ at arbitrary time t ?

[2.] Re-do problem 1 with the matrices for \hat{H} and \hat{M} interchanged.

[3.] We solved the $N=2$ site (spin-1/2) Heisenberg Hamiltonian in class both by 'brute force' (explicit construction and diagonalization) and also by a 'trick' using the rules for adding angular momentum. Do the same 'brute force' solution of the three site case $\hat{H} = J/\hbar^2 (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1)$. Can you also do the case where spins 1 and 3 are not connected: $\hat{H} = J/\hbar^2 (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3)$?

[4.] We also solved the $N=4$ site problem in class using the 'trick'. What are the eigenenergies with an additional 'frustrating' interaction J' :

$$\hat{H} = J/\hbar^2 (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_4 + \vec{S}_4 \cdot \vec{S}_1) + J'/\hbar^2 (\vec{S}_1 \cdot \vec{S}_3 + \vec{S}_2 \cdot \vec{S}_4)$$

Discuss what happens as J'/J increases. We will talk further about this in class after you have had a chance to think about the problem independently. This problem provides a simple illustration of a 'quantum phase transition'.

[5.] How big is the Hilbert space for the spin-1/2 Heisenberg Hamiltonian with N spins? Describe how you might write a program to set up the matrix for \hat{H} . (If you could do this, you could then call a matrix diagonalization library routine and thereby completely solve the problem numerically.) I don't want an actual working code in any specific language, but rather your thoughts on the algorithmic steps which would be useful/necessary. Discuss how large an N is feasible to do with a workstation. (How much memory is required for a given N ? How much cpu time?)

[6.] (Optional) Set up \hat{H} and diagonalize for the $N=4$ spin J - J' Heisenberg model and check the eigenvalues you obtained in Problem 4. How much of it can you do with pencil and paper? Can you do the rest with a computer?

Physics 215B Winter 2013
HW1 Solns

1. \hat{H} is diagonal so $|u_i\rangle$ are eigenvectors.

Can immediately write $|\psi(t)\rangle = \frac{3}{5} e^{-i\omega t} |u_2\rangle + \frac{4}{5} e^{-2i\omega t} |u_3\rangle$

with $\omega \equiv E/\hbar$.

$$\begin{aligned} \langle \hat{H} \rangle(t=0) &= \frac{1}{5} (0 \ 3 \ 4) E \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \frac{1}{5} \begin{pmatrix} 0 \\ 3 \\ 4 \end{pmatrix} \\ &= \frac{E}{25} (0 \ 3 \ 4) \begin{pmatrix} 0 \\ 3 \\ 8 \end{pmatrix} = \frac{41}{25} E \end{aligned}$$

Possible values for measuring M are eigenvalues of \hat{M} : $(-1, 1, 2)$

$-2F, +F, +2F$

$$\langle \hat{M} \rangle(t) = \langle \psi(t) | \hat{M} | \psi(t) \rangle$$

$$= \frac{1}{5} \begin{pmatrix} 0 & 3e^{+i\omega t} & 4e^{+2i\omega t} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} F \frac{1}{5} \begin{pmatrix} 0 \\ 3e^{-i\omega t} \\ 4e^{-2i\omega t} \end{pmatrix}$$

$$= \frac{F}{25} \begin{pmatrix} & & \\ 8e^{-i\omega t} & & \\ 6e^{-i\omega t} & & \end{pmatrix}$$

$$= \frac{F}{25} (24e^{-i\omega t} + 24e^{+i\omega t}) = \frac{48F}{25} \cos \omega t$$

2.

$$\boxed{2.} \quad \text{Now } \hat{H} = F \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} \quad \hat{M} = F \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

$$\begin{aligned} \langle \hat{H} \rangle (t=0) &= \frac{1}{5} (0 \ 3 \ 4) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix} F \begin{pmatrix} 0 \\ 3 \\ 4 \end{pmatrix} \frac{1}{5} \\ &= \frac{F}{25} (0 \ 3 \ 4) \begin{pmatrix} 0 \\ 8 \\ 6 \end{pmatrix} = \frac{F}{25} 48. \end{aligned}$$

