Vorlesung 8

Sunday, 9. June 2019 13:42

3 Spin Qubits

3.0 Reminder

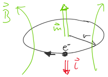
0.1 Spin magnetic moment: $\vec{S}$

- angular moment of a particle
- it's a internal property (like the mass)
- half-integer or integer of $\hbar$

Spin	type	particle
0	Boson	Higgs-Boson
$\frac{1}{2}\hbar$	Fermion	Electron, Neutrino, Quarks
$1\hbar$	Boson	Photon, Gluon, W-Boson, Z-Boson
$\frac{3}{2}\hbar$	Fermion	super symetric particles
$2\hbar$	Boson	Graviton

- since 1925, we have known that e^- has spin $1/2$

3.0.2 Angular magnetic moment $\vec{l}$



current $I = -\frac{e}{\tau} = -\frac{ev}{2\pi r}$

mag. moment $m = IA = -\frac{ev}{2\pi r}\pi r^2$

$= -\frac{evr}{2}$

angular moment

$$\vec{l} = m_e \vec{r} \times \vec{v}$$

quantum number l

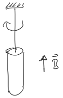
$l_z = m_l \hbar \qquad m_l = 0, \pm 1, \dots \pm l$

$$m_z = -m_l \frac{e\hbar}{2m_e} = -m_l \mu_B$$

$\uparrow$ Bohr Magneton

$\vec{m} = \gamma \vec{l} \qquad \gamma$: gyromagnetic ratio

3.0.3 Einstein-de Haas Effect



angular moment is conserved

$$\vec{J} = \vec{L} + \vec{S} = \text{const.}$$

3.0.4 Hund's rule

- an e^- in an atomic orbital can be described by 4 quantum numbers

1st rule: maximise the spin $\vec{S}$

2nd rule: maximise angular moment $\vec{L}$

3rd rule: total angular moment

$$J = |L \pm S|$$

"$-$" less than half-full orbital

"$+$" more than half-full orbital

Ex: Praseodynium (Pr) $3e^-$ in 4f shell $\sim l = 3$

1. HR: $3e^- \sim S = \frac{3}{2}$

2. HR: $\begin{array}{ccccccc} \uparrow & \uparrow & \uparrow & \_ & \_ & \_ & \_ \\ l_z = 3 & 2 & 1 & 0 & -1 & -2 & -3 \end{array}$

$$L = \sum_i l_i = 3 + 2 + 1 = 6$$

3. HR : $J = |L-S| = |6-\frac{3}{2}| = \frac{9}{2}$

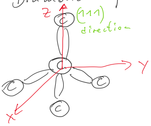
ex: Dy, Tb, Ho

3.1. Magnetic moments in solid state materials

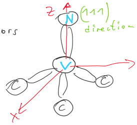
a) Ex: doped insolator: NV-center in diamond

nitrogen ↗ ↖ vacancy

Diamond: fcc with basis $(0,0,0)$, $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$

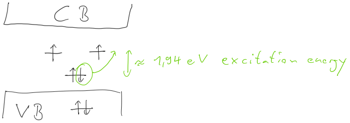


each C has 4 neighbors



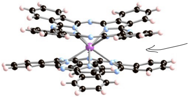
C_{3v} - symmetry

- neutral NV^0: 5 e^- not bounded
- neg. charged NV^-: 6 e^-



b) Ex: mag. molecules

$TbPc_2$ Pc: Phthalocyanine



Tb^{3+}-Ion with 8 e^- in 4f-shell

4f	↑↓	↑	↑	↑	↑	↑	↑
l_z	-3	-2	-1	0	1	2	3

1. Hund's rule: $S = 6 \cdot \frac{1}{2} = 3$
2. HR: $L = \sum_i l_i = 3$
3. HR: $J = L + S = 6$

for rare earth ions, Spin-Orbit interacθ is very strong

$E_{\text{spin-Orbit}} \approx 10\,000\,K$

number of states: $(2J+1) = 13$

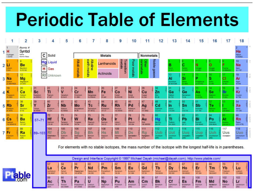
- states are degerate in vaccum
- non-degerate in solid state

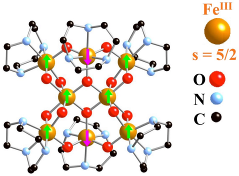
$E_{\text{ligand field}} \approx 1\,000\,K$

