

I. EWALD SUMMATION

The single site energy of a dipole in an electric field is

$$E_i = -\mathbf{S}_i \cdot \mathbf{E}(\mathbf{r}_i). \quad (1)$$

So that the total electrostatic energy of the lattice is

$$U = \sum_i E_i. \quad (2)$$

The electric field produced by a dipole is¹

$$\mathbf{E}(\mathbf{r}) = \frac{3(\hat{\mathbf{r}} \cdot \mathbf{S})\hat{\mathbf{r}} - \mathbf{S}}{r^3} = (\mathbf{S} \cdot \nabla) \nabla \frac{1}{r} \quad (3)$$

On a lattice of N dipoles, equation (1) becomes

$$E_i = -\mathbf{S}_i \cdot \left(\sum_{j \neq i} (\mathbf{S}_j \cdot \nabla) \nabla \frac{1}{r_{ij}} \right) \quad (4)$$

$$= -(\mathbf{S}_i \cdot \nabla) \sum_{j \neq i} (\mathbf{S}_j \cdot \nabla) \frac{1}{r_{ij}} \quad (5)$$

Where (4)→(5) holds because \mathbf{S}_j is not a function of \mathbf{r} , (i.e. the commutation relationship holds: $[\nabla, (\mathbf{S}_j \cdot \nabla)] = \mathbf{0} \quad \forall j$).

Then equation (2) becomes

$$U = \sum_{i < j} \mathbf{S}_i \cdot \mathbf{J}(\mathbf{r}_{ij}) \cdot \mathbf{S}_j \quad (6)$$

Where

$$\mathbf{J}_{\mu\nu}(\mathbf{r}) = -\partial_\mu \partial_\nu \frac{1}{r} \quad (7)$$

To compute an infinite lattice sum we have periodic boundary conditions to unlimited range.

$$U = \sum_n \sum_{i < j} \mathbf{S}_i \cdot \mathbf{J}(\mathbf{r}_{ij} + \mathbf{n}L) \cdot \mathbf{S}_j \quad i, j \in \{1, 2 \dots N\} \quad (8)$$

$$= \sum_{i < j} \mathbf{S}_i \cdot \left(\sum_n \mathbf{J}(\mathbf{r}_{ij} + \mathbf{n}L) \right) \cdot \mathbf{S}_j \quad (9)$$

where L is the linear size of the lattice containing N dipoles in the direction of cubic translation vectors and \mathbf{n} is a vector of integers (in general the lattice can be the size of any parallelepiped with lattice translation vectors, \mathbf{T}) The inner sum is conditionally convergent and can't be approximated by truncation.

Multiplying by $\frac{1}{\sqrt{\pi}} \Gamma\left(\frac{1}{2}\right) = 1$,

$$\frac{1}{r} = \frac{1}{\sqrt{\pi}} \Gamma\left(\frac{1}{2}\right) \frac{1}{r} \quad (10)$$

$$= \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-u} \left(\frac{du}{2\sqrt{ur}} \right) \quad (11)$$

$$= \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-t^2 r^2} dt \quad (12)$$

Where I made the substitution, $u = t^2 r^2$, to go from step (11) ↔ (12). Now the integral is split into two parts

$$\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_0^\alpha e^{-t^2 r^2} dt + \frac{2}{\sqrt{\pi}} \int_\alpha^\infty e^{-t^2 r^2} dt \quad (13)$$

$$= \frac{2}{\sqrt{\pi}} \int_0^\alpha e^{-t^2 r^2} dt + \frac{2}{\sqrt{\pi}} \frac{1}{r} \int_{\alpha r}^\infty e^{-(tr)^2} d(tr) \quad (14)$$

$$= \frac{2}{\sqrt{\pi}} \int_0^\alpha e^{-t^2 r^2} dt + \frac{1}{r} \text{erfc}(\alpha r) \quad (15)$$

So the energy can be decomposed as

$$U = U_{\text{SR}} + U_{\text{LR}} \quad (16)$$

The first term in (15) contributes to the long range part, U_{LR} , and is summed in reciprocal space. The second term in (15) contributes to the short range part, U_{SR} , which is summed in position space.

