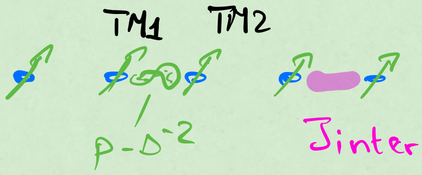
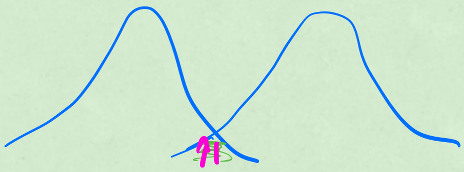
31.10.2022

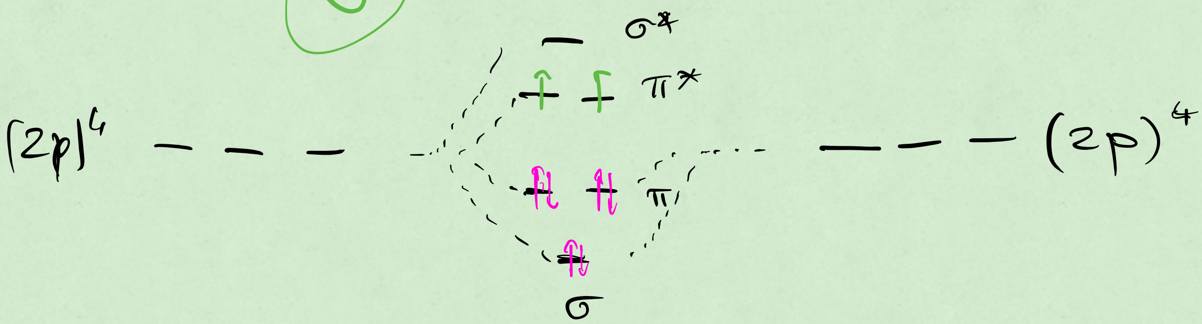


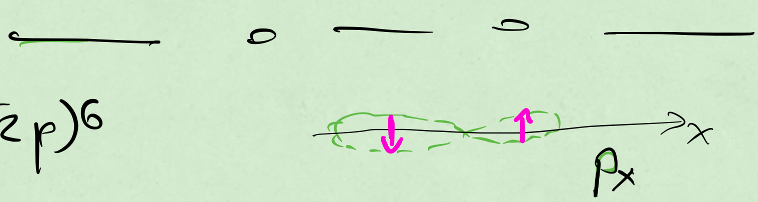


bad for magnetism

S = 1

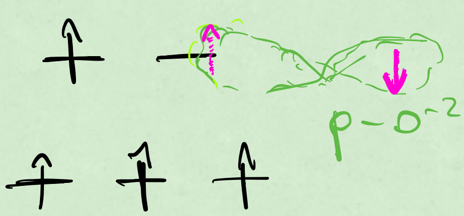
LCMO



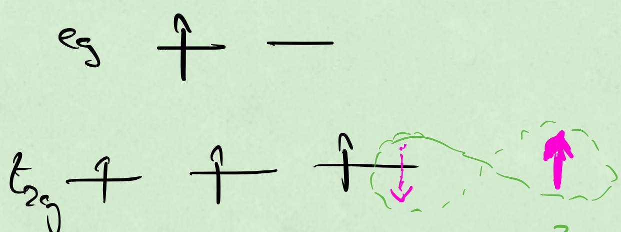


