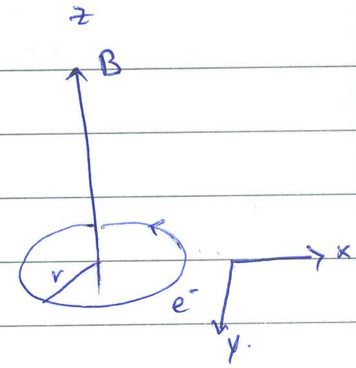
HW-3 Q.2



Consider an electron moving in an orbit of radius $\vec{r}$. At time t, the mag. field is turned on slowly from zero, the change in flux through the current loop induces an emf. Induced emf is given by

$$\mathcal{E} = \oint \bar{E}\cdot d\bar{l} = -d\varphi/dt$$

$$E\, 2\pi r = -d\varphi/dt$$

Torque on electron by induced E $= -eEr$

Also
$$\vec{\tau} = |d\bar{L}/dt| = -eEr = \frac{e}{2\pi}\, d\varphi/dt$$

$$= \frac{e r^2 \mu_0}{2}\, dH/dt$$

$$\varphi = BA$$
$$= \mu_0 H \pi r^2$$

Integrating w.r.t time from zero field, change in angular momentum

$$\Delta L = \frac{e r^2 \mu_0}{2} H.$$

magnetic moment

$$\mu = \frac{-e}{2m_e} L$$

change in ang. mom. changes magnetic moment by an amount

$$\Delta\mu = \frac{-e}{2m_e}\Delta L$$

$$\Delta \mu = -\frac{e^2 r^2 \mu_0 H}{4 m_e}.$$

For all the electrons in the solid,

$$\Delta \mu = -\frac{Z e^2 \mu_0 H}{4 m_e} \langle r^2_{avg} \rangle$$

~~Multiply with n no. of electrons.~~

$$\Delta \mu = \frac{-Z n e^2 \mu_0 H}{6 m_e} \langle r^2_{avg} \rangle$$

average value of the square of projection onto the field direction reduces ~~m~~ μ by a factor $2/3$.

$$\chi = M/H$$

$$\langle x^2 \rangle = \langle y^2 \rangle = 2/3 \langle r^2 \rangle$$

$$\boxed{\chi = -\frac{n \mu_0 Z e^2}{6 m_e} \langle r^2 \rangle_{avg}.}$$

$$x^2 + y^2 + z^2 = r^2$$

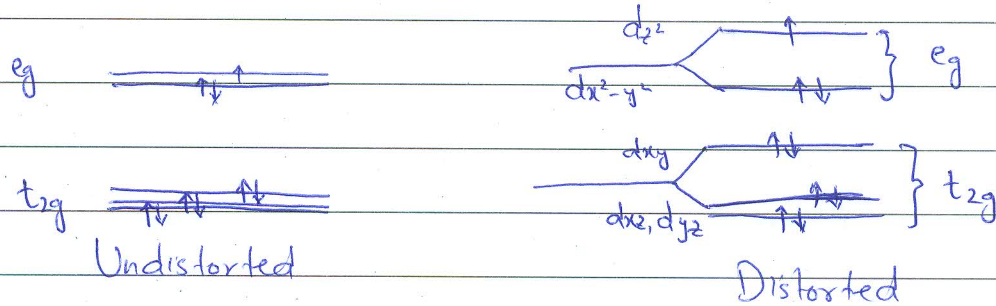
$$3\langle x^2 \rangle = \langle r^2 \rangle$$

$$\langle x^2 \rangle = 1/3 \langle r^2 \rangle$$

Q.4 HW3

Cu^{2+} in an octahedral environment

Cu^{2+} has configuration $3d^9$



An octahedral complex can distort, thus splitting the t_{2g} and e_g levels. The distortion lowers the energy because e_g levels are lowered in energy. saving in energy from lowering of d_{xz}, and d_{yz} levels is exactly balanced by the raising of d_{xy} level.

