Equations (7.4) are simply too difficult to be solved for a large number of unknowns => one has to use symmetry arguments to reduce them.

e.g. Homogeneous system:

$$\langle \hat a^+_{\vec k} \hat a_{\vec k'} \rangle = \frac{1}{V}\int d\vec r \int d\vec r'\, e^{i\vec k\cdot\vec r - i\vec k'\cdot\vec r'} \langle \hat\psi^+(\vec r)\hat\psi(\vec r')\rangle \quad = \quad \text{homogeneity}$$

$$= \frac{1}{V}\int d\vec r \int d\vec r'\, e^{i\vec k\cdot\vec r - i\vec k'\cdot\vec r'} f(\vec r - \vec r') =$$

$\vec R = \frac{\vec r + \vec r'}{2}$ $\quad \vec r = \vec R + \frac{\vec\rho}{2}$

$\vec\rho = \vec r - \vec r'$ $\quad \vec r' = \vec R - \frac{\vec\rho}{2}$

$$= \frac{1}{V}\int d\vec R \int d\vec\rho\; e^{i\vec R(\vec k - \vec k')}\, e^{i\frac{\vec\rho}{2}(\vec k + \vec k')} f(\vec\rho)$$

$$= \delta_{\vec k,\vec k'} \tilde f(\vec k) = \delta_{\vec k,\vec k'} \langle \hat a^+_{\vec k}\hat a_{\vec k}\rangle$$

7.2 Hartree-Fock approximation

The mean-field theory must be slightly modified if we consider iolike particles:

$$\hat a^+_\nu \hat a^+_\mu \hat a_{\mu'} a_{\nu'} \overset{MF}{\approx} \hat a^+_\nu \hat a_{\nu'}\langle \hat a^+_\mu \hat a_{\mu'}\rangle + \hat a_\mu \hat a_{\mu'}\langle \hat a^+_\nu \hat a_{\nu'}\rangle + \quad \Big\}\ \text{Hartree or direct term}$$

$$\pm\Big(\hat a^+_\nu \hat a_{\mu'}\langle \hat a^+_\mu \hat a_{\nu'}\rangle + \hat a^+_\mu \hat a_{\nu'}\langle \hat a^+_\nu \hat a_{\mu'}\rangle + \quad \Big\}\ \text{Fock or exchange term}$$

$$-\langle \hat a^+_\nu \hat a_{\nu'}\rangle\langle \hat a^+_\mu \hat a_{\mu'}\rangle \mp \langle \hat a^+_\nu \hat a_{\mu'}\rangle\langle a^+_\mu \hat a_{\nu'}\rangle \quad \Big\}\ \text{compensating term.} \qquad (7.6)$$

the first sign is valid for bosons, the second for fermions.

From (7.6) it follows that:

$$\langle \hat a^+_\nu \hat a^+_\mu \hat a_{\mu'} \hat a_{\nu'}\rangle_{MF} = \langle \hat a^+_\nu \hat a_{\nu'}\rangle_{MF}\langle \hat a^+_\mu \hat a_{\mu'}\rangle_{MF} \pm \langle \hat a^+_\nu \hat a_{\mu'}\rangle_{MF}\langle \hat a^+_\mu \hat a_{\nu'}\rangle_{MF} \qquad (7.7)$$

Equation (7.7) is exact for non interacting Hamiltonians (Wick's theorem) and, as such it should hold also for the mean field Hamiltonian, which thus must have the form given in (7.6).

Example: Coulomb interaction $\quad \hat V_{ee} \approx \hat V_{MF} = \hat V_{Hartree} + \hat V_{Fock}$

$$\langle \hat V_{Hartree}\rangle = \frac{1}{2}\sum_{\sigma\sigma'}\int d\vec r\int d\vec r'\, \langle \hat\psi^+_\sigma(\vec r)\hat\psi_\sigma(\vec r)\rangle\, v_{ee}(\vec r - \vec r')\langle \hat\psi^+_{\sigma'}(\vec r')\hat\psi_{\sigma'}(\vec r')\rangle \qquad (7.7)$$

$$\langle \hat V_{Fock} \rangle = -\frac{1}{2}\sum_{\sigma\sigma'} \int d\vec r \int d\vec r\,' \langle \hat\psi^+_\sigma(\vec r)\,\hat\psi_{\sigma'}(\vec r\,')\rangle\, v_{ee}(\vec r-\vec r\,')\,\langle \hat\psi^+_{\sigma'}(\vec r\,')\hat\psi_\sigma(\vec r)\rangle \tag{7.8}$$