O^{-2} $(2p)^6$

TM - O_h symmetry

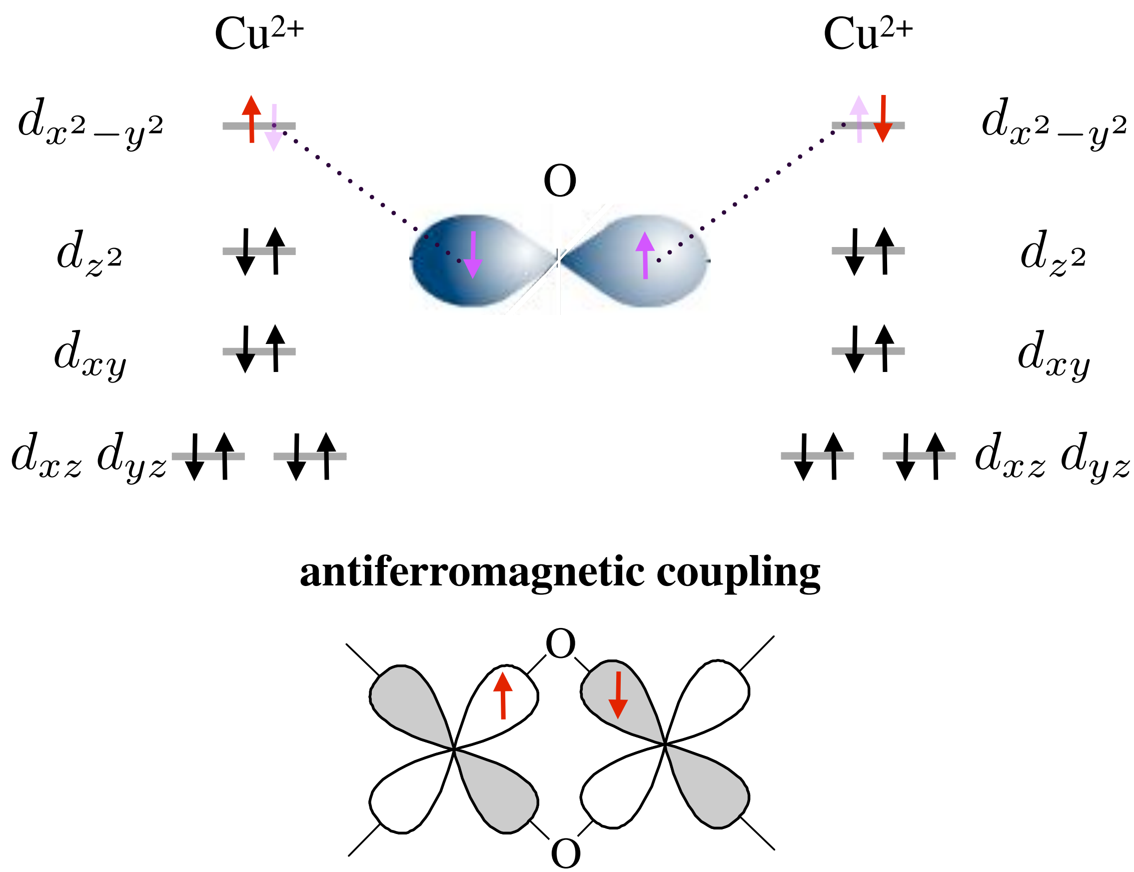


1st Hond-like behavior

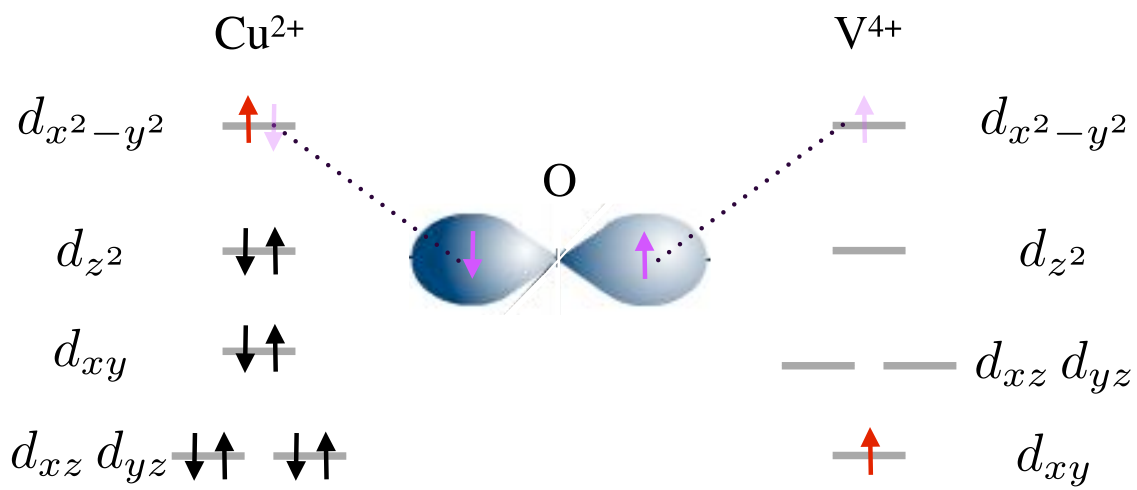


Pauli pr. like behavior

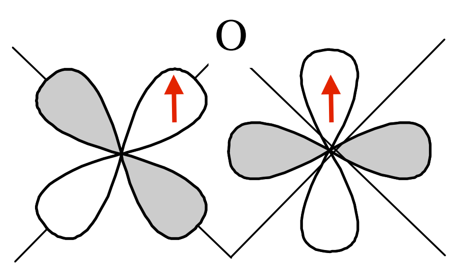
Super exchange between Cu^{2+} and Cu^{2+}