$E_{\text{exange}} \approx 10 - 100\,K$

$E_{\text{dipolar}} \approx 1K$

$E_{\text{nuclear spin}} \approx 1K$


Periodic Table of Elements



Fe$_8$: [Fe$_8$O$_2$(OH)$_{12}$tacn$_6$]$^{8+}$

$\Rightarrow S = 10$

3.2.1 Isotropic mag. Moment

$$\mathcal{H} = \underbrace{g\mu_B \vec{B}\vec{S}}_{\text{Zeeman energy}}$$

$\vec{S}$: stands for $\vec{J} = \vec{L} + \vec{S}$
details ignored
$\vec{s}$: single spin
$\vec{S}$: collective spin

$(2s+1)$ states : $|s,m\rangle$: $|s,-s\rangle, |s,-s+1\rangle, + \dots |s,s\rangle$
often only m : $|m\rangle$: $|-s\rangle, |-s+1\rangle \dots |s\rangle$

Spin operator: $\vec{S} = \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix}$

commutator: $[S_x, S_y] = i(\hbar)S_z$, and cyclic

eigenvalue eq. : $S_z|s,m\rangle = m(\hbar)|s,m\rangle$

$$\vec{S}^2|s,m\rangle = s(s+1)(\hbar^2)|s,m\rangle$$

$$S_\pm = S_x \pm i S_y$$

$$S_\pm|s,m\rangle = \sqrt{s(s+1) - m(m\pm1)}(\hbar)|s,m\pm1\rangle$$

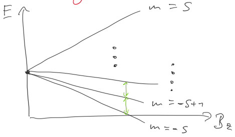
choice: $\vec{B} \parallel z \Rightarrow \mathcal{H} = g\mu_B B_z S_z$

Schrödinger eq. $\mathcal{H}|s,m\rangle = E|s,m\rangle$

$$\Rightarrow E_{m,n} = \langle s,m|\mathcal{H}|s,n\rangle$$

$$= g\mu_B B_z m\, \delta_{m,n} \sim \text{diagonal}$$

Zeeman-Diagram



Quantum bit ?
~ equidistand
~ analog to harmonic oscillator but (2s+1) states

3.2.2 Magnetic anisotropy (cristal field, ligand field)

a) easy axis

$$\mathcal{H} = -D s_z^2 + g\mu_B \vec{B}\vec{s} \quad , D > 0$$

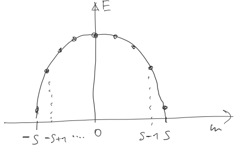
for $\vec{B} \parallel z$

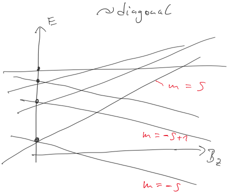
$$\mathcal{H} = -D s_z^2 + g\mu_B B_z s_z$$

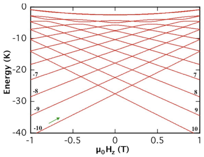
$$E_{m,n} = \langle S,m|\mathcal{H}|S,n\rangle = \left(-Dm^2 + g\mu_B B_z m\right)\delta_{m,n}$$

$\rightsquigarrow$ diagonal

- for $\vec{B} = 0$







Quantum bits ?

yes, non equidistant level

- for $\vec{B} \parallel x$

$$\mathcal{H} = -DS_z^2 + g\mu_B B_x S_x \qquad S_x = \frac{1}{2}\left(S_+ + S_-\right)$$

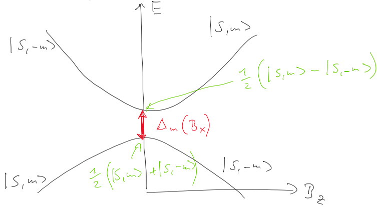
$$E_{m,n} = \langle S,m|\mathcal{H}|S,n\rangle = -Dm^2 + g\mu_B B_x \frac{1}{2}\left[\sqrt{+}\,\delta_{m,n+1} + \sqrt{-}\,\delta_{m,n-1}\right]$$

$\rightsquigarrow$ numerical diagonalization

pertupation theory, 2S-order :

$$\Delta_m(B_x) \approx \frac{2D\,(S+m)!}{[(2m-1)!]^2\,(S-m)!}\left(\frac{g\mu_B B_x}{2D}\right)^{2m}$$

$$\sim \frac{B_x^{2m}}{D^{2m-1}}$$



$\Rightarrow$ nice Qubit, tunable with B_x

b) with transverse anisotropy

$$\mathcal{H} = -DS_z^2 + E' S_x^2 \qquad \text{with } S^2 = S_x^2 + S_y^2 + S_z^2$$

$$\rightsquigarrow \mathcal{H} = -DS_z^2 + \underbrace{E\left(S_x^2 - S_y^2\right)}_{= E/2\,\left(S_+^2 + S_-^2\right)} \qquad D > E > 0$$