If we now specialize the Hartree-Fock approximation to the jellium model:

$$\hat V^{\,jellium}_{ee,\,HF} = \frac{1}{2V}\sum_{\vec q\neq 0}\sum_{\substack{\vec k\vec k'\\ \sigma\sigma'}} \tilde v_{ee}(\vec q)\Big[\langle a^+_{\vec k+\vec q,\sigma} a_{\vec k\sigma}\rangle a^+_{\vec k'-\vec q\sigma'} a_{\vec k'\sigma'} + a^+_{\vec k+\vec q\sigma} a_{\vec k\sigma}\langle a^+_{\vec k'-\vec q\sigma'} a_{\vec k'\sigma'}\rangle\Big]$$

$$-\frac{1}{2V}\sum_{\vec q\neq 0}\sum_{\substack{\vec k\vec k'\\ \sigma\sigma'}}{}' \tilde v_{ee}(\vec q)\Big[\langle a^+_{\vec k+\vec q\sigma} a_{\vec k'\sigma'}\rangle a^+_{\vec k'-\vec q\sigma'} a_{\vec k\sigma} + a^+_{\vec k+\vec q\sigma} a_{\vec k'\sigma'}\langle a^+_{\vec k'-\vec q\sigma'} a_{\vec k\sigma}\rangle\Big]$$

$$-\frac{1}{2V}\sum_{\vec q\neq 0}\sum_{\substack{\vec k\vec k'\\ \sigma\sigma'}} \tilde v_{ee}(\vec q)\Big[\langle a^+_{\vec k+\vec q,\sigma} a_{\vec k\sigma}\rangle\langle a^+_{\vec k'-\vec q\sigma'} a_{\vec k'\sigma'}\rangle - \langle a^+_{\vec k+\vec q\sigma} a_{\vec k'\sigma'}\rangle\langle a^+_{\vec k'-\vec q\sigma'} a_{\vec k\sigma}\rangle\Big] \tag{7.8b}$$

Translational invariance + spin independence of the averages

$$\begin{cases} \langle a^+_{\vec k\sigma} a_{\vec k'\sigma'}\rangle = \delta_{\vec k\vec k'}\delta_{\sigma\sigma'}\,\bar n_{\vec k\sigma} \\ \bar n_{\vec k\uparrow} = \bar n_{\vec k\downarrow} = \bar n_{\vec k} \end{cases}$$

together with the isotropy of the Coul. interaction $v_{ee}(\vec r) = v(r) \Rightarrow \tilde v_{ee}(\vec q) = \tilde v_{ee}(q)$ yield

$$\begin{cases} \hat T_{el} + \hat V^{\,jellium}_{ee,\,HF} = \sum_{\vec k\sigma}\big(\varepsilon_{\vec k} + v_{HF}(k)\big)\, a^+_{\vec k\sigma} a_{\vec k\sigma} + \text{const} \\ v_{HF}(k) = -\frac{1}{V}\sum_{\vec q\neq\vec k}{}' \tilde v_{ee}(|\vec q-\vec k|)\,\bar n_{\vec q} \end{cases} \tag{7.9}$$

proof:

In (7.8b) the Hartree term disappears since it requires $\vec q = 0$, excluded due to the background. The exchange term reads:

$$-\frac{1}{2V}\sum_{\vec q\neq 0}\sum_{\vec k\sigma}\Big(\bar n_{\vec k+\vec q}\, a^+_{\vec k\sigma} a_{\vec k\sigma} + a^+_{\vec k+\vec q\sigma} a_{\vec k+\vec q\sigma}\,\bar n_{\vec k} - \bar n_{\vec k+\vec q}\,\bar n_{\vec k}\Big)\tilde v_{ee}(\vec q) =$$

$$= -\frac{1}{2V}\sum_{\vec q\neq 0}\sum_{\vec k\sigma}\left[a^+_{\vec k\sigma}a_{\vec k\sigma}\left(\bar n_{\vec k+\vec q}+\bar n_{\vec k-\vec q}\right)-\bar n_{\vec k+\vec q}\bar n_{\vec k}\right]\tilde v_{ee}(|\vec q|)\,.$$

$$= -\frac{1}{2V}\sum_{\vec q\neq 0}\sum_{\vec k\sigma}\Big[a^+_{\vec k\sigma}a_{\vec k\sigma}\,\bar n_{\vec k+\vec q}\underbrace{\left(\tilde v_{ee}(\vec q)+\tilde v_{ee}(-\vec q)\right)}_{2\tilde v_{ee}(q)}-\bar n_{\vec k+\vec q}\bar n_{\vec k}\,\tilde v_{ee}(q)\Big]$$

$$\overset{\vec k+\vec q\to\vec q}{=} -\frac{1}{V}\sum_{\vec k\sigma}\left(a^+_{\vec k\sigma}a_{\vec k\sigma}-\frac{1}{2}\bar n_{\vec k}\right)\left[\sum_{\vec q\neq\vec k}\tilde v_{ee}(|\vec q-\vec k|)\,\bar n_{\vec q}\right].$$

The last equation above reproduces (7.9) apart from the trivial kinetic term.

