Variational Mean Field

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Variational Mean Field

In the mean field approximation we assume the density matrix for our system breaks down into single particle density matrices:

$$\rho = \prod_{\alpha} \rho_{\alpha}$$

Then we employ the Bogoliubov inequality which states:

$$F \leq F_{\rho} := \mathrm{Tr}\{H\rho\} + \mathrm{T}\,\mathrm{Tr}\{\rho \ln(\rho)\}$$

This has the nice property of not requiring too much initial intuition about our system such as Landau MFT requires.

Model Hamiltonian

For our model Hamiltonian $H_{ij} = S_i \cdot A_{ij} \cdot S_j$ we get:

$$F_\rho = -\frac{1}{2}\sum_{i,j} \vec{m}_i \cdot \underline{\underline{A}}_{ij} \cdot \vec{m}_j - \sum_i \vec{h}_i \cdot \underline{\underline{g}}_i \cdot \vec{m}_i$$

$$+\mathrm{T}\sum_i \int \mathrm{d}\Omega_i \rho_i(\Omega_i) \ln\Big(\rho_i(\Omega_i)\Big) - \sum_i \lambda_i \left(\int \mathrm{d}\Omega_i \rho_i(\Omega_i) - 1\right)$$

where

$$\vec{m}_i := \mathrm{Tr}\Big\{\vec{S}_i \rho_i\Big\} = \int \mathrm{d}\Omega_i \vec{S}_i(\Omega_i)\rho_i(\Omega_i)$$

Minimization

After functional minimization with respect to each ρ_i and λ_i:

$$\vec{m}_i = \frac{1}{Z_i} \int \mathrm{d}\Omega_i \exp\left\{\beta \vec{\mathcal{H}}_i \cdot \vec{S}_i(\Omega_i)\right\} \vec{S}_i(\Omega_i)$$

where

$$\vec{\mathcal{H}}_i = \vec{h}_i \cdot \underline{\underline{g}}_i + \sum_{j \neq i} \vec{m}_j \cdot \underline{\underline{A}}_{ji}$$

$$Z_i = \int \mathrm{d}\Omega_i \exp\left\{\beta \vec{\mathcal{H}} \cdot \vec{S}_i(\Omega_i)\right\}$$

Analytic Integration

It turns out we can integrate Z_i analytically giving us:

$$Z_i = \sinh\left(\beta \left\| \vec{\mathcal{H}}_i \right\|\right)$$

From this we can actually setup the above self consistent equations

$$\vec{m}_i = \frac{1}{\beta} \frac{\partial \ln Z_i}{\partial \vec{\mathcal{H}}_i} = \hat{\mathcal{H}}_i \left[\coth\left(\beta \left\| \vec{\mathcal{H}}_i \right\|\right) - \frac{1}{\beta \left\| \vec{\mathcal{H}}_i \right\|} \right]$$

High Temperature Limit

Since our goal is to calculate magnetic susceptibility in the high temperature limit we can assume $\beta \left\| \vec{\mathcal{H}}_i \right\| \ll 1$.

$$\vec{m}_i = \hat{\mathcal{H}}_i \left[\frac{1}{\beta \left\| \vec{\mathcal{H}}_i \right\|} + \frac{\beta \left\| \vec{\mathcal{H}}_i \right\|}{3} + \mathcal{O}(\beta^2) - \frac{1}{\beta \left\| \vec{\mathcal{H}}_i \right\|} \right]$$

$$\approx \frac{\beta \vec{\mathcal{H}}_i}{3} = \frac{\beta}{3} \left[\vec{h} \cdot \underline{\underline{g}}_i + \sum_{j \neq i} \vec{m}_j \cdot \underline{\underline{A}}_{ji} \right]$$

Notice we got a set of coupled linear equations!