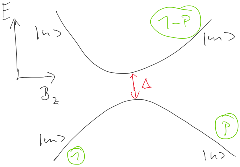
pertubation theory

$$\langle m | [S_\pm^2]^n | -m \rangle = 0 \quad \text{for half-integer spins}$$

⇒ Kramer's Theorem

$$\Delta_m \sim \left(\frac{E}{D}\right)^m \quad \text{for integer spins}$$

3.2.3 Landau-Zener method for finding Δ



- constant field sweep rate

$$\frac{dB}{dt} - \text{const.}$$

$$P = 1 - \exp\left[-c\,\frac{\Delta^2}{dB/dt}\right]$$

$$c = \frac{\pi}{2\hbar g \mu_B |m-n|}$$

- analogous to other qubit system
- e^--tunneling in energy bands

2.4 Dimer

$$\mathcal{H} = -J\,\vec{s}_1\vec{s}_2 \qquad \left.\begin{array}{l} |s_1, m_1\rangle \\ |s_2, m_2\rangle \end{array}\right\} |S, M\rangle$$

total spin $\vec{S} = \vec{s}_1 + \vec{s}_2$, $|s_1 - s_2| \leq S_n \leq s_1 + s_2$

S_n: multipletts

using $\vec{S}^2 = \vec{s}_1^{\,2} + 2\vec{s}_1\vec{s}_2 + \vec{s}_2$ because $\vec{S}, \vec{s}_1, \vec{s}_2$ commute

$$\Rightarrow \mathcal{H} = -\frac{1}{2}J\left(\vec{S}^2 - \vec{s}_1^{\,2} - \vec{s}_2^{\,2}\right)$$

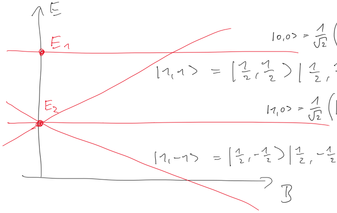
$$\Rightarrow \boxed{E_n = -\frac{J}{2}\left[S_n(S_n+1) - s_1(s_1+1) - s_2(s_2+1)\right]}$$

z.B. $s_1 = s_2 = \frac{1}{2} \curvearrowright S_1 = 0$, $S_2 = 1$ multipletts

$$E_1 = -\frac{J}{2}\left[0(0+1) - \frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}+1\right)\right] = +\frac{3}{4}J$$

$$E_2 = -\frac{J}{2}\left(1(1+1) - \frac{1}{2}\left(\frac{1}{2}+1\right) - \frac{1}{2}\left(\frac{1}{2}+1\right)\right] = -\frac{1}{4}J$$

- ferromag. coupling: $J > 0$



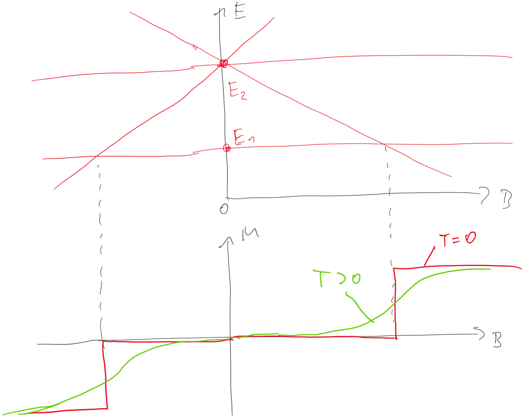
$|0,0\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{1}{2},\tfrac{1}{2}\rangle|\tfrac{1}{2},-\tfrac{1}{2}\rangle - |\tfrac{1}{2},-\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle\right)$

$|1,1\rangle = |\tfrac{1}{2},\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle$

$|1,0\rangle = \frac{1}{\sqrt{2}}\left(|\tfrac{1}{2},\tfrac{1}{2}\rangle|\tfrac{1}{2},-\tfrac{1}{2}\rangle + |\tfrac{1}{2},-\tfrac{1}{2}\rangle|\tfrac{1}{2},\tfrac{1}{2}\rangle\right)$

$|1,-1\rangle = |\tfrac{1}{2},-\tfrac{1}{2}\rangle|\tfrac{1}{2},-\tfrac{1}{2}\rangle$

- antiferromag coupling: $J < 0$



3.2.5 Hyperfine coupling

$$\mathcal{H} = -D S_z^2 + A \underbrace{\vec{S}\vec{I}}_{= \frac{1}{2}\left(\vec{F}^2 - \vec{S}^2 - \vec{I}^2\right)}$$

$$\vec{F} = \vec{S} + \vec{I}$$