We want now to calculate the Hartree-Fock potential $\tilde v_{HF}(k)$. To this purpose we can start assuming $\bar n_{\vec q}=\Theta(k_F-|\vec q|)$ which is the correct result as far as the dispersion is isotropic and monotonous.

$$v_{HF}(k) = -\frac{1}{V}\sum_{\vec q\neq\vec k}\tilde v_{ee}(\vec q-\vec k)\,\bar n_{\vec q}\simeq -\frac{1}{\cancel{V}}\frac{\cancel{V}}{(2\pi)^3}\,2\pi\int_0^{k_F}dq\,q^2\,\frac{\cancel{4\pi}e^2}{\cancel{4\pi}\varepsilon_0}\int_{-1}^{1}d(\cos\theta_q)\,\frac{1}{k^2+q^2-2qk\cos\theta_q}$$

$$= -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\pi}\int_0^{k_F}dq\,q^2\,\frac{1}{k^2+q^2}\int_{-1}^{1}d(\cos\theta_q)\,\frac{1}{1-\frac{2qk}{k^2+q^2}\cos\theta_q}=$$

$$= -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\pi}\int_0^{k_F}dq\,\frac{q^{\cancel{2}}\,\cancel{k^2+q^2}}{2\cancel{q}k\,\cancel{(k^2+q^2)}}\ln\left|\frac{1+\frac{2qk}{k^2+q^2}}{1-\frac{2qk}{k^2+q^2}}\right| = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\pi}\int_0^{k_F}dq\,\frac{q}{k}\ln\left|\frac{k+q}{k-q}\right|$$

$$= -\frac{e^2}{4\pi\varepsilon_0}\frac{k_F}{\pi}\left(1+\frac{k_F^2-k^2}{2k_Fk}\ln\left|\frac{k+k_F}{k-k_F}\right|\right)\qquad(7.8)$$

Where the last equality has been obtained by applying the standard integral

$$\int x\ln(a+bx)\,dx = \frac{1}{2}\left(x^2-\frac{a^2}{b^2}\right)\ln(a+bx)-\frac{1}{2}\left(\frac{x^2}{2}-\frac{ax}{b}\right)$$

proof of (7.8)

$$\int_0^{k_F} dq \; \frac{q}{k} \ln \left| \frac{k+q}{k-q} \right| = k \int_0^{k_F/k} dx \; x \ln \left| \frac{1+x}{1-x} \right|$$

. $k < k_F$

$$= k \left[\int_0^{1^-} dx \; x \ln \left(\frac{1+x}{1-x} \right) + \int_{1^+}^{k_F/k} dx \; x \ln \frac{1+x}{-1+x} \right] =$$

$$= k \left\{ \left[\frac{1}{2} (x^2 - 1) \ln (1+x) - \frac{1}{2} \left(\frac{x^2}{2} - x \right) \right] \Big|_0^{1^-} - \left[\frac{1}{2} (x^2 - 1) \ln (1-x) - \frac{1}{2} \left(\frac{x^2}{2} + x \right) \right]_0^{1^-} \right.$$

$$\left. \left[\frac{1}{2} (x^2 - 1) \ln (1+x) - \frac{1}{2} \left(\frac{x^2}{2} - x \right) \right]_{1^+}^{k_F/k} - \left[\frac{1}{2} (x^2 - 1) \ln |-1+x| - \frac{1}{2} \left(\frac{x^2}{2} + x \right) \right]_{1^+}^{k_F/k} \right.$$

$$k \left\{ \cancel{\frac{1}{4}} + \cancel{\frac{3}{4}} + \frac{1}{2} \left(\frac{k_F^2}{k^2} - 1 \right) \ln \left(1 + \frac{k_F}{k} \right) - \frac{1}{2} \left(\cancel{\frac{k_F^2}{2k^2}} - \frac{k_F}{k} \right) - \cancel{\frac{1}{4}} \right.$$

$$\left. - \frac{1}{2} \left(\frac{k_F^2}{k^2} - 1 \right) \ln \left(-1 + \frac{k_F}{k} \right) + \frac{1}{2} \left(\cancel{\frac{k_F^2}{2k^2}} + \frac{k_F}{k} \right) - \cancel{\frac{3}{4}} \right\} =$$

$$= k \left\{ \frac{k_F}{k} + \frac{1}{2} \left(\frac{k_F^2}{k^2} - 1 \right) \ln \frac{1 + \frac{k_F}{k}}{-1 + \frac{k_F}{k}} \right\} = k_F \left(1 + \frac{k_F^2 - k^2}{2 k k_F} \ln \left(\frac{k_F + k}{k_F - k} \right) \right)$$

