Variational Mean Field

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

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

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

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

and λ_i are Lagrange multipliers that fix the normalization. Note $\vec{S}_i(\Omega_i)$ is a unit vector pointing in the direction of the solid angle Ω_i.

Minimization

One needs to minimize with respect to each ρ_i and λ_i:

$$0 = \frac{\partial F}{\partial \rho_i} = -\frac{1}{2}\sum_{j \neq i} \vec{S}_i(\Omega_i) \cdot \underline{\underline{A}}_{ij} \cdot \vec{m}_j + \vec{m}_j \cdot \underline{\underline{A}}_{ji} \cdot \vec{S}_i(\Omega_i)$$

$$-\vec{h}_i \cdot \underline{\underline{g}}_i \cdot \vec{S}_i(\Omega_i) + \mathrm{T}\left[\ln\left(\rho_i(\Omega_i)\right) + 1\right] - \lambda_i$$

$$0 = \frac{\partial F}{\partial \lambda_i} = \left(\int \mathrm{d}\Omega_i \rho_i(\Omega_i) - 1\right)$$

Quick Aside

Since they both describe the same couplings we know $\vec{m}_i \cdot \underline{\underline{A}}_{ij} \cdot \vec{m}_j = \vec{m}_j \cdot \underline{\underline{A}}_{ji} \cdot \vec{m}_i$. Then let us rewrite the first equation as

$$0 = -\vec{\mathcal{H}}_i \cdot \vec{S}_i(\Omega_i) + \mathrm{T}\left[\ln\left(\rho_i(\Omega_i)\right) + 1\right] - \lambda_i$$

where

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

*NOTE: The aforementioned equality holds for all possible $\{m_i, m_j\}$ so $\underline{\underline{A}}_{ji} = \underline{\underline{A}}_{ij}^T$ (notice the subscripts). I only mention this since this fact is used in the code.

Minimization

From the first equation we get:

$$\rho_i(\Omega_i) = \exp\left\{ \frac{1}{T} \left(\vec{\mathcal{H}}_i \cdot \vec{S}_i(\Omega_i) \right) \right\} \exp\left\{ \frac{\lambda_i}{T} - 1 \right\}$$

From the second equation we can determine

$$\exp\left\{ \frac{\lambda_i}{T} - 1 \right\} = \frac{1}{\int \mathrm{d}\Omega_i \exp\left\{ \frac{1}{T} \left(\vec{\mathcal{H}}_i \cdot S_i(\Omega_i) \right) \right\}}$$

Minimization

Combining all the above we find

$$\rho_i(\Omega_i) = \frac{1}{Z_i}\exp\left\{\frac{1}{T}\left(\vec{\mathcal{H}}_i \cdot S_i(\Omega_i)\right)\right\}$$

where

$$Z_i := \int \mathrm{d}\Omega_i \exp\left\{\frac{1}{T}\left(\vec{\mathcal{H}}_i \cdot S_i(\Omega_i)\right)\right\}$$

Notice if we examine the contents of $\vec{\mathcal{H}}$ the above turns out to be a self consistent equation in the $\{\rho_i\}_{i\in\mathrm{LAT}}$. A simplification can be made. It turns out ρ_i only depends on the average spin of neighboring sites, $\vec{m}_i$.

Minimization

So let us try to determine these average spins, then we will have solved the problem. By definition

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

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

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

Another set of self-consistent equations.

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 setup the above self consistent equations through the following trick

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

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

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

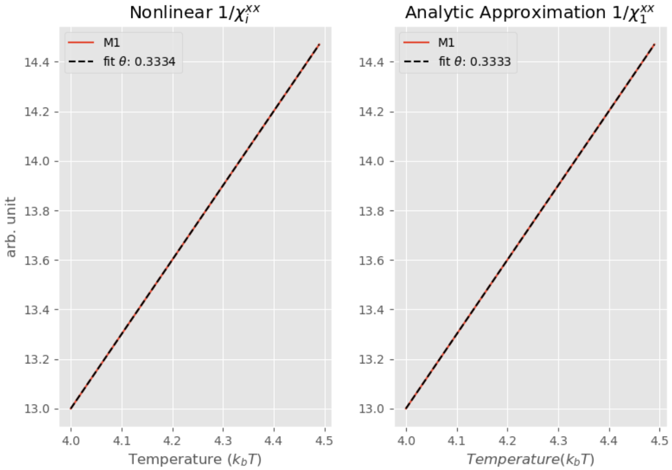
A Solution for Susceptibility

We need to solve the following set of matrix equations

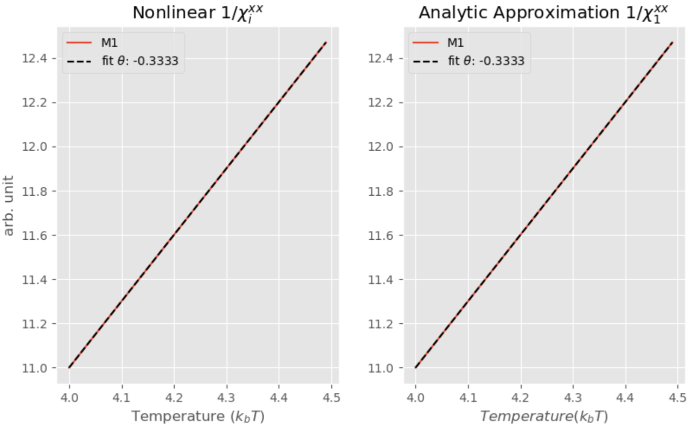
$$\underline{\underline{g}}_i = \frac{3}{\beta}\underline{\underline{\chi}}_i + \sum_{j\neq i}\underline{\underline{\chi}}_j \cdot \underline{\underline{A}}_{ji}$$

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.

