Consider an Iron-56 (^{56}Fe) atom ($Z_{Fe} = 26$) in its ground state experiencing a weak external magnetic field B in the z direction. The interaction is given by:

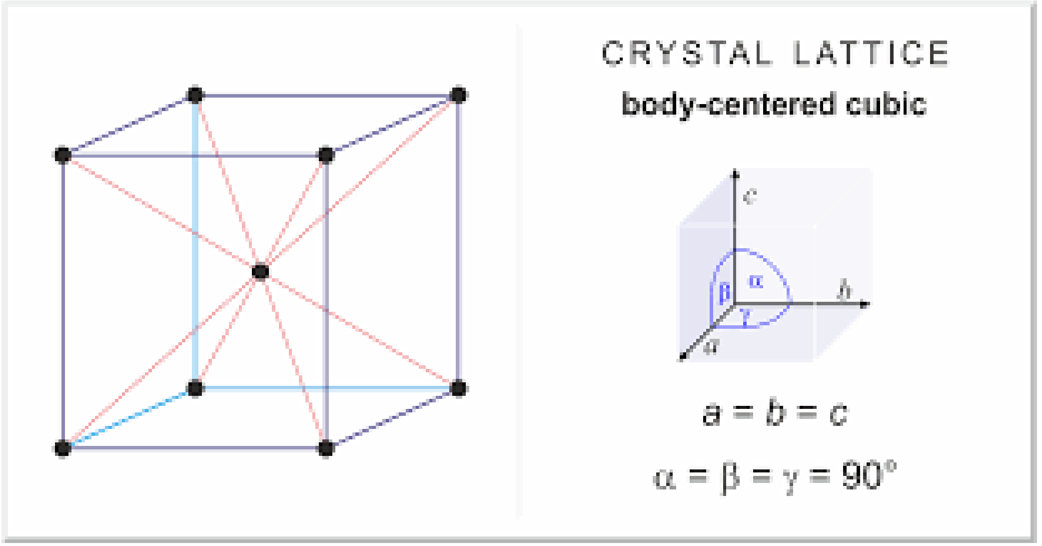
$$\mathbf{H} = -\frac{eB}{2mc}(L_z + 2S_z)$$

a. Find *J, L* and *S* of the ground state and write the atomic orbital $^{2S+1}L_J$ of the ground state.

b. Find the *z* component of the magnetic moment of an Iron atom for any M_J projection and calculate the Lande *g*-factor of Iron

c. An iron atom sits in a Body Centered Cubic BCC arrangement (see figure) with a lattice constant of a_0. Calculate the magnetic field felt by the center atom only considering nearest neighbor interactions assuming their magnetic moments are from an M=+4 and points entirely in the positive Z direction.

d. If a magnetic field with a strength B is pointed along the Z direction. Calculate the energy splitting of all 2J+1 projection states of the center atom by the applied field and its neighbors.

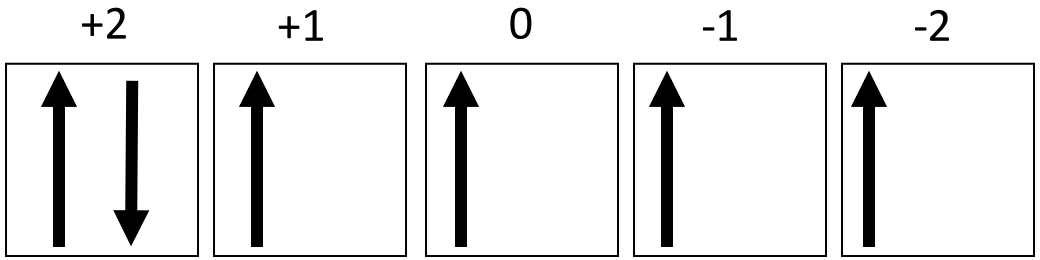


Useful Equation:

$$\vec{B}(\vec{r},\vec{m}) = \frac{1}{4\pi}\frac{3\hat{r}(\hat{r}\cdot\vec{m})-\vec{m}}{|\vec{r}|^3}$$

a. Find *J, L and S* of the ground state and write the Atomic orbital $^{2S+1}L_J$ of the ground state.