Possible values of M measurement are eigenvalues $E, E, 2E$

$$\begin{aligned} \text{Eigenstates of } \hat{H} \text{ are } |e_1\rangle &= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} & |e_2\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} & |e_3\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \\ E_1 &= F & E_2 &= 2F & E_3 &= -2F \end{aligned}$$

$$|\psi(t)\rangle = \sum_n e^{-i\omega_n t} |e_n\rangle \langle e_n | \psi(t=0) \rangle \quad \omega_n = E_n/\hbar$$

Define $\omega = F/\hbar$

$$\begin{aligned} &= e^{-i\omega t} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \cdot \phi + e^{-2i\omega t} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{2}} \frac{7}{5} + e^{+2i\omega t} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \frac{1}{\sqrt{2}} \left(\frac{-1}{5}\right) \\ &\quad \uparrow \\ &\quad \frac{1}{\sqrt{2}} (0 \ 1 \ 1) \begin{pmatrix} 0 \\ 3/5 \\ 4/5 \end{pmatrix} \end{aligned}$$

$$|\psi(t)\rangle = \left(\frac{7}{10} e^{-2i\omega t} - \frac{1}{10} e^{2i\omega t} \right) |u_2\rangle + \left(\frac{7}{10} e^{-2i\omega t} + \frac{1}{10} e^{2i\omega t} \right) |u_3\rangle$$

3,

2 // cant d

$$\langle \hat{M} \rangle(t) = \langle \psi(t) | \hat{M} | \psi(t) \rangle$$

$$= \frac{1}{10} \begin{pmatrix} 0 & 7e^{+2i\omega t} & -e^{-2i\omega t} & 7e^{+2i\omega t} & -e^{-2i\omega t} \end{pmatrix} E \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} 0 \\ 7e^{-2i\omega t} & -e^{2i\omega t} \\ 7e^{-2i\omega t} & +e^{2i\omega t} \end{pmatrix} \frac{1}{10}$$

$$= \frac{E}{100} \left\{ \begin{aligned} & (7e^{2i\omega t} - e^{-2i\omega t})_1 (7e^{-2i\omega t} - e^{2i\omega t}) \\ & + (7e^{2i\omega t} + e^{-2i\omega t})_2 (7e^{-2i\omega t} + e^{2i\omega t}) \end{aligned} \right\}$$

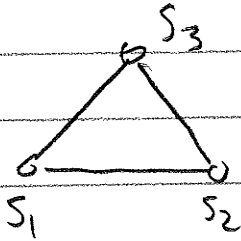
$$= \frac{E}{100} \left\{ \begin{aligned} & 49 - 7e^{4i\omega t} - 7e^{-4i\omega t} + 1 \\ & + 98 + 14e^{-4i\omega t} + 14e^{4i\omega t} + 2 \end{aligned} \right\}$$

$$= \frac{E}{100} \left\{ 150 + 14 \cos 4\omega t \right\}$$

$$\langle \hat{M} \rangle(t) = 1.5E + \frac{7}{50} \cos 4\omega t$$

4.

3



$$\hat{H} = \frac{J}{\hbar^2} (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1)$$