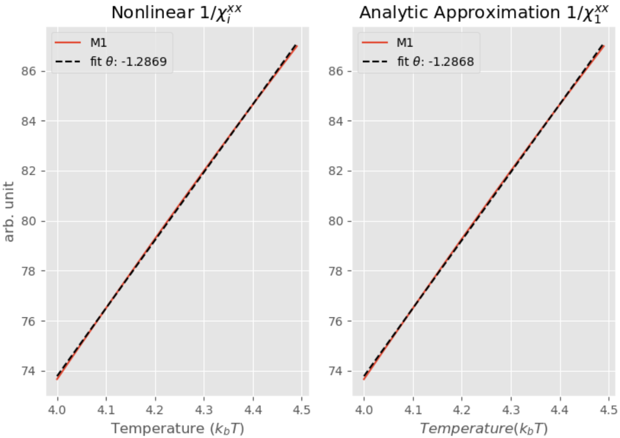
Two Site Isotropic FM



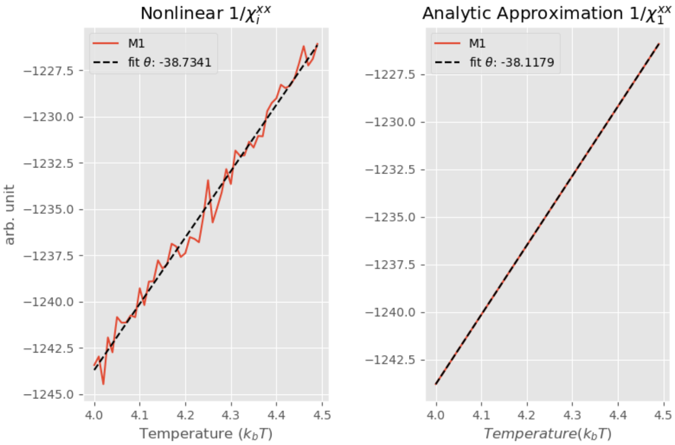
Two Site Isotropic AFM



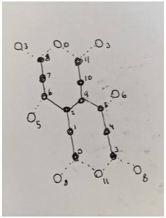
Two Site Small Anisotropy



Two Site Large Anisotropy



Our System



$$\underline{\underline{\chi}}_0 = F\left(\underline{\underline{\chi}}_1, \underline{\underline{\chi}}_8, \underline{\underline{\chi}}_{11}\right) \qquad \underline{\underline{\chi}}_6 = F\left(\underline{\underline{\chi}}_2, \underline{\underline{\chi}}_5, \underline{\underline{\chi}}_7\right)$$

$$\underline{\underline{\chi}}_1 = F\left(\underline{\underline{\chi}}_0, \underline{\underline{\chi}}_2\right) \qquad \underline{\underline{\chi}}_7 = F\left(\underline{\underline{\chi}}_6, \underline{\underline{\chi}}_8\right)$$

$$\underline{\underline{\chi}}_2 = F\left(\underline{\underline{\chi}}_1, \underline{\underline{\chi}}_6, \underline{\underline{\chi}}_9\right) \qquad \underline{\underline{\chi}}_8 = F\left(\underline{\underline{\chi}}_0, \underline{\underline{\chi}}_3, \underline{\underline{\chi}}_7\right)$$

$$\underline{\underline{\chi}}_3 = F\left(\underline{\underline{\chi}}_4, \underline{\underline{\chi}}_8, \underline{\underline{\chi}}_{11}\right) \qquad \underline{\underline{\chi}}_9 = F\left(\underline{\underline{\chi}}_2, \underline{\underline{\chi}}_5, \underline{\underline{\chi}}_{10}\right)$$

$$\underline{\underline{\chi}}_4 = F\left(\underline{\underline{\chi}}_3, \underline{\underline{\chi}}_5\right) \qquad \underline{\underline{\chi}}_{10} = F\left(\underline{\underline{\chi}}_9, \underline{\underline{\chi}}_{11}\right)$$

$$\underline{\underline{\chi}}_5 = F\left(\underline{\underline{\chi}}_4, \underline{\underline{\chi}}_6, \underline{\underline{\chi}}_9\right) \qquad \underline{\underline{\chi}}_{11} = F\left(\underline{\underline{\chi}}_0, \underline{\underline{\chi}}_3, \underline{\underline{\chi}}_{10}\right)$$