① $H = J\sum_{\langle ij\rangle} \vec{S}_i\cdot\vec{S}_j$

a) $J<0$ (Feromagnet)

$$\langle\vec{S}\rangle = -S\,B_S(\beta g\mu_B S\vec{B}_{eF})\,;\quad \vec{B}_{eF} = \frac{Jz}{g\mu_B}\langle\vec{S}\rangle\,;\quad z=6$$

$$\langle\vec{S}\rangle = -S\,B_S\left(\beta J z S\langle\vec{S}\rangle\right)$$

$$\langle\vec{S}\rangle = -S\,\frac{S+1}{3S}\beta J z S\langle\vec{S}\rangle + \dots = \frac{S(S+1)|J|z}{3k_BT}\langle\vec{S}\rangle + \dots$$

$$T_c = \frac{2S(S+1)|J|}{k_B}$$

1/2⁻

b) $H_{MFA} = J\sum_i \vec{S}_i\cdot\langle\vec{S}_j\rangle - J\sum_{\langle ij\rangle}\langle\vec{S}_i\rangle\langle\vec{S}_j\rangle$

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$$E_{MFA} = \langle H_{MFA}\rangle = J\sum_{\langle ij\rangle}\langle\vec{S}_i\rangle\cdot\langle\vec{S}_j\rangle = J\frac{Nz}{2}S^2\cos 120^\circ = -\frac{3}{2}JS^2\times N$$

c) $\vec{B}_A^{ef} = \frac{J}{g\mu_B}\left(3\langle\vec{S}_B\rangle + 3\langle\vec{S}_C\rangle\right) = -\frac{3J}{g\mu_B}\langle\vec{S}_A\rangle$ v smeri magnetizacije na podmreži A

$\langle\vec{S}_B\rangle + \langle\vec{S}_C\rangle = -\langle\vec{S}_A\rangle$

++

$$\vec{B}_B^{ef} = -\frac{3J}{g\mu_B}\langle\vec{S}_B\rangle$$

$$\vec{B}_C^{ef} = -\frac{3J}{g\mu_B}\langle\vec{S}_C\rangle$$

d) $\langle\vec{S}_A\rangle = -S\,B_S\left(\beta g\mu_B S\vec{B}_A^{ef}\right) = +S\,B_S\left(\beta\cdot 3JS\langle\vec{S}_A\rangle\right)$

$$\langle\vec{S}_A\rangle = \frac{S(S+1)}{3k_BT}3J\langle\vec{S}_A\rangle + \dots \Rightarrow T_c = \frac{S(S+1)J}{k_B}$$

enačbi za $\langle\vec{S}_B\rangle$ in $\langle\vec{S}_C\rangle$ sta enaki!

++

① e) $H = J\sum_{\langle ij\rangle} \vec{S_i}\cdot\vec{S_j} + g\mu_B \sum_i \vec{S_i}\cdot\vec{B_0}$

$$E_{MFA} = J\sum_{\langle ij\rangle} \langle\vec{S_i}\rangle\cdot\langle\vec{S_j}\rangle + g\mu_B \sum_i \langle\vec{S_i}\rangle\cdot\vec{B_0} =$$

$$= \frac{1}{2}J\left[\frac{N}{3}\langle\vec{S_A}\rangle\cdot\left(3\langle\vec{S_B}\rangle+3\langle\vec{S_C}\rangle\right) + \frac{N}{3}\langle\vec{S_B}\rangle\cdot\left(3\langle\vec{S_A}\rangle+3\langle\vec{S_C}\rangle\right) + \frac{N}{3}\langle\vec{S_C}\rangle\cdot\left(3\langle\vec{S_A}\rangle+3\langle\vec{S_B}\rangle\right)\right] + g\mu_B\frac{N}{3}\left(\langle\vec{S_A}\rangle+\langle\vec{S_B}\rangle+\langle\vec{S_C}\rangle\right)\cdot\vec{B_0} =$$