. $k > k_F$

$$k \left\{ \left[\frac{1}{2} (x^2 - 1) \ln (1+x) - \frac{1}{2} \left(\frac{x^2}{2} - x \right) \right]_0^{k_F/k} - \left[\frac{1}{2} (x^2 - 1) \ln (1-x) - \frac{1}{2} \left(\frac{x^2}{2} + x \right) \right]_0^{k_F/k} \right\} =$$

$$= k \left\{ \frac{1}{2} \left(\frac{k_F^2}{k^2} - 1 \right) \ln \left(1 + \frac{k_F}{k} \right) - \frac{1}{2} \left(\cancel{\frac{k_F^2}{k^2}} - \frac{k_F}{k} \right) - \frac{1}{2} \left(\frac{k_F^2}{k^2} - 1 \right) \ln \left(1 - \frac{k_F}{k} \right) + \frac{1}{2} \left(\cancel{\frac{k_F^2}{k^2}} + \frac{k_F}{k} \right) \right\}$$

$$= k \left\{ \frac{k_F}{k} + \frac{1}{2} \frac{k_F^2 - k^2}{k^2} \ln \left(\frac{k + k_F}{k - k_F} \right) \right\} = k_F \left(1 + \frac{k_F^2 - k^2}{2 k k_F} \ln \left(\frac{k + k_F}{k - k_F} \right) \right)$$

The 2 cases can be put together into

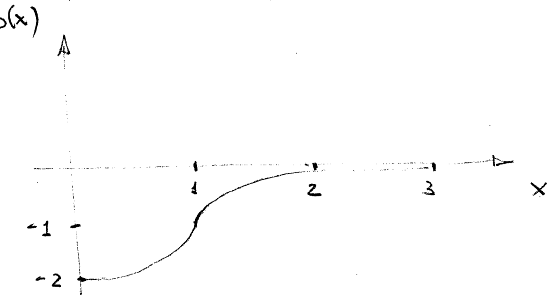
$$k_F \left(1 + \frac{k_F^2 - k^2}{2 k k_F} \ln \left| \frac{k + k_F}{k - k_F} \right| \right)$$

The Hartree-Fock spectrum thus reads:

$$\varepsilon^{HF}_{\vec{k}\sigma} = \frac{\hbar^2 k^2}{2m} - \frac{e^2}{4\pi\varepsilon_0}\frac{k_F}{\pi}\left(1 + \frac{k_F^2 - k^2}{2k_F k}\ln\left|\frac{k+k_F}{k-k_F}\right|\right)$$

The dispersion relation of the effective single particle model is clearly isotropic. Moreover the correction to the free particle can be written as:

$$\begin{cases} v_{HF}(k) = \dfrac{e^2}{4\pi\varepsilon_0}\dfrac{k_F}{\pi} S(k/k_F) \\[2ex] S(x) = -1 - \dfrac{1-x^2}{2x}\ln\left|\dfrac{x+1}{x-1}\right| \end{cases}$$



$$\frac{\partial S}{\partial x} = -\frac{1}{2}\frac{-2x^2-(1-x^2)}{x^2}\ln\left|\frac{x+1}{x-1}\right| - \frac{1-x^2}{2x}\left|\frac{x-1}{x+1}\right| \begin{cases} \dfrac{(\cancel{x}-1)-(\cancel{x}+1)}{(x-1)^2} & x \geq 1 \\[2ex] \dfrac{1-\cancel{x}+(\cancel{x}+1)}{(1-x)^2} & x < 1 \end{cases}$$

$$= \frac{x^2+1}{2x^2}\ln\left|\frac{x+1}{x-1}\right| \mp \frac{\cancel{x-1}}{\cancel{2}x}\,|\cancel{x-1}|\,\frac{\cancel{2}}{\cancel{(x-1)^2}} =$$

$$= \frac{1}{2x}\left(\frac{1+x^2}{x}\ln\left|\frac{x+1}{x-1}\right| - 2\right) \geq 0 \quad \Leftrightarrow \quad \ln\left|\frac{x+1}{x-1}\right| \geq \frac{2x}{1+x^2} \quad \checkmark$$

Since $S(x)$ is monotonously increasing, the initial Ansatz is correct. Notice though that the Fermi energy must be adjusted

$$\varepsilon_F^{HF} = \frac{\hbar^2 k_F^2}{2m} + \frac{e^2}{4\pi\varepsilon_0}\frac{k_F}{\pi}S(1) = \frac{\hbar^2 k_F^2}{2m} - \frac{e^2}{4\pi\varepsilon_0}\frac{k_F}{\pi} \qquad (7.9)$$