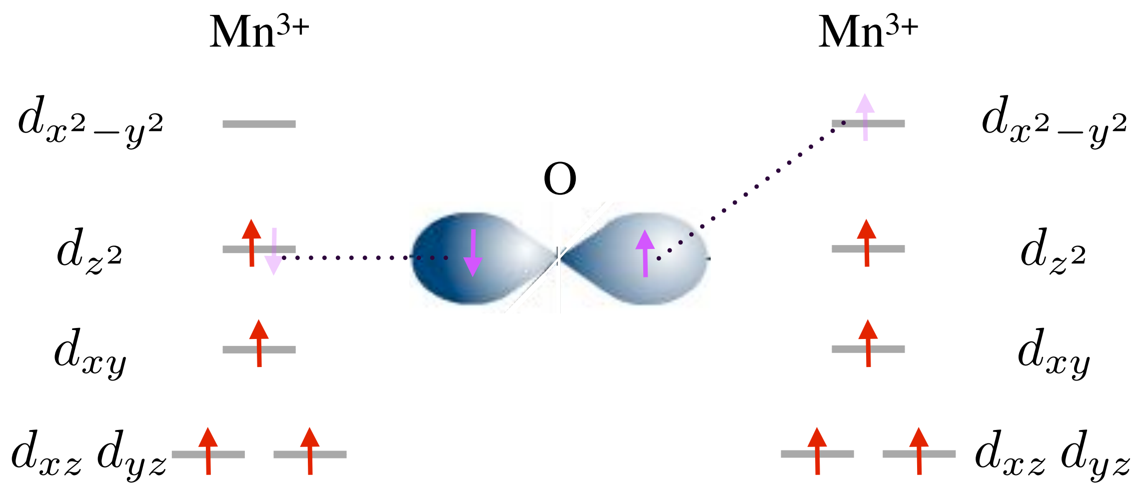
Super exchange between Cu^{2+} and V^{4+}



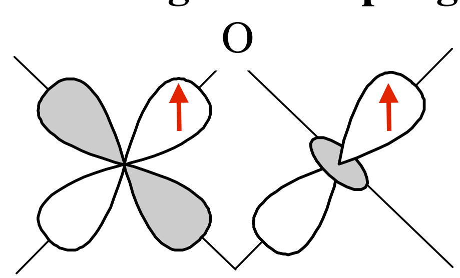
ferromagnetic coupling



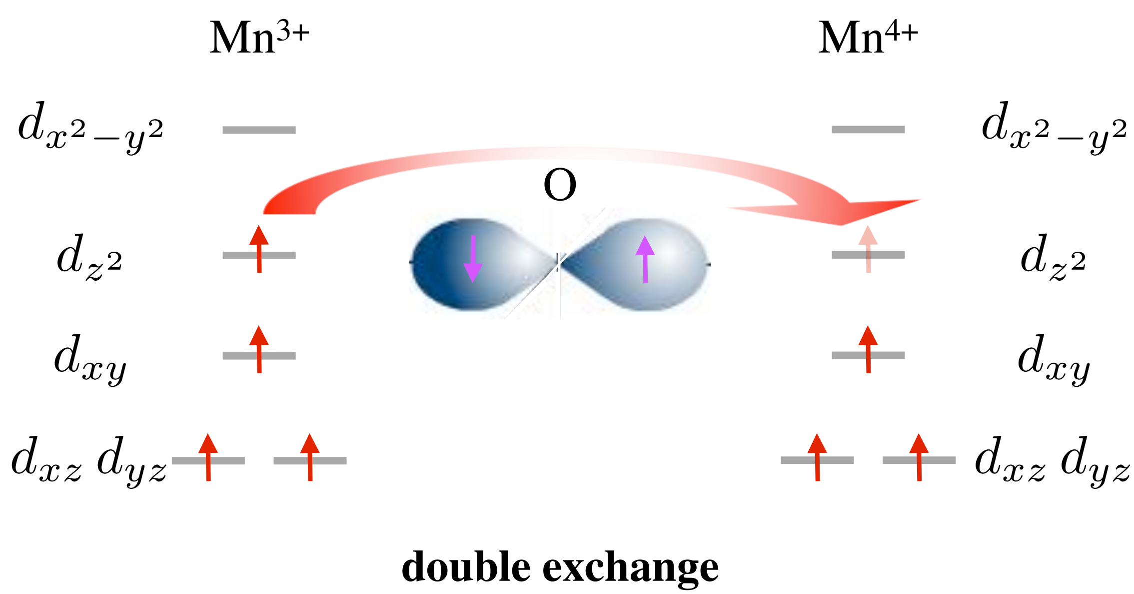
Super exchange between Mn^{3+} and Mn^{3+}



