ELECTRIC-FIELD MAPPED AVERAGING FOR IDEAL HEISENBERG MODEL

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This time we consider a system of rigid 2D Heisenberg dipoles interacting with an external field $\mathbf{E}$. Let θ be the angle that $\boldsymbol{\mu}$ makes with $\mathbf{E}$, and we use θ as the coordinate describing the orientation, $0 \leq \theta \leq 2\pi$. such that such that the total energy of a configuration is given by

$$u = -E\mu \sum_{i}^{N} \cos\theta_i. \tag{1}$$

We note that $\theta = 0/2\pi$ is the preferred (low-energy) orientation. And the corresponding Boltzmann factor and partition function would be

$$\begin{aligned} p &= \exp[\beta E\mu\cos\theta_i] \\ q &= \int_0^{2\pi} p\, d\theta_i = 2\pi I_0(\beta E\mu) \end{aligned} \tag{2}$$

Now we can try to solve eq(12) in our JCTC paper:

$$\frac{\partial}{\partial E}\left(\frac{p}{q}\right) + \nabla\cdot\left(\frac{p}{q}\mathbf{v}^E\right) = 0; \tag{3}$$

$$\frac{\beta\mu e^{\beta E\mu\cos\theta_i}\left(\cos\theta_i I_0(\beta E\mu) - I_1(\beta E\mu)\right)}{2\pi I_0(\beta E\mu)^2} + \frac{e^{\beta E\mu\cos\theta_i}\left(\left(v^E\right)' - \beta E\mu\sin\theta_i v^E\right)}{2\pi I_0(\beta E\mu)} = 0 \tag{4}$$

I_0 and I_1 are Bessel Functions. Note we could divide both side on eq:(4) by $e^{\beta E\mu\cos\theta_i}/2\pi I_0(\beta E\mu)$ we would have:

$$\left(v^E\right)' - \beta E\mu\sin\theta_i v^E = \frac{\beta\mu\left(\cos\theta_i I_0(\beta E\mu) - I_1(\beta E\mu)\right)}{I_0(\beta E\mu)} \tag{5}$$

the general function for eq(5) would be

$$v^E = e^{-\beta E\mu\cos\theta_i}\int \frac{\beta\mu\left(\cos\theta_i I_0(\beta E\mu) - I_1(\beta E\mu)\right)}{I_0(\beta E\mu)}\exp(\beta E\mu\cos\theta_i)\, d\theta_i; \tag{6}$$

We are interested v^E and $v^{EE} = \partial v^E/\partial E$ in the case when electric field $\mathbf{E} \to 0$

$$\begin{aligned} v^E &= -\beta\mu\sin\theta_i \\ v^{EE} &= \frac{1}{2}\beta^2\mu^2\cos\theta_i\sin\theta_i \end{aligned} \tag{7}$$

Then necessary Jacobian derivatives would be

$$
\begin{aligned}
J_E &= \frac{\partial v^E}{\partial \theta_i} = -\beta\mu \sum_i^N \cos\theta_i \\
J_{EE} - J_E J_E &= \frac{\partial v^{EE}}{\partial \theta_i} + v^E \frac{\partial^2 v^E}{\partial \theta_i^2} \\
&= \frac{1}{2}\beta^2\mu^2 \sum_i^N (-1 + 2\cos 2\theta_i)
\end{aligned} \tag{8}
$$

The necessary energy derivatives would be

$$
\begin{aligned}
\mathcal{U}_E &= u_E - v^E \beta F = -\beta\mu \sum_i^N \cos\theta_i + \beta^2\mu \sum_i^N F_i \sin\theta_i \\
\mathcal{U}_{EE} &= u_{EE} - \beta F \left(v_{EE} + v_E \frac{\partial v_E}{\partial \theta_i} \right) + v_E \phi v_E - 2V_E F_E \\
&= \frac{-3}{2} \sum_i^N F_i \beta^3 \mu^2 \sin\theta_i \cos\theta_i - 2 \sum_i^N \beta^2 \mu^2 \sin^2\theta_i \\
&+ \sum_i^N \sum_i^N \beta^3 \mu^2 \sin\theta_i \phi_{ij} \sin\theta_i
\end{aligned} \tag{9}
$$

where $Fi = -\partial u/\partial\theta_i$ and $\phi_{ij} = \partial^2 u/\partial\theta_i \partial\theta_j$. Note that torque on atom i is also $\tau_i = -\partial u/\partial\theta_i$ so $F_i = \tau_i$. If combine eq(8) and eq(9), we can get $\mathcal{A}_E$ and $\mathcal{A}_{EE}$ for X or Y direction.