1.

$$n = \int_0^\infty f(E)\, g(E)\, dE$$

$$n = \int_0^\infty \frac{1}{e^{(E-\mu)\beta}+1} \times \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

When an external mag. field is applied, $E \longrightarrow E \pm \mu_0 B$

$$n_\uparrow = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{1}{e^{(E+\mu_0 B-\mu)\beta}+1} E^{1/2}\, dE \quad \text{——} \quad (1)$$

$$n_\uparrow = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{1}{e^{(E-\mu_0 B-\mu)\beta}+1} E^{1/2}\, dE. \quad \text{——} \quad (2).$$

(1) and (2) can be written as

$$n_\uparrow = 1/\lambda^3\, f_{3/2}(z)\, z e^{\mu_0 B/K_B T} \qquad \text{where } z = e^{+\mu/K_B T}$$

$$n_\downarrow = 1/\lambda^3\, f'_{3/2}(z)\, z e^{-\mu_0 B/K_B T} \qquad \lambda = \left(\frac{2\pi\hbar^2}{m K_B T}\right)^{1/2}$$

$$f_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{dx\, x^{n-1}}{z^{-1} e^{x}+1}$$

$$M = \mu_B (n_\uparrow - n_\downarrow) = \mu_B \frac{1}{\lambda^3} f_{3/2}(z) z \left[e^{\mu_B B / k_B T} - e^{-\mu_B B / k_B T} \right]$$

At high temperatures, and low mag. fields, $f_{3/2}(z) \approx z$

$$M = \frac{2 \mu_B z}{\lambda^3} \sinh\left(\mu_B B / k_B T \right).$$

For n-electrons

$$n = n_\uparrow + n_\downarrow = \frac{2z}{\lambda^3} \cosh\left(\mu_B B / k_B T \right)$$

Normalizing M

$$M \approx \frac{n \, 2\mu_B z / \lambda^3 \sinh\left(\mu_B B / k_B T \right)}{2z/\lambda^3 \cosh\left(\mu_B B / k_B T \right)}$$

$$M \approx n \mu_B \tanh\left(\mu_B B / k_B T \right)$$

At high temp, $\tanh(x) \approx x$

$$M = n \mu_B^2 B / k_B T$$

Susceptibility

$$\chi = \frac{\mu_0 M}{B}$$

$$\boxed{\chi \approx \frac{\mu_0 \mu_B^2 n}{k_B T}}$$

HW-3. Q.5

$$V = D\left(x^4 + y^4 + z^4 - \tfrac{3}{5} r^4\right)$$

In spherical co-ordinates

$$x = r\sin\theta\cos\varphi$$

$$y = r\sin\theta\sin\varphi$$

$$z = r\cos\theta.$$

converting V into spherical co-ordinates will give us

$$V = \frac{Dr^4}{8}\left[\sin^4\theta\left(e^{i4\varphi} + e^{-i4\varphi} + 6\right) + 8\cos^2\theta - 24/5\right]$$

$|2\rangle, |1\rangle, |0\rangle, |-1\rangle, |-2\rangle$ can be ~~read~~ read off from the spherical Harmonics table.

Matrix element

$$H = \begin{pmatrix} \langle 2|H|2\rangle & \langle 2|H|1\rangle & \langle 2|H|0\rangle & \langle 2|H|-1\rangle & \langle 2|H|-2\rangle \\ \langle 1|H|2\rangle & \langle 1|H|1\rangle & \langle 1|H|0\rangle & \langle 1|H|-1\rangle & \langle 1|H|-2\rangle \\ \langle 0|H|2\rangle & \langle 0|H|1\rangle & \langle 0|H|0\rangle & \langle 0|H|-1\rangle & \langle 0|H|-2\rangle \\ \langle -1|H|2\rangle & \langle -1|H|2\rangle & \langle -1|H|0\rangle & \langle -1|H|-1\rangle & \langle -1|H|-2\rangle \\ \langle -2|H|2\rangle & \langle -2|H|2\rangle & \langle -2|H|0\rangle & \langle -2|H|-1\rangle & \langle -2|H|-2\rangle \end{pmatrix}$$