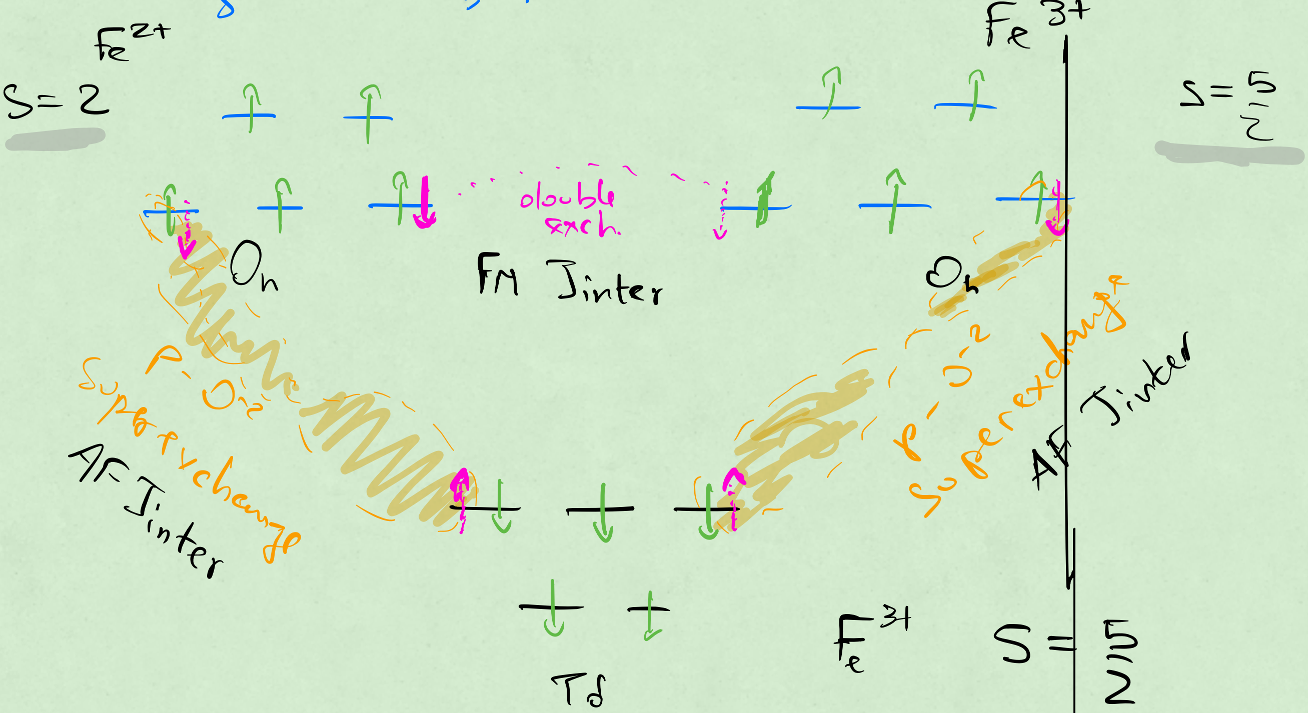
ferromagnetic coupling

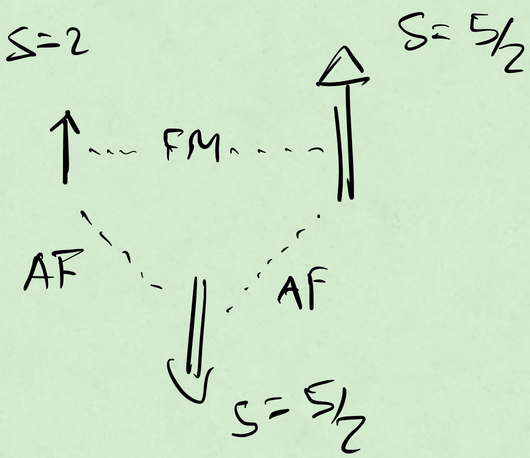


Double exchange Mn^{3+} and Mn^{4+} mediated by the electron-transfer



Magnetite Fe_3O_4





unit cell has

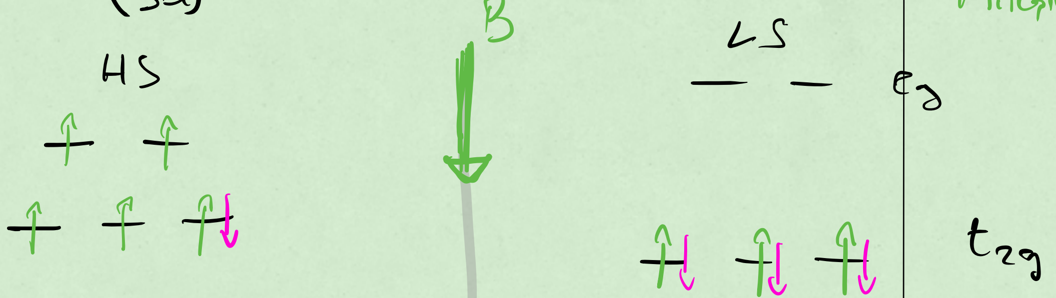
$$\mu = S g_s \mu_B = 4 \mu_B$$

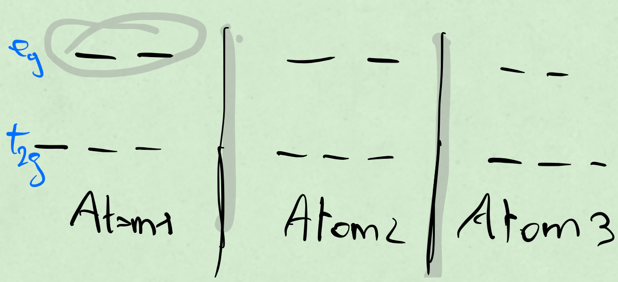