Fe(26) electronic configuration: [Ar] $4s^2 3d^6$



Hund's Rules For Atomic Ground State:

- Max S
- Max L
- If shell ≤ ½ full: Min J
- If shell > ½ full: Max J

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

$$L = \sum m_l = 2 \qquad S = \sum m_s = 2 \qquad J = L + S \implies {}^5\mathbf{D}_4$$

b. Find the z component of the magnetic moment of an Iron atom for any M_J projection and calculate the Lande g-factor

$$H = -m \cdot B$$

$$\mathbf{H} = -\frac{eB}{2mc}(L_z + 2S_z)$$

$$\hat{m}_z = \frac{e}{2mc}(L_z + 2S_z)$$

~~$|L, S, M_L, M_s\rangle$~~ → $|L, S, J, M_J\rangle$

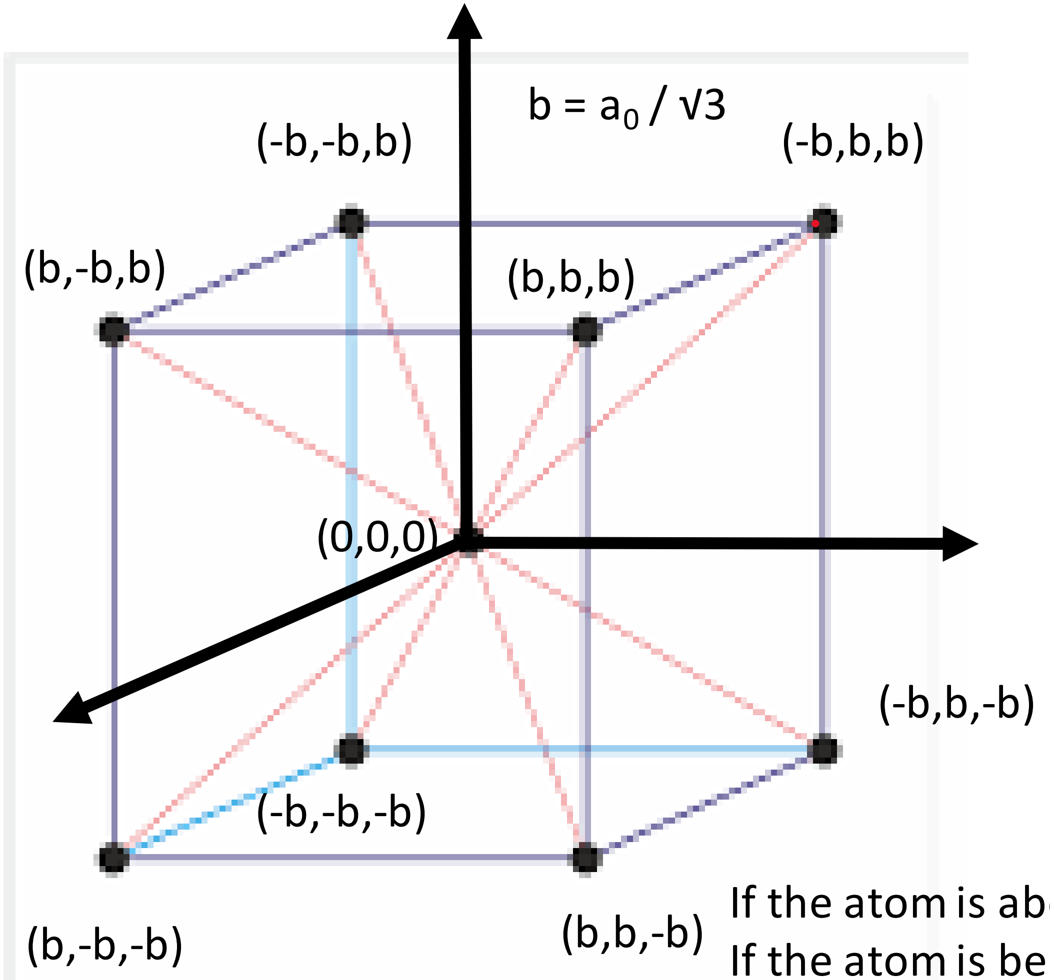
$$m_z = g\frac{e\hbar}{2mc}\vec{J} \cdot \hat{z} = M_J g\frac{e\hbar}{2mc}$$

We can express the magnetic dipole moment as J • z instead of (J + S) • z because of a trick using the wigner eckhart theorem which is shown the notes and results in the value of g shown below

$$g = 1 + \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)} = 1 + \frac{4(4+1)+2(2+1)-2(2+1)}{2*4*(4+1)} = \frac{3}{2}$$

Proof of this result is in lecture notes*

c. An iron atom sits in a Body Centered Cubic BCC arrangement (see figure) with a lattice constant of a_0. Calculate the magnetic field felt by the center atom only considering nearest neigh0or interactions assuming their magnetic moments are from M=+4 and point entirely in the positive z direction



$$\vec{B}(\vec{r},\vec{m}) = \frac{1}{4\pi}\frac{3\hat{r}(\hat{r}\cdot\vec{m})-\vec{m}}{|\vec{r}|^3}$$

If magnetic moment is entirely in +z $M_J = 4$

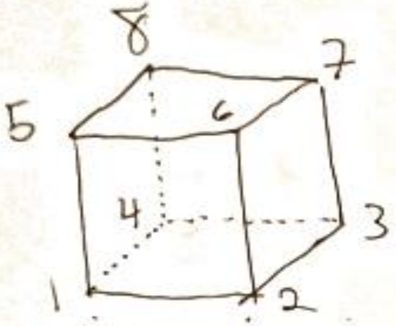
$$B_{tot}(r=0) = \sum_{i=1}^{8} \vec{B}(\vec{r}_i,\vec{m})$$

For all corners $|(\hat{r}\cdot\vec{m})|$ is the same with a value of 1/√3
But the sign of the final contribution will be different.