The ground state contribution per particle in HF is given by

$$\varepsilon_{G,HF} = \frac{1}{N_{el}}\sum_{\vec{k}\sigma} v_{HF}(\vec{k})\,\bar{n}_{\vec{k}} = \frac{1}{N_{el}}\sum_{\substack{\vec{k}\sigma \\ \vec{q}\neq\vec{k}}}\left(-\frac{1}{V}\right)\tilde{v}_{ee}(\vec{q}-\vec{k})\,\bar{n}_{\vec{q}}\left(\bar{n}_{\vec{k}} - \frac{1}{2}\bar{n}_{\vec{k}}\right)$$ the counterterm

$$= -\frac{1}{2VN_{el}}\sum_{\vec{q}\neq 0}\sum_{\vec{k}\sigma}\tilde{v}_{ee}(\vec{q})\,\theta(k_F - |\vec{k}+\vec{q}|)\,\theta(k_F - |\vec{k}|)$$

same result of the 1st order perturbation theory!

The long wavelength expansion of the Hartree-Fock dispersion reads:

$$\frac{\hbar^2 k^2}{2m} + \frac{e^2}{4\pi\varepsilon_0}\frac{k_F}{\pi}\left[S(0) + \frac{1}{2}S''(0)\frac{k^2}{k_F^2}\right] = -\frac{e^2}{2\pi\varepsilon_0}\frac{k_F}{\pi} + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m} + \frac{2}{3k_F^2\hbar^2}\frac{e^2}{4\pi\varepsilon_0}\right)$$

<u>proof</u>:

$$S(x) \overset{x\to 0}{=} -1 - \frac{1-x^2}{2x}\left(x - \cancel{\frac{x^2}{2}} + \frac{x^3}{3} - \left(-x - \cancel{\frac{x^2}{2}} - \frac{x^3}{3}\right)\right)$$

$$= -2 - \frac{1}{3}x^2 + x^2 = -2 + \frac{2}{3}x^2 + o(x^2)$$

The Hartree-Fock approximation can thus interpreted, at very low momenta within an effective mass

$$\frac{1}{m^*} = \frac{1}{m}\left(1 + \frac{1}{3\pi}\frac{2m}{\hbar^2 k_F^2}\cdot\frac{e^2}{4\pi\varepsilon_0}k_F\right) = \frac{1}{m}\left(1 + \alpha r_s\right) \qquad (7.10)$$

The low r_s limit reproduces the free particle theory. For high r_s the theory breaks down, since the interaction becomes strong. The most problematic feature of the Hartree-Fock approximation, though, is that it predicts a vanishing density of states at the Fermi energy.

$$\rho(\varepsilon) = \frac{1}{V}\sum_{\vec{k}\sigma}\delta(\varepsilon - \underbrace{\varepsilon_{\vec{k}} - V_{HF}(k)}_{-\varepsilon_{TOT}(k)}) = \frac{1}{\pi^2}\int_0^\infty dk\, k^2\,\delta(\varepsilon - \varepsilon_{\vec{k}} - V_{HF}(k)) = \frac{1}{\pi^2}k^2(\varepsilon)\left|\frac{\partial \varepsilon_{TOT}}{\partial k}\right|^{-1} \qquad (7.11)$$

The Hartree-Fock (mean-field) approach gives a good estimate of the ground state properties. It is though a bad approx for the excitation energies of the system. Many-body corrections to the HF model lead to <u>SCREENING</u> of the Coulomb interaction and thus to a regularization of the theory.

7.3 Mean-field treatment of the Heisenberg model

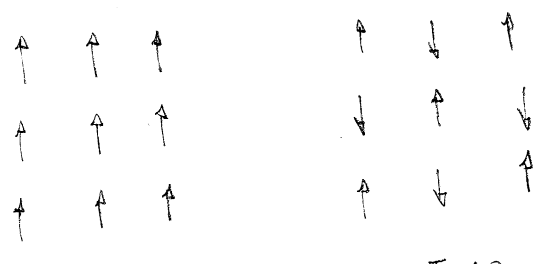
The Heisenberg model is a nice example of effective Hamiltonian emerging as low energy approximation of the Coulomb interaction.