$$U_{\text{LR}} = \sum_{i < j} \mathbf{S}_i \cdot \mathbf{A}_{ij} \cdot \mathbf{S}_j \quad (17)$$

$$\mathbf{A}_{ij}^{\mu\nu} = - \sum_n \frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \int_0^\alpha e^{-t^2 |\mathbf{r}_{ij} + \mathbf{n}L|^2} dt \quad (18)$$

$$= - \frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \sum_n \int_0^\alpha e^{-t^2 |\mathbf{r}_{ij} + \mathbf{n}L|^2} dt \quad (19)$$

$$= - \frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu M(\mathbf{r}) \Big|_{\mathbf{r}=\mathbf{r}_{ij}} \quad (20)$$

Where

$$M(\mathbf{r}) = \sum_n \int_0^\alpha e^{-t^2 |\mathbf{r} + \mathbf{n}L|^2} dt \quad (21)$$

$$= \int \left[\sum_n \delta(\mathbf{r}' - \mathbf{n}L) \int_0^\alpha e^{-t^2 |\mathbf{r} + \mathbf{r}'|^2} dt \right] d^3 \mathbf{r}' \quad (22)$$

$$= \int \left[\frac{1}{V} \sum_G e^{i\mathbf{G} \cdot \mathbf{r}'} \int_0^\alpha e^{-t^2 |\mathbf{r} + \mathbf{r}'|^2} dt \right] d^3 \mathbf{r}' \quad (23)$$

$$= \frac{1}{V} \sum_G e^{-i\mathbf{G} \cdot \mathbf{r}} \int \left[e^{i\mathbf{G} \cdot (\mathbf{r}' + \mathbf{r})} \int_0^\alpha e^{-t^2 |\mathbf{r} + \mathbf{r}'|^2} dt \right] d^3 (\mathbf{r}' + \mathbf{r}) \quad (24)$$

$$= \frac{2\pi \sqrt{2\pi}}{V} \sum_G e^{-i\mathbf{G} \cdot \mathbf{r}} \mathcal{F} \left[\int_0^\alpha e^{-t^2 r^2} dt \right] (\mathbf{G}) \quad (25)$$

$$= \frac{2\pi \sqrt{2\pi}}{V} \sum_G e^{-i\mathbf{G} \cdot \mathbf{r}} \int_0^\alpha \frac{1}{2\sqrt{2}t^3} e^{-G^2/4t^2} dt \quad (26)$$

$$= \frac{\pi \sqrt{\pi}}{V} \sum_G e^{-i\mathbf{G} \cdot \mathbf{r}} \int_\infty^{G^2/4\alpha^2} \frac{1}{t^3} e^{-u} \left(\frac{-2t^3 du}{G^2} \right) \quad (27)$$

$$= \frac{2\pi \sqrt{\pi}}{V} \sum_G \frac{1}{G^2} e^{-i\mathbf{G} \cdot \mathbf{r}} \int_{G^2/4\alpha^2}^\infty e^{-u} du, \quad u = \frac{G^2}{4t^2} \quad (28)$$

$$= \frac{2\pi \sqrt{\pi}}{V} \sum_G \frac{1}{G^2} e^{-G^2/4\alpha^2} e^{-i\mathbf{G} \cdot \mathbf{r}} \quad (29)$$

Where \mathcal{F} is the 3D Fourier transform which, for this case, decouples into the product of 3 1D Fourier transforms of a Gaussian.

The reciprocal space sum transformation is used in (22)→(23)²

$$\sum_n \delta(\mathbf{r} - \mathbf{n}L) = \frac{1}{V} \sum_G e^{-i\mathbf{G} \cdot \mathbf{r}} \quad (30)$$

which is true inside of the integral. For the 1D case,

$$\int L \sum_n \delta(x - nL) dx = \sum_n \int_{(x-nL)/2}^{(x+nL)/2} \delta(x - nL) dx \quad (31)$$

$$= \sum_n \int_{(x-nL)/2}^{(x+nL)/2} \sum_G e^{-iG(x-nL)} dx \quad (32)$$

$$= \int \sum_G e^{-iGx} dx \quad (33)$$

which can be easily generalized to the 3D case.