$$S_1^z S_2^z + \frac{1}{2} (S_1^+ S_2^- + S_1^- S_2^+)$$

Basis $|S_1^z S_2^z S_3^z\rangle$

$$\hat{H} |+++ \rangle = J \frac{3}{4} |+++ \rangle$$

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

Do rest in head Matrix of \hat{H}

$ +++ \rangle$	$\frac{3}{4}J$	0	0	0	0	0	0	0
$ ++-\rangle$	0	$-\frac{J}{4}$	$\frac{J}{2}$	$\frac{J}{2}$	0	0	0	0
$ +-+\rangle$	0	$\frac{J}{2}$	$-\frac{J}{4}$	$\frac{J}{2}$	0	0	0	0
$ -++ \rangle$	0	$\frac{J}{2}$	$\frac{J}{2}$	$-\frac{J}{4}$	0	0	0	0
$ ---+\rangle$	0	0	0	0	$-\frac{J}{4}$	$\frac{J}{2}$	$\frac{J}{2}$	0
$ --+\rangle$	0	0	0	0	$\frac{J}{2}$	$-\frac{J}{4}$	$\frac{J}{2}$	0
$ +--\rangle$	0	0	0	0	$\frac{J}{2}$	$\frac{J}{2}$	$-\frac{J}{4}$	0
$ ---\rangle$	0	0	0	0	0	0	0	$\frac{3}{4}J$

Need eigenvalues of 3×3 matrix

$$\frac{J}{4} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$$

~~matrix~~

5,

3// cont'd Get eigenvalues of $\begin{pmatrix} 0 & 2 & 2 \\ 2 & 0 & 2 \\ 2 & 2 & 0 \end{pmatrix} \frac{J}{4}$

and subtract $\frac{J}{4}$ at end. By inspection $\lambda = -2$

works (and is doubly degenerate). But do it the long way:

$$-\lambda(\lambda^2 - 4) - 2(-2\lambda - 4) + 2(4 + 2\lambda) = 0$$

$$-\lambda^3 + 4\lambda + 4\lambda + 8 + 8 + 4\lambda = 0$$

$$\lambda^3 - 12\lambda - 16 = 0$$

$$(\lambda + 2)^2(\lambda - 4) = 0$$

$$\lambda = -2, -2, 4$$

So eigenvalues are

$$\frac{J}{4} (-2, -2, 4) - \frac{J}{4} =$$

diagonal shift.

Complete list of eigenvalues: $\frac{3J}{4}, -\frac{3J}{4}, -\frac{3J}{4}, \frac{3J}{4}$

and $\begin{matrix} \uparrow & \uparrow \\ |+++ \rangle & |+-+ \rangle \\ |--+ \rangle & |++ \rangle \end{matrix}$ and same for $\begin{matrix} |--+\rangle \\ |-+-\rangle \\ |+-+\rangle \end{matrix}$

\Rightarrow There are only 2 eigenvalues: $\pm \frac{3J}{4}$ each 4-fold degenerate

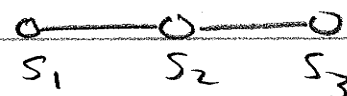
Eigenvectors include $|+++ \rangle; |--+ \rangle$ for $\lambda = \frac{3J}{4}$

$\frac{1}{\sqrt{3}} |+++ \rangle + |+-+ \rangle + |++ \rangle$ for $\lambda = -\frac{3J}{4}$

etc.

3/cont'd Do the "open boundary case"

$$H = \frac{J}{k^2} (\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3)$$



$$\hat{H} |+++ \rangle = J \frac{1}{2} |+++ \rangle$$

$$\hat{H} |++- \rangle = \frac{J}{2} |+-+ \rangle$$

Do rest in head to get matrix of \hat{H}

$$\begin{array}{l} |+++ \rangle \\ |++- \rangle \\ |+-+ \rangle \\ |-++ \rangle \\ |--+ \rangle \\ |-+- \rangle \\ |+-- \rangle \\ |--- \rangle \end{array} \begin{pmatrix} \frac{1}{2}J & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}J & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2}J & -\frac{1}{2}J & \frac{1}{2}J & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}J & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}J & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2}J & -\frac{1}{2}J & \frac{1}{2}J & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}J & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2}J \end{pmatrix}$$

Need eigenvalues of $\frac{J}{2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$$\begin{aligned} & -\lambda [(-\lambda-1)(-\lambda) - 1] - [0\lambda - 0] \\ & = -\lambda [\lambda^2 + \lambda - 1] + \lambda \\ & = -\lambda^3 - \lambda^2 + 2\lambda = -\lambda(\lambda^2 + \lambda - 2) = -\lambda(\lambda+2)(\lambda-1) \end{aligned}$$

7.