$$\hat{H} = -2 \sum_{\alpha\beta} J_{\alpha\beta} \hat{\vec{S}}_\alpha \cdot \hat{\vec{S}}_\beta \tag{7.12}$$

where $\hat{S}_\alpha$ is the spin operator for an ion of site α on the lattice and $J_{\alpha\beta}$ is the strength of the interaction between the magnetic moments at sites α and β. The interaction (due to screening) it is usually short range and, in first approximation we can restrict to the nearest neighbours:

$$J_{\alpha\beta} = \begin{cases} J_0 & \text{if } \alpha \text{ and } \beta \text{ are neighbours} \\ 0 & \text{otherwise} \end{cases}$$

If $J_0 > 0$ we expect a parallel orientation of the spins on the lattice to minimize the free energy (ferromagnetic state) while for $J_0 < 0$, at least for a square lattice, we expect the antiparallel configuration to be favourable (antiferromagnetism)



$J_0 > 0$ $\qquad$ $J_0 < 0$

The spin operators in (7.12) refer to DISTINGUISHABLE particles since the lattice site cannot be interchanged (at low energies). Thus, the mean field version of (7.12) reads:

$$\hat{H}_{MF} = -2 \sum_{\alpha\beta} \langle \hat{\vec{S}}_\alpha \rangle \cdot \hat{\vec{S}}_\beta + \langle \hat{\vec{S}}_\beta \rangle \cdot \hat{\vec{S}}_\alpha - \langle \hat{\vec{S}}_\alpha \rangle \cdot \langle \hat{\vec{S}}_\beta \rangle . \tag{7.13}$$

Now comes the (non-trivial) assumption over the mean values:

$$\langle \hat{\vec{S}}_\alpha \rangle = \langle S_z \rangle \vec{e}_z \qquad (7.14)$$

i.e. we assume the ensemble average to be UNIFORM and directed in a preferential direction $\vec{e}_z$. If we introduce the uniform magnetization $\vec{m} = g\mu_B \langle S_z \rangle \vec{e}_z$ where g is the giromagnetic factor associated to the ion and $\mu_B = \frac{q\hbar}{2m_q}$ is the corresponding Bohr magneton,

$$\hat{H}_{MF} = -2J_0 n \langle S_z \rangle \sum_\alpha \left(\hat{S}_{z,\alpha} - \frac{1}{2}\langle S_z \rangle \right) =$$

$$= -\frac{2J_0 n}{g\mu_B}\, \vec{m} \cdot \sum_\alpha \left(\hat{\vec{S}}_\alpha - \frac{1}{2g\mu_B}\vec{m} \right)$$

$$= -\frac{2J_0 n}{g^2\mu_B^2}\, m \sum_\alpha g\mu_B \hat{S}_{z,\alpha} + \frac{J_0 n N}{g^2\mu_B^2} m^2 \qquad (7.15)$$

where n is the number of nearest neighbours in the lattice.
An external magnetic field in the z direction adds a Zeemann term

$$\hat{H}^B_{MF} = -\Big(\underbrace{\frac{2J_0 n}{g^2\mu_B^2} m}_{} + B_{ext} \Big) \sum_\alpha g\mu_B \hat{S}_{z,\alpha} + \frac{J_0 n N}{g^2\mu_B^2} m^2 \qquad (7.16)$$

"internal" magnetic field associated to the magnetization $\vec{m}$.

In order to access the statistical properties of the system we calculate first the partition function for $\hat{H}^B_{MF}$. If we assume $S_z = \pm\frac{1}{2}$ and $g=2$

$$Z_{MF} = \mathrm{Tr}\left\{ e^{-\beta \hat{H}^B_{MF}} \right\} = e^{-\beta \frac{J_0 n m^2 N}{g^2\mu_B^2}} \mathrm{Tr}\left\{ \exp\left[\beta \left(\frac{2J_0 n}{g^2\mu_B^2} m + B_{ext} \right) \sum_\alpha g\mu_B \hat{S}_{z,\alpha} \right] \right\}$$

$$= e^{-\beta \frac{J_0 n m^2 N}{4\mu_B^2}} \left(e^{-\beta B(m)\mu_B} + e^{\beta B(m)\mu_B} \right)^N \qquad (7.17)$$

where $B(m) = \frac{J_0 n}{2\mu_B^2} m + B_{ext}$. The exponent N indicate that we are in presence of N non interacting identical particles.