	S	$\mu^{th}_{[\mu_B]}$	μ^{exp}
Fe^{2+}	2	4	2.2
Co^{2+}	3/2	3	1.7
Ni^{2+}	1	2	0.6

th.
- assumes HS
- quenching of L

LOCAL MOM. MAGNETISM

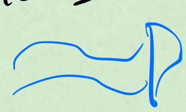
Fe^{2+} $(3d)^6$ ~ o —

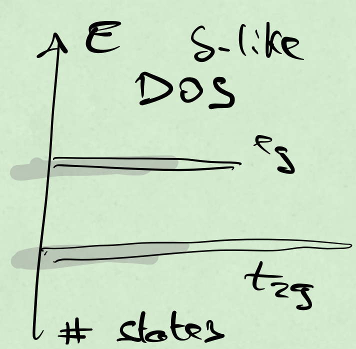




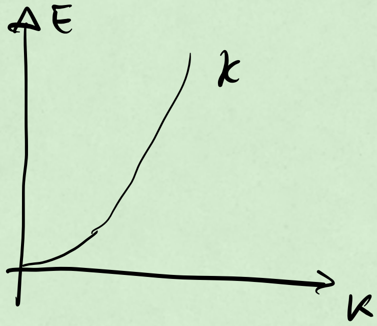
Separated Atoms

. . . . .