The long-range coupling matrix is

$$A_{ij}^{\mu\nu} = -\frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \frac{2\pi\sqrt{\pi}}{V} \sum_G \frac{1}{G^2} e^{-G^2/4\alpha^2} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}} \quad (34)$$

$$= -\frac{4\pi}{V} \sum_G \frac{1}{G^2} e^{-G^2/4\alpha^2} (\partial_\mu \partial_\nu e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}}) \quad (35)$$

$$= \frac{4\pi}{V} \sum_G \frac{G_\mu G_\nu}{G^2} e^{-G^2/4\alpha^2} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}} \quad (36)$$

The singular $\mathbf{r}_{ij} + \mathbf{n}L = \mathbf{0}$ term which was included in the integral represents dipole interaction with its own field. This term may be subtracted directly.

$$- \frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \int_0^\alpha e^{-t^2 r^2} dt \Big|_{r=0} \quad (37)$$

$$= - \int_0^\alpha \left(\frac{8}{\sqrt{\pi}} t^4 r_\mu r_\nu e^{-t^2 r^2} - \frac{4}{\sqrt{\pi}} t^2 \delta_{\mu\nu} e^{-t^2 r^2} \right) \Big|_{r=0} dt \quad (38)$$

$$= \frac{4\alpha^3}{3\sqrt{\pi}} \delta_{\mu\nu} \quad (39)$$

So we have the correction to (17)

$$U_{LR} = \frac{1}{2} \sum_{ij}^N \left(\mathbf{S}_i \cdot \mathbf{A}_{ij} \cdot \mathbf{S}_j - \frac{4\alpha^3}{3\sqrt{\pi}} \delta_{ij} S_i^2 \right) \quad (40)$$

The short range contribution to the energy is

$$U_{SR} = \frac{1}{2} \sum_{ij}^N \mathbf{S}_i \cdot \mathbf{B}_{ij} \cdot \mathbf{S}_j \quad (41)$$

where \mathbf{B} is the short range coupling matrix

$$B_{ij}^{\mu\nu} = - \sum_n \frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \int_\alpha^\infty e^{-t^2 r_{ij}^2} dt \quad (42)$$

$$= - \sum_n \int_\alpha^\infty \left(\frac{8}{\sqrt{\pi}} t^4 r_{ij}^\mu r_{ij}^\nu e^{-t^2 r_{ij}^2} - \frac{4}{\sqrt{\pi}} t^2 \delta_{\mu\nu} e^{-t^2 r_{ij}^2} \right) dt \quad (43)$$

Computing the first integral

$$\frac{8}{\sqrt{\pi}} r^\mu r^\nu \int_\alpha^\infty t^4 e^{-t^2 r^2} dt \quad (44)$$

$$= \frac{8}{\sqrt{\pi}} \frac{r^\mu r^\nu}{r^5} \int_{(\alpha r)^2}^\infty u^2 e^{-u} \frac{du}{2\sqrt{u}}, \quad u = t^2 r^2 \quad (45)$$

Integrating by parts twice

$$\frac{4}{\sqrt{\pi}} \frac{r^\mu r^\nu}{r^5} \int_{(\alpha r)^2}^\infty u^{3/2} e^{-u} du \quad (46)$$

$$= \frac{4}{\sqrt{\pi}} \frac{r^\mu r^\nu}{r^5} \left[\int_{(\alpha r)^2}^\infty \frac{3}{2} u^{1/2} e^{-u} du + \alpha^3 r^3 e^{-\alpha^2 r^2} \right] \quad (47)$$

$$= \frac{4}{\sqrt{\pi}} \frac{r^\mu r^\nu}{r^5} \left[\frac{3}{2} \left[\int_{(\alpha r)^2}^\infty e^{-u} \frac{du}{2\sqrt{u}} + \alpha r e^{-\alpha^2 r^2} \right] + \alpha^3 r^3 e^{-\alpha^2 r^2} \right] \quad (48)$$

$$= \frac{r^\mu r^\nu}{r^5} \left[3\text{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r (3 + 2\alpha^2 r^2) e^{-\alpha^2 r^2} \right] \quad (49)$$