The free energy for the system reads

$$F = -\frac{1}{\beta}\ln Z_{MF} = \frac{J_0 n N}{4\mu_B^2} m^2 - \frac{N}{\beta}\ln\left(e^{-\beta B(m)\mu_B} + e^{\beta B(m)\mu_B}\right)$$

The minimization condition needed to calculate the mean field parameter m reads:

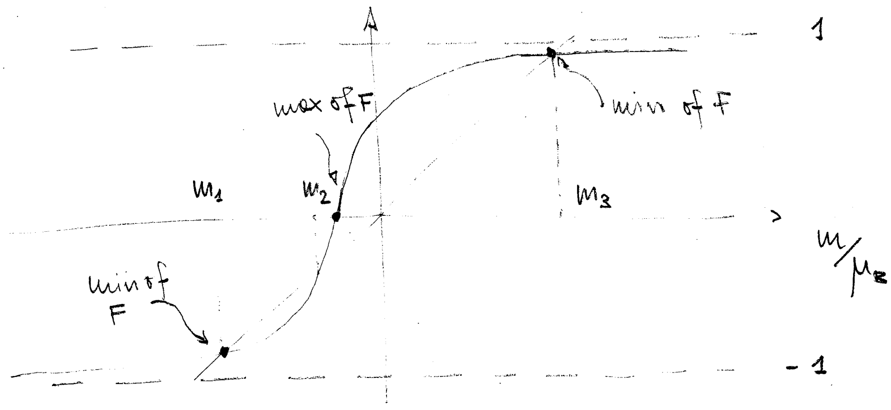
$$0 = \frac{\partial F}{\partial m} = \frac{J_0 n N}{2\mu_B^2} m - \frac{N}{\cancel{\beta}} \frac{e^{\beta B(m)\mu_B} - e^{-\beta B(m)\mu_B}}{e^{-\beta B(m)\mu_B}+e^{\beta B(m)\mu_B}} \frac{dB(m)}{dm}\cancel{\beta}\mu_B$$

$$= \frac{J_0 n N}{2\mu_B^2}\left(m - \mu_B \tanh\left(\beta B(m)\mu_B\right)\right)$$

In other terms:

$$\frac{m}{\mu_B} = \tanh\left(\frac{J_0 n}{2k_BT}\frac{m}{\mu_B} + \frac{\mu_B B_{ext}}{k_B T}\right) \qquad (7.18)$$

The condition (7.18) is satisfied either once or 3 times since $F \to \infty$ both for $m \to -\infty$ and $m \to +\infty$ the single solution is a minimum. In the case of 3 solutions $m_1 < m_2 < m_3$ $F(m_1)$ and $F(m_3)$ are minima and $F(m_2)$ is a maximum of the free energy. Moreover, if $B_{ext} = 0$ $m_1 = -m_3$ and $m_2 = 0$. Moreover $|m_i| < \mu_B \Rightarrow$ all solutions are physical



$$\frac{m}{\mu_B} = -\frac{2\mu_B B_{ext}}{n J_0}$$ is the crossing point

If we consider at first $B_{ext}=0$, the ferromagnetic solutions correspond to $|m|=\mu_B$. It is reached only for $\frac{J_0 h}{2k_BT}\to\infty$ i.e. $k_BT \ll hJ_0$. Antiferromagnetic ordering cannot be captured by the proposed mean field.

The critical temperature at which some degree of magnetization appears is given when the slope of the tanh in the origin is larger than 1.

$$\frac{J_0 h}{2k_BT} > 1 \quad \Rightarrow \quad k_BT < \frac{hJ_0}{2} \quad \Rightarrow \quad T_c = \frac{hJ_0}{2k_B} \tag{7.19}$$

It is also interesting to test how the equilibrium magnetization varies with the external magnetic field and obtain the magnetic susceptibility

$$\chi(B_{ext},T) = \left(\frac{\partial \bar{m}}{\partial B_{ext}}\right)_T \quad \text{where } \bar{m} \text{ is the "stable" solution}$$

of the equation (7.18) or, in its inverse form:

$$\tanh^{-1}\left(\frac{m}{\mu_B}\right) = \frac{T_c}{T}\frac{m}{\mu_B} + \frac{\mu_B B_{ext}}{k_BT} \tag{7.20}$$

The magnetic susceptibility has a different form for $T<T_c$ or $T>T_c$ as it should be since the system is undergoing a phase transition from paramagnetic to ferromagnetic. In particular:

$$\chi \approx 1\ \frac{\mu_B^2}{k}\ \frac{1}{T-T_c} \qquad \text{for } T \gtrsim T_c \tag{7.21a}$$

$$\chi \approx \frac{\mu_B^2}{2k}\ \frac{1}{T_c-T} \qquad \text{for } T \lesssim T_c \tag{7.21b}$$

which indicates that, close to the transition temperature, a small variation of the magnetic field causes a large variation of the magnetization.

proof of (7.21).