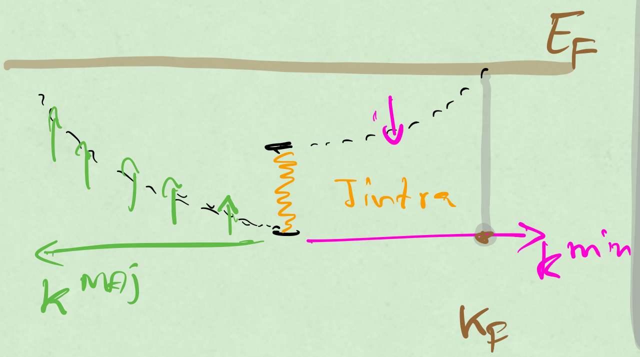


ITINERANT MAGNETISM

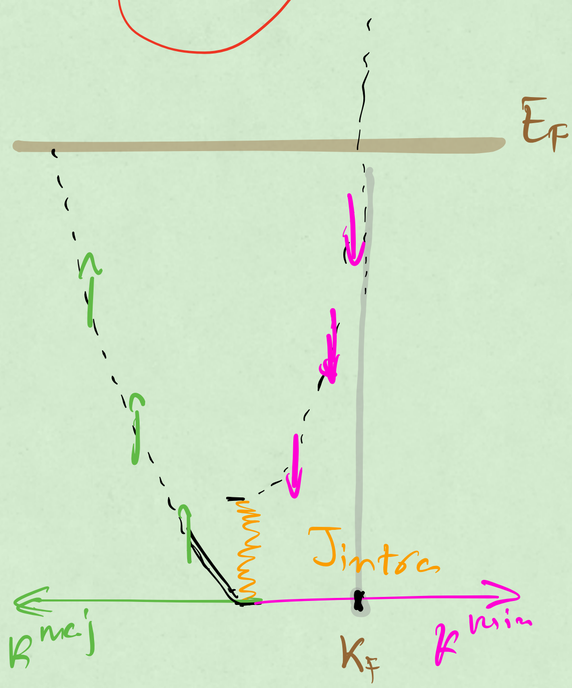


How do I split bands to recreate HS vs LS configuration

HS



LS



$K_F^{HS} > K_F^{LS}$

High DOS

"flat" band

low DOS

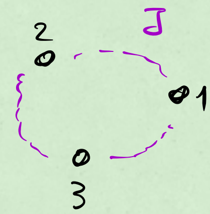
"parabolic" band

Workshop assignment @6-week

(on the blackboard.)

Ring with $N=3$ spins $1/2$

$$\mathcal{H} = -J\left(\hat{S}_1 \cdot \hat{S}_2 + \hat{S}_2 \cdot \hat{S}_3 + \hat{S}_3 \cdot \hat{S}_1\right)$$



In the previous assignment we have computed the eigenvalues of $\mathcal{H}$ and their degeneracy using the $|S_{13}, S_{123}\rangle$ states. Table:

S_{13}	S_{123}	$E\,(J)$	dim
0	1/2	3/4	2
1	1/2	3/4	2
1	3/2	$-3/4$	4

Today we want to express the operators $\mathcal{H}$, $\hat{S}^z_{123}$, and T [translation] on the single particle basis and progressively build (numerically) a basis of common eigenst

The fact that a basis of common eig. can $\exists$ is guaranteed by

$$[\mathcal{H}, \hat{S}^z] = [\mathcal{H}, T] = [T, \hat{S}^z] = 0$$

state of single particle basis can be mapped into integer numbers

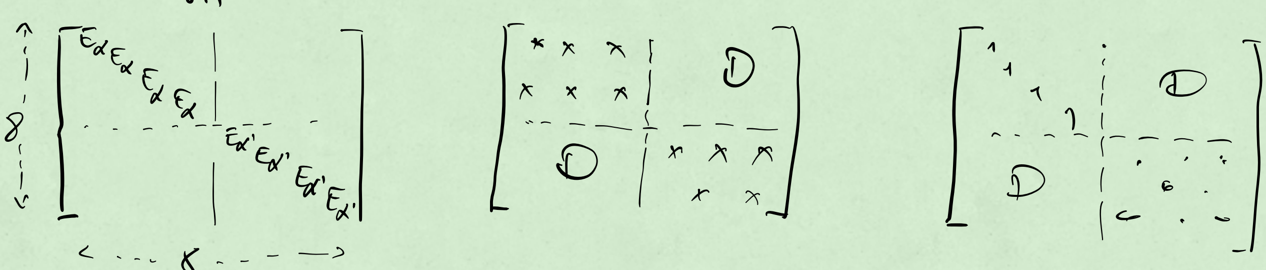
int	bin	
0	(0 0 0)	$\vert - - - \rangle$
1	(0 0 1)	$\vert - - + \rangle$
$\vdots$		$\vdots$
6	(1 1 0)	$\vert + + - \rangle$
7	(1 1 1)	$\vert + + + \rangle$

On this basis only $\hat{S}^z_{123}$ is diagonal. In fact

$$\hat{S}^z_{123} = \hat{S}^z_1 + \hat{S}^z_2 + \hat{S}^z_3 \quad \dots$$

we then diagon. numerically the matrix $\mathcal{H}$
let $|E_\alpha, \alpha\rangle$ be the corresponding eigenvector
on this basis

$\mathcal{H}$ $\qquad\qquad$ $\hat{S}^z$ $\qquad\qquad$ T



diag $\qquad\qquad$ block diag $\qquad\qquad$ Block diag

N.B. Each block is characterized by the same eigenv. E_α

Q How do we create states on which $\mathcal{H}$ and $\hat{S}^z$ are simultaneously diagonal?