Eigenvalues are $\frac{J}{2} \{ -2, 0, 1, 1 \}$

each 2 fold degenerate

N.B. A check on eigenvalues is that their

sum should equal the trace of original matrix. This works!

Eigenvectors are $|+++ \rangle$ and $|--- \rangle$ (eigenvalue $\frac{J}{2}$)

Also $\frac{1}{\sqrt{2}} (|+- \rangle - |-+ \rangle)$ (eigenvalue ϕ)

$\frac{1}{\sqrt{2}} (|-+ \rangle - |+ - \rangle)$

The other vectors of eigenvalue $\frac{J}{2}$ determined by

$$\begin{pmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow x=y=z$$

So $\frac{1}{\sqrt{3}} (|++ \rangle + |+ - \rangle + |-+ \rangle)$ Eigenvalue $\frac{J}{2}$

and $\frac{1}{\sqrt{3}} (|-- \rangle + |-+ \rangle + |+ - \rangle)$

Finally $-J$
$$\begin{pmatrix} +2 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow y = -2x = -2z$$

So $\frac{1}{\sqrt{6}} (|++ \rangle - 2|+- \rangle + |+++ \rangle)$ Eigenvalue $-J$

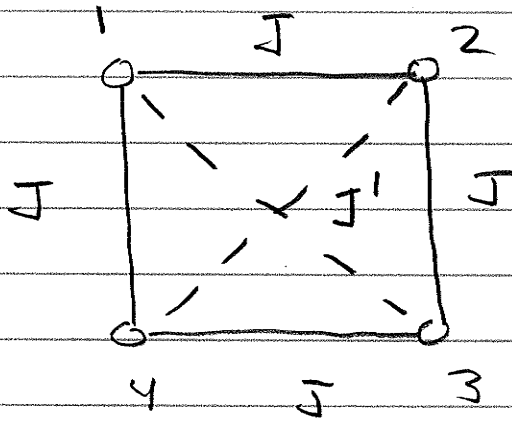
$\frac{1}{\sqrt{6}} (|-- \rangle - 2|-+ \rangle + |+ - \rangle)$

8.

4 We rewrite \hat{H} as

$$\hat{H} = \frac{J}{2\hbar^2} \left[(s_1 + s_2 + s_3 + s_4)^2 - (s_1 + s_3)^2 - (s_2 + s_4)^2 \right]$$

$$+ \frac{J'}{2\hbar^2} \left[(s_1 + s_3)^2 + (s_2 + s_4)^2 - s_1^2 - s_2^2 - s_3^2 - s_4^2 \right]$$



To solve problem rapidly (you could also construct the 16×16 matrix and diagonalize it!) you

use the rules for adding angular momentum, eg

$$\frac{1}{2} + \frac{1}{2} = 0, 1 \quad \text{and} \quad 1 + 1 = 0, 1, 2.$$

You also recall that J^2 gives $j(j+1)\hbar^2$

when acting on $|j m\rangle$

9.

4/cont'd

So we look at the different cases and compute E

$S_1 + S_3$	$S_2 + S_4$	$S_1 + S_2 + S_3 + S_4$	E
0	0	0	$-3J/2$
0	1	1	$-J/2$
1	0	1	$-J/2$
1	1	0	$-2J + J/2$
		1	$-J + J/2$
		2	$+J + J/2$

A typical calculation is like this (for $S_1 + S_3 = 1$, $S_2 + S_4 = 0$)