All off-diagonal terms vanish except $V_{2,-2}$, $V_{-2,2}$. The evaluation of non-zero matrix elements are straightfoward but tedious. For example

$$V_{1,1} = \int_0^\infty r^6 R^2(r)\, dr \; D/8 \int_0^\pi \left(6\sin^2\theta + 8\cos^4\theta - 24/5\right) \times 4\sin^3\theta \cos^2\theta \, d\theta \times \int_0^{2\pi} d\varphi .$$

$$= -4A$$

This calculation can also be performed in mathematica.

[Mathematica file attached.]

$$H = \begin{pmatrix} \frac{5184\pi D a^4}{5} & 0 & 0 & 0 & 5184\pi D a^4 \\ 0 & \frac{-20736 D a^4 \pi}{5} & 0 & 0 & 0 \\ 0 & 0 & \frac{31104}{5}\pi D a^4 & 0 & 0 \\ \overset{0}{\cancel{5184\pi D a^4}} & 0 & 0 & \frac{-20736}{5}\pi D a^4 & 0 \\ 5184\pi D a^4 & 0 & 0 & 0 & \frac{5184}{5}\pi D a^4 \end{pmatrix}$$

Eigenvalues will be | Eigenvectors

Eigenvalues	Eigenvectors
$A + 5A\left(1 + \frac{4\mu_B^2 B^2}{25A^2}\right)^{1/2}$	$\frac{\|2\rangle + x_+\|-2\rangle}{(1+x_+^2)^{1/2}}$
$-4A + \mu_B B$	$\|1\rangle$
$6A$	$\|0\rangle$
$-4A - \mu_B B$	$\|-1\rangle$
$A - 5A\left(1 + \frac{4\mu_B^2 B^2}{25A^2}\right)^{1/2}$	$\frac{\|2\rangle + x_-\|-2\rangle}{(1+x_-^2)^{1/2}}$

where

$$x_\pm = \pm\left(1 + \left(\frac{2\mu_B B}{5A}\right)^2\right)^{1/2} - \frac{2\mu_B B}{5A}$$

so if $K_B T \ll A$, we can only populate the lowest states which are a triplet if $A > 0$ or a doublet if $A < 0$.

Then

$$Z = \begin{cases} 1 + e^{-\mu_B B/K_B T} + e^{\mu_B B/K_B T} & A > 0 \\ 1 + e^{-2\mu_B^2 B^2/5A K_B T} & A < 0. \end{cases}$$

For $A > 0$

$$Z = 1 + e^{-\mu_0 B / k_B T} + e^{+\mu_0 B / k_B T}$$

$$F = -N k_B T \ln Z$$

$$M = -\partial F / \partial B$$

we have already done this calculation in class and previous assignment, so

$$M = \frac{N \mu_B^2 B}{2 k_B T}$$

$$\boxed{\chi = \frac{N \mu_0 \mu_B^2}{2 k_B T}}$$ Curie's law.

Now for $A < 0$

$$Z = 1 + e^{-2\mu_B^2 B^2 / 5 A k_B T}$$

same recipe $M = -\partial F / \partial B$

$$= -\frac{N \mu_B^2 B}{5A}$$

$$\boxed{\chi = \frac{\mu_0 N \mu_B^2}{5A}}$$

HW-3 Q.3

(a)