Let us differentiate (7.20) on both sides with respect of B_{ext}

$$\frac{1}{\mu_B}\left(\frac{\partial \bar{m}}{\partial B_{ext}}\right)\frac{1}{1-\left(\frac{m}{\mu_B}\right)^2} = \frac{T_c}{T\mu_B}\frac{\partial \bar{m}}{\partial B_{ext}} + \frac{\mu_B}{k_B T} \qquad \left(\frac{\partial f^{-1}(x)}{\partial x} = \frac{1}{f'(f^{-1}(x))}\right)$$

By isolating $\frac{\partial \bar{m}}{\partial B_{ext}}$

$$\frac{\partial \bar{m}}{\partial B_{ext}}\left[\frac{1}{1-\left(\frac{m}{\mu_B}\right)^2} - \frac{T_c}{T}\right] = \frac{\mu_B^2}{k_B T} \Rightarrow \frac{\partial \bar{m}}{\partial B_{ext}} = \frac{\mu_B^2}{k_B T}\frac{1-\left(\frac{m}{\mu_B}\right)^2}{1-\frac{T_c}{T}\left(1-\left(\frac{m}{\mu_B}\right)^2\right)} \quad (7.2$$

if $T \gtrsim T_c \Rightarrow \frac{m}{\mu_B} \ll 1 \Rightarrow \chi \approx \frac{\mu_B^2}{k}\frac{1}{T-T_c}$

For $T \lesssim T_c$ we can find a close expression for $\frac{m}{\mu_B}$ by using the expansion $\tanh x \simeq x - \frac{x^3}{3}$ $(B_{ext}=0)$.

$$\frac{m}{\mu_B} = \frac{T_c}{T}\frac{m}{\mu_B} - \frac{1}{3}\left(\frac{T_c}{T}\frac{m}{\mu_B}\right)^3 \Leftrightarrow 1 = \frac{T_c}{T}\left(1-\frac{1}{3}\left(\frac{T_c}{T}\right)^2\left(\frac{m}{\mu_B}\right)^2\right)$$

and, in other terms $\frac{m}{\mu_B} = \left[3\left(\frac{T}{T_c}\right)^3\left(\frac{T_c}{T}-1\right)\right]^{1/2} \cong \left[3\left(1-\frac{T}{T_c}\right)\right]^{1/2}$. (7.22b)

By substituting in (7.22) we obtain:

$$\chi(T,B) \cong \frac{\mu_B^2}{k}\frac{1-3\frac{T_c-T}{T_c}}{T-T_c\left(1-3\frac{T_c-T}{T_c}\right)} \cong \frac{\mu_B^2}{2k}\frac{1}{T_c-T}$$

Analogously one can also calculate the specific heat associated to the model

$$E = \langle H \rangle_{MF} = -\frac{2nNJ_0 m^2}{g^2\mu_B^2} = -\frac{1}{2}N k_B T_c\left(\frac{m}{\mu_B}\right)^2 \quad (7.23)$$

The specific heat is the variation of the Energy per volume ($\tilde{=}$ per ion) with respect to the temperature:

$$C(T) = \frac{1}{N}\frac{\partial E}{\partial T} \tag{7.24}$$

The combination of (7.23) and (7.24) yields:

$$C(T) = -k_B T_c \left(\frac{m}{\mu_B}\right)\frac{\partial}{\partial T}\left(\frac{m}{\mu_B}\right)$$

where m is the minimum solution of the self-consistency equation (7.18). If we differentiate (7.20) with respect to the temperature

$$\frac{1}{1-\left(\frac{m}{\mu_B}\right)^2}\frac{\partial}{\partial T}\left(\frac{m}{\mu_B}\right) = -\frac{T_c}{T^2}\frac{m}{\mu_B} + \frac{T_c}{T}\frac{\partial}{\partial T}\left(\frac{m}{\mu_B}\right)$$

$$\Rightarrow \frac{\partial}{\partial T}\left(\frac{m}{\mu_B}\right) = \left[\frac{T_c}{T} - \frac{1}{1-\left(\frac{m}{\mu_B}\right)^2}\right]^{-1}\frac{T_c}{T^2}\frac{m}{\mu_B}$$ and eventually for the specific heat

$$C(T) = -k_B\frac{T_c^2}{T^2}\left(\frac{m}{\mu_B}\right)^2\left[\frac{T_c}{T} - \frac{1}{1-\left(\frac{m}{\mu_B}\right)^2}\right]^{-1} \tag{7.25}$$

The asymptotic behaviour $T \to T_c^-$ can thus be obtained by inserting (7.22b)

$$C(T) \tilde{=} -k_B\frac{T_c^2}{T^2}\,3\left(1-\frac{T}{T_c}\right)\left[\frac{T_c}{T} - \frac{1}{1-3\left(1-\frac{T}{T_c}\right)}\right]^{-1} \tilde{=} \frac{3}{2}k \quad \text{for } T \to T_c^-$$

On the other side for $T \to T_c^+$ $\quad m = 0 \quad \to \quad \frac{\partial E}{\partial T} = 0.$