Local Susceptibility

The susceptibility is found by differentiating with respect to external field h and and taking the limit $h \to 0$.

$$\underline{\underline{\chi}}_i := \left.\frac{\partial \vec{m}_i}{\partial \vec{h}}\right|_{h=0} = \frac{\beta}{3}\left[\underline{\underline{g}}_i + \sum_{j \neq i} \underline{\underline{A}}_{ij} \cdot \underline{\underline{\chi}}_j\right]$$

where

$$\underline{\underline{\chi}}_i = \begin{bmatrix} \frac{\partial m_i^x}{\partial h^x} & \frac{\partial m_i^x}{\partial h^y} & \frac{\partial m_i^x}{\partial h^z} \\ \frac{\partial m_i^y}{\partial h^x} & \frac{\partial m_i^y}{\partial h^y} & \frac{\partial m_i^y}{\partial h^z} \\ \frac{\partial m_i^z}{\partial h^x} & \frac{\partial m_i^z}{\partial h^y} & \frac{\partial m_i^z}{\partial h^z} \end{bmatrix}$$

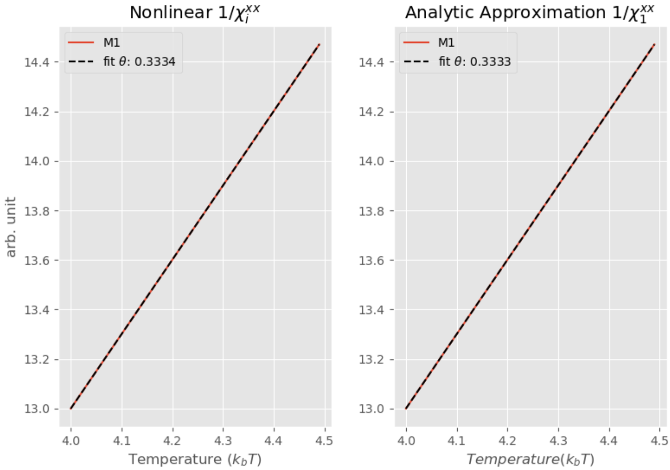
A Solution for Susceptibility

We need to solve the following set of matrix equations

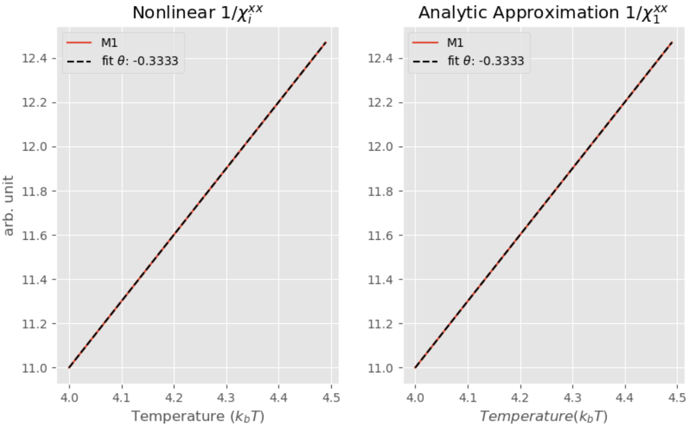
$$\underline{\underline{g}}_i = \frac{3}{\beta}\underline{\underline{\chi}}_i + \sum_{j \neq i} \underline{\underline{\chi}}_j \cdot \underline{\underline{A}}_{ji}$$

An infinite set of linear equations. Typically one makes some simplifying assumptions. If we think the system is ferromagnetic we assume uniform magnetization and local susceptibility.