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

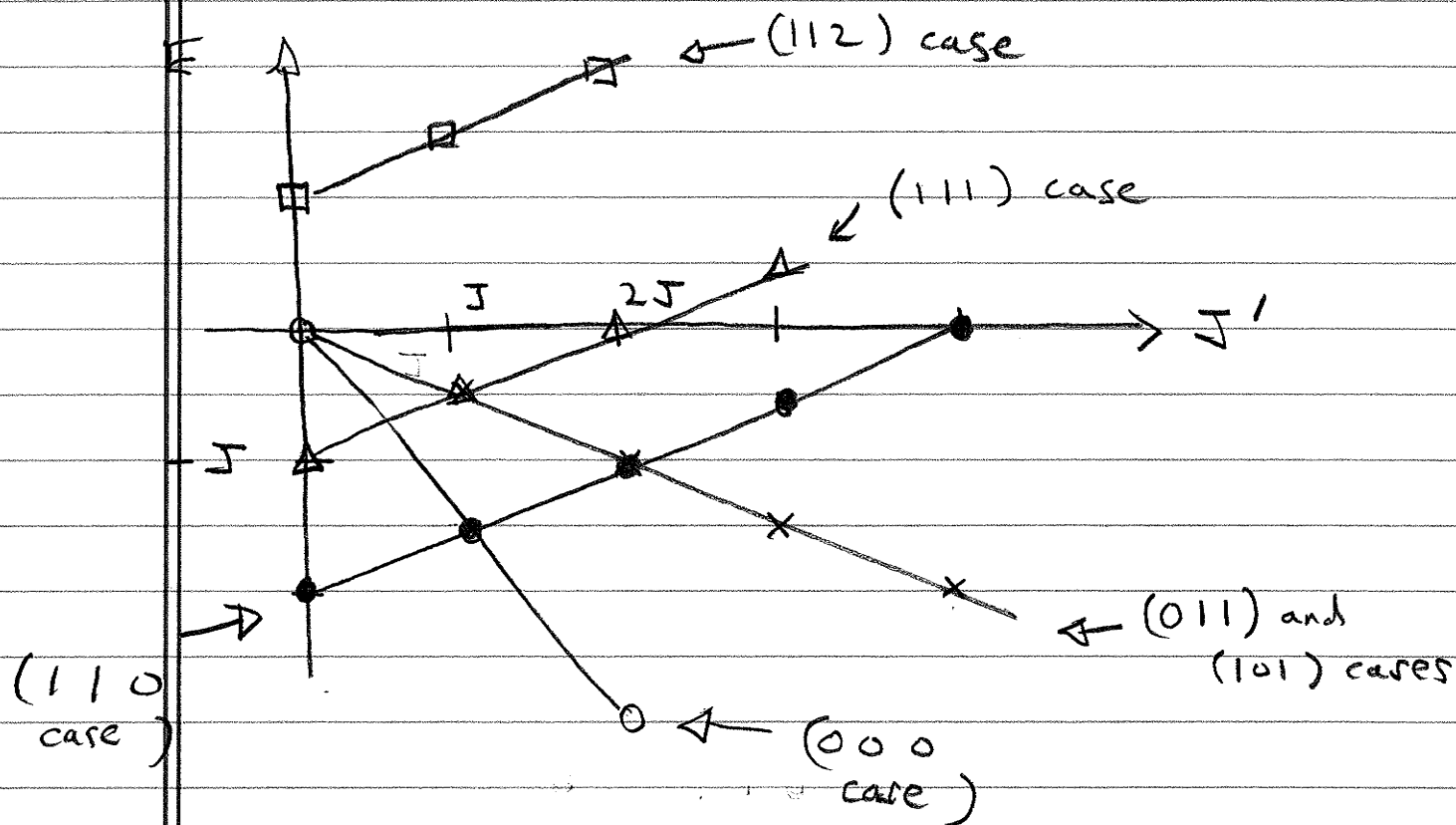
\downarrow $2t^2$ \downarrow $-2t^2$ \downarrow \emptyset

$$+ \frac{J'}{2t^2} \left[(S_1 + S_3)^2 + (S_2 + S_4)^2 - S_1^2 - S_2^2 - S_3^2 - S_4^2 \right]$$