$$
\begin{aligned}
\mathcal{A}_E &= -\langle J_E \rangle + \langle U_E \rangle = \beta^2 \mu \sum_i^N F_i \sin\theta_i \\
\mathcal{A}_{EE} &= -\langle J_{EE} - J_E J_E \rangle + \langle \mathcal{U}_E \rangle - Var[J_E - \mathcal{U}_E] \\
&= -\frac{N\beta^2\mu^2}{2} - \frac{3}{2}\beta^3\mu^2 \sum_i^N F_i \sin\theta_i \cos\theta_i \\
&+ \beta^3\mu^2 \sum_i^N \phi_{ij} \sin\theta_i \sin\theta_i - Var\left[\beta^2 \mu \sum_i^N F_i \sin\theta_i \right]
\end{aligned} \tag{10}
$$

Now, we sum over X and y direction for these terms: $-\frac{N\beta^2\mu^2}{2}$,$-\frac{3}{2}\beta^3\mu^2 \sum_i^N F_i \sin\theta_i \cos\theta_i$, $\beta^3\mu^2 \sum_i^N \phi_{ij} \sin\theta_i \sin\theta_i$ and $Var\left[-\beta^2\mu \sum_i^N F_i \sin\theta_i \right]$.

$$
\sum_{x,y} \left\langle -\sum_i^N \frac{\beta^2\mu^2}{2} \right\rangle = -N\beta^2\mu^2 \tag{11}
$$

$$\sum_{x,y}\left\langle \frac{3}{2}\beta^3\mu^2\sum_i^N F_i\sin\theta_i\cos\theta_i\right\rangle = \left\langle \frac{3}{2}\beta^3\mu^2\sum_i^N \tau_i\sin\theta_i\cos\theta_i\right\rangle$$

$$= \left\{ \begin{array}{c} \left\langle \frac{3}{2}\beta^3\mu^2\sum_i^N \tau_i\sin 2\theta_i\right\rangle \\ \left\langle 3\beta^3\mu^2\sum_i^N \tau_i e_{xi}e_{yi}\right\rangle \end{array} \right. \tag{12}$$

where e_{xi} and e_{yi} are x and y component of dipole $\overrightarrow{e_i}$

$$\sum_{x,y}\left\langle \beta^3\mu^2\sum_i^N \phi_{ij}\sin\theta_i\sin\theta_j\right\rangle = \left\langle \beta^3\mu^2\sum_i^N\sum_j^N \phi_{ij}(\sin\theta_i\sin\theta_j+\cos\theta_i\cos\theta_i)\right\rangle$$

$$= \left\langle \beta^3\mu^2\sum_i^N \phi_{ij}\cos(\theta_i-\theta_j)\right\rangle \tag{13}$$

For the $Var\left[\beta^2\mu\sum_i^N F_i\sin\theta_i\right]$ has two parts: $\beta^4\mu^2\left\langle (\sum_i^N F_i\sin\theta_i)^2\right\rangle$ and $\beta^4\mu^2\left\langle (\sum_i^N F_i\sin\theta_i)\right\rangle^2$.

$$\sum_{x,y}\left\langle \left(\sum_i^N F_i\sin\theta_i\right)^2\right\rangle = \sum_{x,y}\left\langle \left(\sum_i^N \tau_i\overrightarrow{e_i}\cdot\overrightarrow{Y}\right)^2\right\rangle = \sum_{x,y}\left\langle \left(\overrightarrow{Y}\cdot\left(\sum_i^N \tau_i\overrightarrow{e_i}\right)\right)^2\right\rangle$$

$$= \left\langle \left(\sum_i^N \tau_i\overrightarrow{e_i})\right)^2\right\rangle = \left\langle \overrightarrow{A}^2\right\rangle \tag{14}$$

where vector $\overrightarrow{A} = \left(\sum_i^N \tau_i\overrightarrow{e_i})\right)$

$$\sum_{x,y}\left\langle \sum_i^N F_i\sin\theta_i\right\rangle^2 = \sum_{x,y}\left\langle \left(\sum_i^N \tau_i\overrightarrow{e_i}\cdot\overrightarrow{Y}\right)\right\rangle^2 = \langle A_x\rangle^2 + \langle A_y\rangle^2 \tag{15}$$

Where A_x and A_y are x and y component of $\overrightarrow{A}$. In Sum, if we combine eq(11),(12),(13),(14)and (15)

$$\mathcal{A}_{EE} = -N\beta^2\mu^2 + \left\langle \frac{3}{2}\beta^3\mu^2\sum_i^N \tau_i\sin 2\theta_i\right\rangle + \left\langle \beta^3\mu^2\sum_i^N\sum_j^N \phi_{ij}\cos(\theta_i-\theta_j)\right\rangle$$

$$- var\left[\sum_i^N \tau_i\overrightarrow{e_i}\right] \tag{16}$$