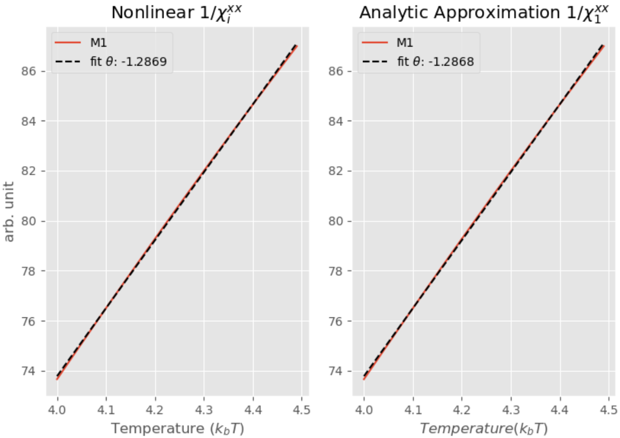
Two Site Isotropic FM



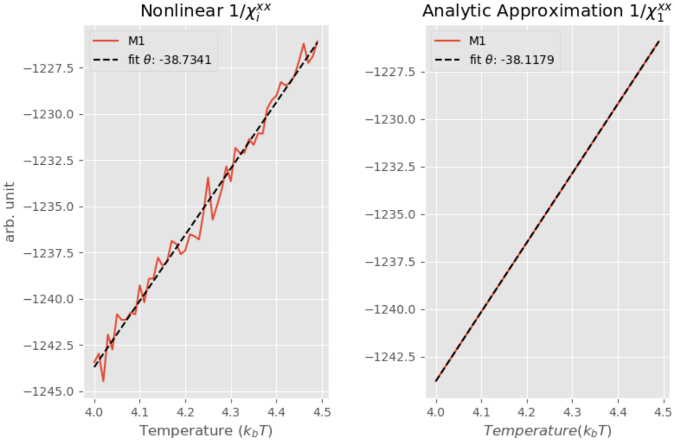
Two Site Isotropic AFM



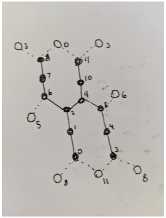
Two Site Small Anisotropy



Two Site Large Anisotropy



Our System



$$\underline{\underline{\chi}}_0 = F\left(\underline{\underline{\chi}}_1, \underline{\underline{\chi}}_8, \underline{\underline{\chi}}_{11}\right)$$

$$\underline{\underline{\chi}}_1 = F\left(\underline{\underline{\chi}}_0, \underline{\underline{\chi}}_2\right)$$

$$\underline{\underline{\chi}}_2 = F\left(\underline{\underline{\chi}}_1, \underline{\underline{\chi}}_6, \underline{\underline{\chi}}_9\right)$$

$$\underline{\underline{\chi}}_3 = F\left(\underline{\underline{\chi}}_4, \underline{\underline{\chi}}_8, \underline{\underline{\chi}}_{11}\right)$$

$$\underline{\underline{\chi}}_4 = F\left(\underline{\underline{\chi}}_3, \underline{\underline{\chi}}_5\right)$$

$$\underline{\underline{\chi}}_5 = F\left(\underline{\underline{\chi}}_4, \underline{\underline{\chi}}_6, \underline{\underline{\chi}}_9\right)$$

$$\underline{\underline{\chi}}_6 = F\left(\underline{\underline{\chi}}_2, \underline{\underline{\chi}}_5, \underline{\underline{\chi}}_7\right)$$

$$\underline{\underline{\chi}}_7 = F\left(\underline{\underline{\chi}}_6, \underline{\underline{\chi}}_8\right)$$

$$\underline{\underline{\chi}}_8 = F\left(\underline{\underline{\chi}}_0, \underline{\underline{\chi}}_3, \underline{\underline{\chi}}_7\right)$$

$$\underline{\underline{\chi}}_9 = F\left(\underline{\underline{\chi}}_2, \underline{\underline{\chi}}_5, \underline{\underline{\chi}}_{10}\right)$$

$$\underline{\underline{\chi}}_{10} = F\left(\underline{\underline{\chi}}_9, \underline{\underline{\chi}}_{11}\right)$$

$$\underline{\underline{\chi}}_{11} = F\left(\underline{\underline{\chi}}_0, \underline{\underline{\chi}}_3, \underline{\underline{\chi}}_{10}\right)$$