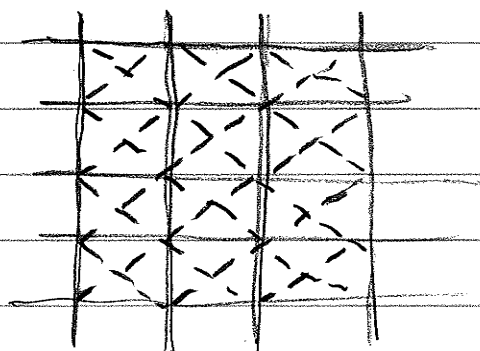
\downarrow $2t^2$ \downarrow \emptyset \downarrow \downarrow \downarrow \downarrow \downarrow $-4(3/4)t^2$

↓ Material from now on we will discuss in class
(ie not expected on your HW solns)

4/cont'd. Let's plot these energies



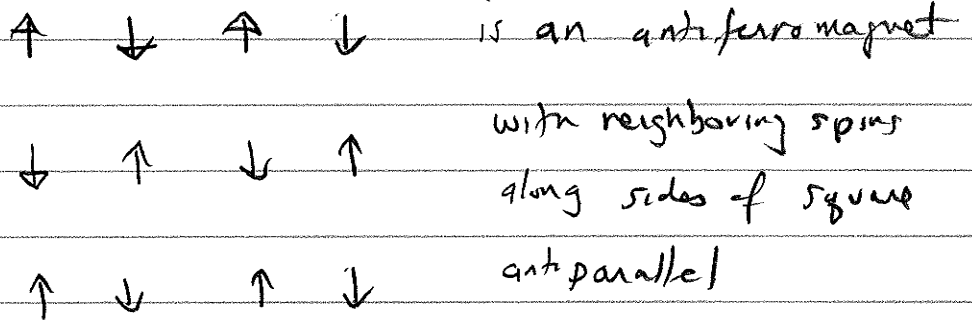
What you can see is that the lowest energy is (110) for $J' < J$ but switches to (000) at $J' > J$. This "level crossing" becomes an actual phase transition if one studies a big lattice:



of J bonds and J' bonds

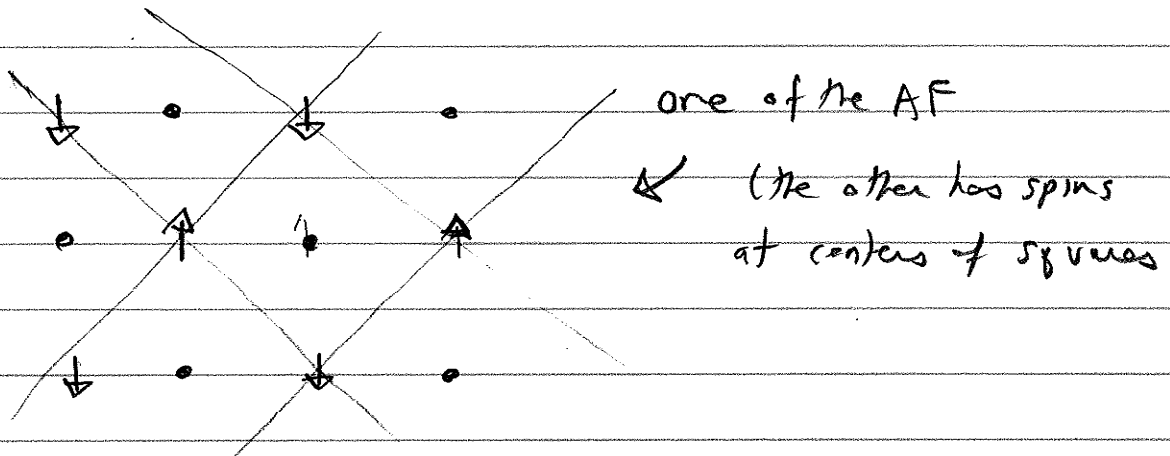
11.

4 cont'd. More specifically for $J' \ll J$ the ground state



two interpenetrating
But if J' dominates one has \wedge antiferromagnets

with spins along diagonals antiparallel



Amazingly the physics of the model for intermediate

$J' \approx J$ is not resolved!!