$$= \frac{JNS^2}{6}\left[3\cos\alpha+3\cos\alpha+3\cos\alpha+3\cos2\alpha+3\cos\alpha+3\cos2\alpha\right] + g\mu_B\frac{N}{3}SB_0\left(1+\cos\alpha+\cos\alpha\right) =$$

$$= JNS^2\left(2\cos\alpha+\cos2\alpha\right) + \frac{1}{3}g\mu_B B_0 SN\left(1+2\cos\alpha\right)$$

$$\frac{dE_{MFA}}{d\alpha} = 0 = J\cancel{N}S^{\cancel{2}}\left(-\cancel{2}\sin\alpha - \sin2\alpha\cdot\cancel{2}\right) + \frac{2}{3}g\mu_B B_0 \cancel{S}\cancel{N}\left(-\sin\alpha\right)$$

$$-JS\sin2\alpha = \left(JS+\frac{1}{3}g\mu_B B_0\right)\sin\alpha$$

$$-2JS\sin\alpha\cos\alpha = \left(JS+\frac{1}{3}g\mu_B B_0\right)\sin\alpha$$

↳ • $\sin\alpha = 0 \Rightarrow \alpha = 0$ ali π

• $-2JS\cos\alpha_0 = JS + \frac{1}{3}g\mu_B B_0$

$$\underline{\underline{\cos\alpha_0 = -\frac{1}{2} - \frac{1}{6}\frac{g\mu_B B_0}{JS}}} \Rightarrow B_0 \leq \frac{3JS}{g\mu_B} \equiv B_0^{max}$$

$E_{MFA}(\alpha=0) = N\left(3JS^2 + g\mu_B B_0 S\right)$: feromagnetna ureditev

$E_{MFA}(\alpha=\pi) = N\left(-JS^2 - \frac{1}{3}g\mu_B B_0 S\right)$

$E_{MFA}(\alpha_0) = N\left(-\frac{3}{2}JS^2 - \frac{1}{18}\frac{(g\mu_B B_0)^2}{J}\right)$

↳ to je osnovno stanje za $B_0 < B_0^{max}$

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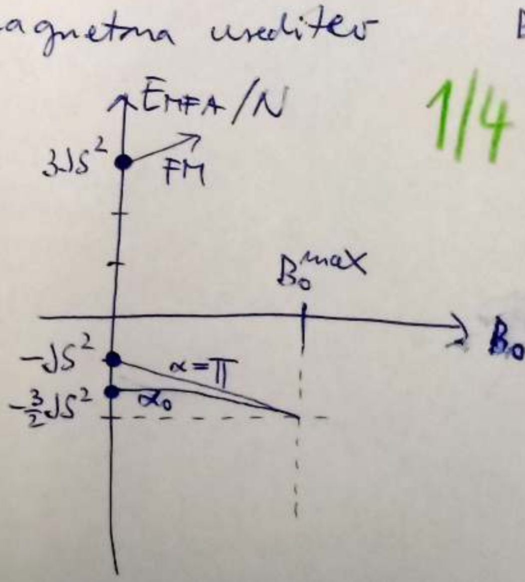
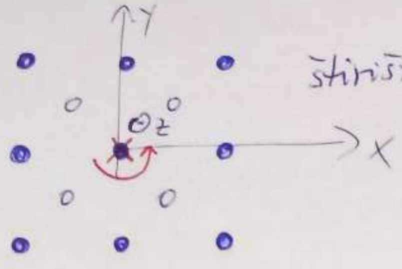
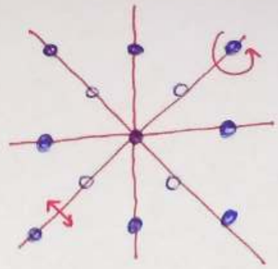


(2) a)



štirištevna os (z)



dvoštevne osi, zrcalne ravnine (⊥ na ravnino lista)