$$\psi_{n\ell m}(r) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi)$$

$n=2,\quad \ell=1,\quad m_\ell = 1, 0, -1.$

$$\psi_{211} = R_{21}(r)\, Y_1^{1}(\theta,\varphi)$$

$$\psi_{210} = R_{21}(r)\, Y_1^{0}(\theta,\varphi)$$

$$\psi_{21-1} = R_{21}\, Y_1^{-1}(\theta,\varphi)$$

$$\psi_{p+} = R_{21}(r)\left[-\tfrac{1}{\sqrt{2}}\left(Y_1^{1}(\theta,\varphi) - Y_1^{-1}(\theta,\varphi)\right)\right]$$

$$\psi_{p-} = R_{21}(r)\left[\tfrac{i}{\sqrt{2}}\left(Y_1^{1}(\theta,\varphi) + Y_1^{-1}(\theta,\varphi)\right)\right]$$

(b)

$$\hat{L}_x = -i\hbar\left(y\,\partial/\partial z - z\,\partial/\partial y\right)$$

in spherical co-ordinates

$$\hat{L}_x = i\hbar\left(\sin\varphi\,\partial/\partial\theta + \cot\theta\cos\varphi\,\partial/\partial\varphi\right)$$

$$\Rightarrow \quad \psi_{px} = -\frac{R_{21}(r)}{\sqrt{2}}\left(Y_1^{1}(\theta,\varphi) + Y_1^{-1}(\theta,\varphi)\right)$$

$$\psi_{px} = \underbrace{-\frac{i}{2\sqrt{2}}\sqrt{\frac{1}{6a_0^3}}\left(r/a_0\right)e^{-r/2a_0}}_{\text{say } A(r)} \sin\theta \sin\varphi$$

$$\psi_{px} = -A(r)\sin\theta\sin\varphi$$

$$\hat{L}_x \psi_{px} = -A(r)\, i\hbar \left[\sin\varphi \frac{\partial}{\partial\theta}(\sin\theta) + \cot\theta\cos\varphi . \sin\theta \frac{\partial}{\partial\varphi}(\sin\varphi) \right]$$

$$= -A(r)\, i\hbar \left[\sin\varphi\cos\theta + \cot\theta\sin\theta \cancel{\sin}\cos^2\varphi \right]$$

$$\langle L_x \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_{px}^* \hat{L}_x \psi_{px}\, r^2 dr \sin\theta\, d\theta\, d\varphi$$

using Mathematica (see attached file).

$$\langle L_x \rangle = 0$$

Similarly, for ψ_{py}, ψ_{pz}

$$\langle L_x \rangle = 0$$

Orbital angular momentum is quenched. $J = S$.

(c)

$\hat{L}^2$ in spherical co-ordinates

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right]$$

$$\psi_{px} = \underbrace{\tfrac{i}{2}\sqrt{\tfrac{3}{\pi}}\, R_{21}}_{\text{say } A(r)} \sin\theta \sin\varphi .$$

$$\hat{L}^2|\psi_{px}\rangle = -\hbar^2 A(r) \left[\frac{1}{\sin\theta} \sin\varphi \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\sin\theta\right) + \frac{1}{\sin^2\theta} . \sin\theta \times \frac{\partial^2}{\partial\varphi^2} \sin\varphi \right]$$

This simplifies as

$$= -\hbar^2 A(r) \frac{\sin\varphi}{\sin\theta} (\cos 2\theta - 1)$$

$$\hat{L}^2|\psi_{px}\rangle = -\frac{i}{2}\sqrt{\tfrac{3}{\pi}}\, R_{21}\, \hbar^2 \frac{\sin\varphi}{\sin\theta} (\cos 2\theta - 1)$$

ψ =

$$\langle \hat{L}^2 \rangle = \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi_{px}^* \hat{L}_x \psi_{px}\, r^2 \sin\theta\, dr\, d\theta\, d\varphi$$

$$\boxed{\langle \hat{L}^2 \rangle = 2\hbar^2}$$

(d)

linear combination of wavefns are no longer the eigenfunctions of angular momentum operators L_x, L_y, L_z. so each component of ang. momentum averages to zero.