A we need to diag. $\hat{S}^z$ on the blocks characterized by the same eigenvalue E_α.
Concretely for this problem one has

$$E_\alpha = -\frac{3}{4} \qquad \alpha = 1,2,3,4$$

$$E_{\alpha'} = \frac{3}{4} \qquad \alpha' = 5,6,7,8$$

Achtung these are not the single particle states even if they are enumerated with integers

After having performed this additional block diagonalization we create the simultaneous eigenstates of $\mathcal{H}$ and $\hat{S}^z_T$ $|E_\alpha, \alpha, M, \mu\rangle$:

$$\mathcal{H}\,|E_\alpha,\alpha;M,\mu\rangle = E_\alpha\,|E_\alpha,\alpha;M,\mu\rangle$$

$$\hat{S}^z_T\,|E_\alpha,\alpha;M,\mu\rangle = M\,|E_\alpha,\alpha;M,\mu\rangle$$

$\mathcal{H}$ and $\hat{S}^z$ are diagonal on this basis by constuction

T is, however, not completely diagonal yet: it mixes up states associated with $E = \frac{3}{4}$ & $M = \frac{1}{2}$

The corresponding matrix reads

$$A = \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \qquad \text{with} \quad a = -0.5$$

$$b = -0.86603\ldots$$

We diagonalize the matrix A. Note that we should not expect real eigenvalue because it's not symmetric (nor hermitean).

$$\begin{vmatrix} a-\lambda & b \\ -b & a-\lambda \end{vmatrix} = (a-\lambda)^2 + b^2 = 0$$

$$\Rightarrow a-\lambda = \pm\sqrt{-b^2} \Rightarrow \lambda_\pm = a \pm i b$$

one can further note that $a = \cos\left(\frac{2\pi}{3}\right)$

$b = \sin\left(\frac{2\pi}{3}\right)$

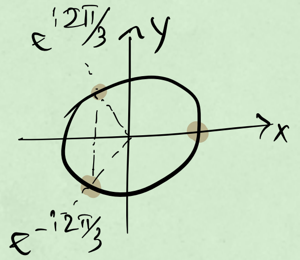
therefore $\lambda_\pm = \cos\left(\frac{2\pi}{3}\right) \pm i \sin\left(\frac{2\pi}{3}\right) = e^{i\,2\pi/3}$

This is to be expected because

$T^N = \mathbb{I}$ by definition so the eigenvalues of T can only be roots of the units

$\lambda = e^{ik}$ with $k = \frac{2\pi}{N} n$ with $n = 0, 1 \dots, N-1$

for $N=3$ the possible values on the $\mathbb{C}$ plane are



With this knowledge we should be able to identify univocally each basis state by defining the values of E, M, K

From the knowledge of the eigenvectors

$$\begin{pmatrix} a & b \\ -b & a \end{pmatrix}\begin{pmatrix} 1 \\ i \end{pmatrix} = \begin{pmatrix} a+ib \\ -b+ia \end{pmatrix} = (a+ib)\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$\begin{pmatrix} a & b \\ -b & a \end{pmatrix}\begin{pmatrix} 1 \\ -i \end{pmatrix} = \begin{pmatrix} a-ib \\ -b-ia \end{pmatrix} = (a-ib)\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

One could, in principle, build the set of eigenstates on which $\mathcal{H}$ $\hat{S}_T^2$ T are simultaneously diagonal e.g.

$$\left.\begin{array}{l} E = 3/4 \\ M = 1/2 \\ K = \frac{2\pi}{3} \end{array}\right\} \quad |E, M, K\rangle = \frac{|7\rangle + i|8\rangle}{\sqrt{2}}$$

where $|7\rangle$ and $|8\rangle$ refer to the last 2 eigenvectors of the basis set $|E_\alpha\, \alpha; M, \mu\rangle$

--- o --- o ---

Using similar arguments one can treat the ring with N=4 spins ½. In this case the energy eigenstates are those computed in the last assignment, possible values of $M = \pm 2, \pm 1, 0$ and those of $K = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}$.