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inverzija ($\vec{r} \to -\vec{r}$), zrcaljenje preko ravnine xy ($z \to -z$), ...

b) $d_{xy}(\vec{r}) = xy\,f(r)$

$d_{xz}(\vec{r}) = xz\,F(r)$

$d_{yz}(\vec{r}) = yz\,F(r)$

$d_{x^2-y^2}(\vec{r}) = \frac{x^2-y^2}{2}F(r)$

$d_{z^2}(\vec{r}) = \frac{2z^2-x^2-y^2}{2\sqrt{3}}F(r)$

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$$\langle xy|\overset{y\to -y}{\varphi(\vec{r})}|xz\rangle = \langle xy|\overset{x\to -x}{\varphi(\vec{r})}|yz\rangle =$$
$$= \langle xy|\overset{x\to -x}{\varphi(\vec{r})}|x^2-y^2\rangle = \langle xy|\overset{x\to -x}{\varphi(\vec{r})}|z^2\rangle =$$
$$= \langle xz|\overset{x\to -x}{\varphi(\vec{r})}|yz\rangle = \langle xz|\overset{x\to -x}{\varphi(\vec{r})}|x^2-y^2\rangle =$$
$$= \langle xz|\overset{x\to -x}{\varphi(\vec{r})}|z^2\rangle = \langle yz|\overset{y\to -y}{\varphi(\vec{r})}|x^2-y^2\rangle =$$
$$= \langle yz|\overset{y\to -y}{\varphi(\vec{r})}|z^2\rangle = \langle x^2-y^2|\overset{x\to y,\, y\to -x}{\varphi(\vec{r})}|z^2\rangle = 0$$

z rdečo so navedene simetrijske operacije zaradi katerih je matrični element enak ∅

$$\langle xz|\varphi(\vec{r})|xz\rangle \overset{x\to y,\, y\to -x}{=} \langle yz|\varphi(\vec{r})|yz\rangle$$

$|xz\rangle$ in $|yz\rangle$ ostaneta degenerirani

$$\langle xy|\varphi(\vec{r})|xy\rangle = \int x^2y^2F^2(r)\varphi(\vec{r})d\vec{r} \equiv I_1 \qquad I_3 \equiv \int x^4F^2(r)\varphi(\vec{r})d\vec{r}$$
$$\langle xz|\varphi(\vec{r})|xz\rangle = \int x^2z^2F^2(r)\varphi(\vec{r})d\vec{r} \equiv I_2 \qquad I_4 \equiv \int z^4F^2(r)\varphi(\vec{r})d\vec{r}$$
$$\langle yz|\varphi(\vec{r})|yz\rangle = \int y^2z^2F^2(r)\varphi(\vec{r})d\vec{r} \overset{x\to y,\, y\to -x}{=} I_2$$
$$\langle x^2-y^2|\varphi(\vec{r})|x^2-y^2\rangle = \int \frac{(x^4-2x^2y^2+y^4)}{4}F^2(r)\varphi(\vec{r})d\vec{r} = \frac{1}{2}I_3 - \frac{1}{2}I_1$$
$$\langle z^2|\varphi(\vec{r})|z^2\rangle = \int \frac{1}{12}(2z^2-x^2-y^2)^2F^2(r)\varphi(\vec{r})d\vec{r} =$$
$$= \int\left(\frac{1}{3}z^4 + \frac{1}{12}x^4 + \frac{1}{12}y^4 - \frac{4}{12}z^2x^2 - \frac{4}{12}z^2y^2 + \frac{2}{12}x^2y^2\right)F^2(r)\varphi(\vec{r})d\vec{r} =$$
$$\overset{x\to y,\, y\to -x}{=} \frac{1}{3}I_4 + \frac{1}{6}I_3 - \frac{2}{3}I_2 + \frac{1}{6}I_1$$

Integrali I_1, I_2, I_3 in I_4 so neodvisni, zato v splošnem ostaneta degenerirani samo orbitali $|xz\rangle$ in $|yz\rangle$.