Computing the second integral in (44) only requires integration by parts once

$$- \frac{4}{\sqrt{\pi}} \delta_{\mu\nu} \int_\alpha^\infty t^2 e^{-t^2 r_{ij}^2} dt \quad (50)$$

$$= - \frac{4}{\sqrt{\pi}} \frac{\delta_{\mu\nu}}{r_{ij}^3} \int_{(\alpha r_{ij})^2}^\infty u e^{-u} \frac{du}{2\sqrt{u}} \quad (51)$$

$$= - \frac{4}{\sqrt{\pi}} \frac{\delta_{\mu\nu}}{r_{ij}^3} \left[\int_{(\alpha r_{ij})^2}^\infty e^{-u} \frac{du}{2\sqrt{u}} + \frac{1}{2} \alpha r_{ij} e^{-\alpha^2 r_{ij}^2} \right] \quad (52)$$

$$= - \frac{\delta_{\mu\nu}}{r_{ij}^3} \left[\text{erfc}(\alpha r_{ij}) + \frac{2}{\sqrt{\pi}} \alpha r_{ij} e^{-\alpha^2 r_{ij}^2} \right] \quad (53)$$

So the final expression for the lattice sum is

$$\begin{aligned} \sum_n J(\mathbf{r}_{ij} + \mathbf{n}L) &= \mathbf{A}_{ij} + \mathbf{B}_{ij} - \frac{4\alpha^3}{3\sqrt{\pi}} \delta_{ij} \mathbf{1} \\ \mathbf{A}_{ij} &= \frac{4\pi}{V} \sum_G \frac{\mathbf{G} \otimes \mathbf{G}}{G^2} e^{-G^2/4\alpha^2} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}} \\ \mathbf{B}_{ij} &= \sum_n \frac{1}{|\mathbf{r}_{ij} + \mathbf{n}L|^5} \left(|\mathbf{r}_{ij} + \mathbf{n}L|^2 X(|\mathbf{r}_{ij} + \mathbf{n}L|) \mathbf{1} \right. \\ &\quad \left. + (\mathbf{r}_{ij} + \mathbf{n}L) \otimes (\mathbf{r}_{ij} + \mathbf{n}L) Y(|\mathbf{r}_{ij} + \mathbf{n}L|) \right) \\ X(r) &= \text{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r e^{-\alpha^2 r^2} \\ Y(r) &= 3\text{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r (3 + 2\alpha^2 r^2) e^{-\alpha^2 r^2} \end{aligned}$$

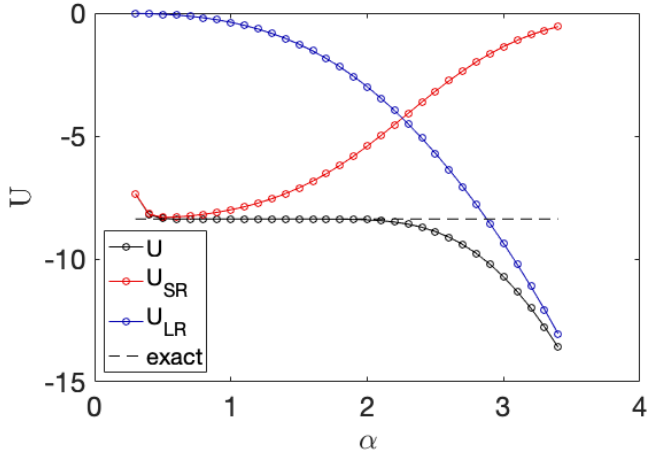


FIG. 1. Convergence of the Ewald summation with splitting parameter, α , for an FCC lattice in the ferromagnetic state. The energy converges to the exact value in the range $\alpha \in [1, 2]$. The summation has bad convergence for a poor choice of α . The Ewald summation was performed with a length constraint cutoff: $|\mathbf{r}| < 10$, and, $|\mathbf{G}| < (2\pi/L) \times 10$. Long range contributions to the energy are dominant if α is chosen to be large (as expected).

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⁷ Stasiak, Pawel, "Theoretical studies of frustrated magnets with dipolar interactions," (2009).

⁸ A. Del Maestro and M. Gingras, *Journal of Physics: Condensed Matter* **16**, 3339 (2004).