For each corner at a position (rx, ry, rz) the vector r when calculating the magnetic field will be (-rx,-ry,-rz). The dipole moment as stated in the problem is in the +z direction.

If the atom is above the center $(\hat{r}\cdot\vec{m})$ is negative since the z component of r is negative
If the atom is below the center $(\hat{r}\cdot\vec{m})$ is positive since the z component of r is negative.

$$m_i = |m|\hat{z} = m(0,0,1)$$



$\vec{r}_1 = \frac{a_0}{\sqrt{3}}(-1, 1, 1)$; $\hat{r}_1 \cdot \vec{m} = \frac{m}{\sqrt{3}}$

$\vec{r}_2 = \frac{a_0}{\sqrt{3}}(-1, -1, 1)$; $\hat{r}_2 \cdot \vec{m} = \frac{m}{\sqrt{3}}$

$\vec{r}_3 = \frac{a_0}{\sqrt{3}}(1, -1, 1)$; $\hat{r}_3 \cdot \vec{m} = \frac{m}{\sqrt{3}}$

$\vec{r}_4 = \frac{a_0}{\sqrt{3}}(1, 1, 1)$; $\hat{r}_4 \cdot \vec{m} = m/\sqrt{3}$

$\vec{r}_5 = \frac{a_0}{\sqrt{3}}(-1, 1, -1)$; $\hat{r}_5 \cdot \vec{m} = -m/\sqrt{3}$

$\vec{r}_6 = \frac{a_0}{\sqrt{3}}(-1, -1, -1)$; $\hat{r}_6 \cdot \vec{m} = -m/\sqrt{3}$

$\vec{r}_7 = \frac{a_0}{\sqrt{3}}(1, -1, -1)$; $\hat{r}_7 \cdot \vec{m} = -m/\sqrt{3}$

$\vec{r}_8 = \frac{a_0}{\sqrt{3}}(1, 1, -1)$; $\hat{r}_8 \cdot \vec{m} = -m/\sqrt{3}$

$\hat{r}_1(\hat{r}_1 \cdot \vec{m}) = m/3(-1, 1, 1)$

$\hat{r}_2(\hat{r}_2 \cdot \vec{m}) = m/3(-1, -1, 1)$

$\hat{r}_3(\hat{r}_3 \cdot \vec{m}) = m/3(1, -1, 1)$

$\hat{r}_4(\hat{r}_4 \cdot \vec{m}) = m/3(1, 1, 1)$

$\hat{r}_5(\hat{r}_5 \cdot \vec{m}) = m/3(1, -1, 1)$

$\hat{r}_6(\hat{r}_6 \cdot \vec{m}) = m/3(1, 1, 1)$

$\hat{r}_7(\hat{r}_7 \cdot \vec{m}) = m/3(-1, 1, 1)$

$\hat{r}_8(\hat{r}_8 \cdot \vec{m}) = m/3(-1, -1, 1)$

$$B_{tot} = \sum_i \frac{3 \cdot r_i(\hat{r}_i \cdot \hat{m}) - \vec{m}}{|\vec{r}|^3}$$

$$(\hat{r}_i(\hat{r}_i \cdot m) - \vec{m}) \cdot \hat{z} = 0$$

$$\sum_i r_i(\hat{r}_i \cdot \hat{m}) \cdot \hat{x} = 0$$

$$\sum_i \hat{r}_i(\hat{r}_i \cdot \hat{m}) \cdot \hat{y} = 0$$

$$B_{tot} = 0$$

Total field felt by neighbors is Zero. With all neighbors magnetically alligned the center atom feels no net magnetic field from them.

d. If a magnetic field with a strength B is pointed along the Z direction. Calculate the energy splitting of all 2J+1 projection states of the center atom by the applied field and its neighbors.

$$\Delta E = -m_z \left| B_z \right|$$

$$= -g \frac{e\hbar}{2mc} M_J |B_z|$$

$$M_J = (\text{-}4,\text{-}3,\text{-}2,\text{-}1,0,1,2,3,4)$$