5 Each of the N spins has 2 choices $S_i^z = \pm 1/2$
 so the Hilbert space has dimension 2^N . (We
 did $N=2$ which had a $2^2=4$ dim space
 and $N=4$ which had a $2^4=16$ dim space.)

The basic idea of writing a code to
 generate the matrix is this: ① You use a bunch
 of loops to allow the different values of $\{S_i^z\}$

② For each $\{S_i^z\}$ you compute the associated
 basis number n . ③ You then act with \hat{H} by

looking for neighboring $(+-)$ pairs of S_i^z
 and you exchange them $(-+)$ you compute

the new basis number m with that exchange and then

set $H_{nm} = J/2$. ④ To get the diagonal

entries H_{nn} just compute $J \sum_{\langle ij \rangle} S_i^z S_j^z$.

SEE
 PAGE
 15
 FOR
 SOME
 MORE
 DETAILS

5 cont'd

How big N is doableCPU consideration To diagonalize a matrix of dimension D takes D^3 operations. A computer can do $\sim 10^9$

operations per second (GHz chip), so to diagonalize

the matrix for an N site spin $1/2$ Heisenberg model

will take CPU time (in seconds)

$$T \sim (2^N)^3 / 10^9$$

N	T (sec)
5	$2^{15} / 10^9 \sim 3 \cdot 10^{-5}$ sec
10	$2^{30} / 10^9 \sim 1$ sec
15	$2^{45} / 10^9 \sim 3 \cdot 10^4$ sec $\sim 1/2$ day
20	$2^{60} / 10^9 \sim 10^9$ sec ~ 30 years

20 sites takes 30 years!

So limit
is ~ 15 sites
from CPU
considerations

5 cont'd

Memory consideration

To store a # in a computer you use 64 bits = 8 bytes

so to store a matrix of dimension D takes D^2 numbers (ignoring sparsity) or $8D^2$ bytes,

A typical computer memory might be 16 Gbytes

so to store the matrix $8D^2 < 16 \cdot 10^9$

$$D < \sqrt{2 \cdot 10^9} \sim 50000$$

recall $D = 2^N$ so this puts a limit

$$2^N = 50000$$

$$N = \frac{\ln(50000)}{\ln 2} = 16$$



limit from memory considerations

Interesting that CPU and
memory limit roughly the same!

Discuss in class (perhaps). Not expecting

you to know this:

A specific way to assign a basis # to

a basis vector $|s_1^z s_2^z s_3^z \dots s_N^z\rangle$ is

$$n = s_1^z + \frac{1}{2} + 2(s_2^z + \frac{1}{2}) + 4(s_3^z + \frac{1}{2}) \\ + 8(s_4^z + \frac{1}{2}) + \dots$$

Thus, for example, for $N = 4$ sites

$$|----\rangle \longrightarrow n = 0$$

$$|+---\rangle \longrightarrow n = 1$$

$$| - + -- \rangle \longrightarrow n = 2$$

$$|++--\rangle \longrightarrow n = 3$$

⋮

$$|++++\rangle \longrightarrow n = 15$$

To "undo" this and get $\{s_1^z, s_2^z, s_3^z, \dots\}$ from n

notice the following eqns work!

$$s_1^z + 1/2 = \text{mod}(n, 2)$$

This works because all the $s_2^z + 1/2, s_3^z + 1/2, \dots$ are multiplied by powers of 2 so give \emptyset when you take $\text{mod}(\cdot, 2)$!

Once you get s_1^z the trick to get s_2^z is

$$\frac{1}{2} [n - (s_1^z + 1/2)] = s_2^z + 1/2 + 2(s_3^z + 1/2) + \dots$$

$$\text{so } s_2^z - 1/2 = \text{mod}\left(\frac{1}{2} [n - (s_1^z + 1/2)], 2\right)$$

by same reasoning that gave us $s_1^z + 1/2$.

So we have exhibited a way to assign a basis number n to each $\{s_1^z, s_2^z, \dots, s_N^z\}$ and also given the basis number how to get $\{s_i^z\}$.