

## 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 is<sup>1</sup>

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

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 and  $\mathbf{n}$  is a cubic translation vector of the simulation box which contains the lattice (in general the simulation box can be the size of any parallelepiped with lattice translation vectors,  $\mathbf{T}$ ). So the lattice constant of the simulation box lattice is  $L$ .

The inner sum is conditionally convergent and can't be approximated by truncation.

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

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

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

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

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,  $U_{\text{LR}}$ , and is summed in reciprocal space. The second term in (15) contributes to the short range part,  $U_{\text{SR}}$ , 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 replacement is used in (22)→(23)<sup>2</sup>

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

The long-range coupling matrix is

$$A_{ij}^{\mu\nu} = -\frac{2}{\sqrt{\pi}} \partial_{\mu} \partial_{\nu} \frac{2\pi\sqrt{\pi}}{V} \sum_{\mathbf{G}} \frac{1}{G^2} e^{-G^2/4a^2} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}} \quad (31)$$

$$= -\frac{4\pi}{V} \sum_{\mathbf{G}} \frac{1}{G^2} e^{-G^2/4a^2} (\partial_{\mu} \partial_{\nu} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}}) \quad (32)$$

$$= \frac{4\pi}{V} \sum_{\mathbf{G}} \frac{G_{\mu} G_{\nu}}{G^2} e^{-G^2/4a^2} e^{-i\mathbf{G} \cdot \mathbf{r}_{ij}} \quad (33)$$

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

$$- \frac{2}{\sqrt{\pi}} \partial_{\mu} \partial_{\nu} \int_0^{\alpha} e^{-t^2 r^2} dt \Big|_{r=0} \quad (34)$$

$$= - \int_0^{\alpha} \left( \frac{8}{\sqrt{\pi}} t^4 r_{\mu} r_{\nu} e^{-t^2 r^2} - \frac{4}{\sqrt{\pi}} t^2 \delta_{\mu\nu} e^{-t^2 r^2} \right) \Big|_{r=0} dt \quad (35)$$

$$= \frac{4\alpha^3}{3\sqrt{\pi}} \delta_{\mu\nu} \quad (36)$$

So we have the correction to (17)

$$U_{\text{LR}} = \frac{1}{2} \sum_{ij} \left( \mathbf{S}_i \cdot \mathbf{A}_{ij} \cdot \mathbf{S}_j - \frac{4\alpha^3}{3\sqrt{\pi}} \delta_{ij} S_i^2 \right) \quad (37)$$

The short range contribution to the energy is

$$U_{\text{SR}} = \frac{1}{2} \sum_{ij} \mathbf{S}_i \cdot \mathbf{B}_{ij} \cdot \mathbf{S}_j \quad (38)$$

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

Define  $\mathbf{r}_{ijn} = \mathbf{r}_{ij} + \mathbf{nL}$

$$B_{ij}^{\mu\nu} = - \sum_{\mathbf{n}} \frac{2}{\sqrt{\pi}} \partial_{\mu} \partial_{\nu} \int_{\alpha}^{\infty} e^{-t^2 r_{ijn}^2} dt \quad (39)$$

$$= - \sum_{\mathbf{n}} \int_{\alpha}^{\infty} \left( \frac{8}{\sqrt{\pi}} t^4 r_{ijn}^{\mu} r_{ijn}^{\nu} e^{-t^2 r_{ijn}^2} - \frac{4}{\sqrt{\pi}} t^2 \delta_{\mu\nu} e^{-t^2 r_{ijn}^2} \right) dt \quad (40)$$

Computing the first integral

$$\frac{8}{\sqrt{\pi}} r^{\mu} r^{\nu} \int_{\alpha}^{\infty} t^4 e^{-t^2 r^2} dt \quad (41)$$

$$= \frac{8}{\sqrt{\pi}} \frac{r^{\mu} r^{\nu}}{r^5} \int_{(\alpha r)^2}^{\infty} u^2 e^{-u} \frac{du}{2\sqrt{u}}, \quad u = t^2 r^2 \quad (42)$$

Integrating by parts twice

$$\frac{4}{\sqrt{\pi}} \frac{r^{\mu} r^{\nu}}{r^5} \int_{(\alpha r)^2}^{\infty} u^{3/2} e^{-u} du \quad (43)$$

$$= \frac{4}{\sqrt{\pi}} \frac{r^{\mu} r^{\nu}}{r^5} \left[ \int_{(\alpha r)^2}^{\infty} \frac{3}{2} u^{1/2} e^{-u} du + \alpha^3 r^3 e^{-\alpha^2 r^2} \right] \quad (44)$$

$$= \frac{4}{\sqrt{\pi}} \frac{r^{\mu} r^{\nu}}{r^5} \left[ \frac{3}{2} \left[ \int_{(\alpha r)^2}^{\infty} e^{-u} \frac{du}{2\sqrt{u}} + \alpha r e^{-\alpha^2 r^2} \right] + \alpha^3 r^3 e^{-\alpha^2 r^2} \right] \quad (45)$$

$$= \frac{r^{\mu} r^{\nu}}{r^5} \left[ 3\text{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r (3 + 2\alpha^2 r^2) e^{-\alpha^2 r^2} \right] \quad (46)$$

Computing the second integral in (40) only requires integration by parts once

$$- \frac{4}{\sqrt{\pi}} \delta_{\mu\nu} \int_{\alpha}^{\infty} t^2 e^{-t^2 r^2} dt \quad (47)$$

$$= - \frac{4}{\sqrt{\pi}} \frac{\delta_{\mu\nu}}{r^3} \int_{(\alpha r)^2}^{\infty} u e^{-u} \frac{du}{2\sqrt{u}} \quad (48)$$

$$= - \frac{4}{\sqrt{\pi}} \frac{\delta_{\mu\nu}}{r^3} \left[ \int_{(\alpha r)^2}^{\infty} e^{-u} \frac{du}{2\sqrt{u}} + \frac{1}{2} \alpha r e^{-\alpha^2 r^2} \right] \quad (49)$$

$$= - \frac{\delta_{\mu\nu}}{r^3} \left[ \text{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r e^{-\alpha^2 r^2} \right] \quad (50)$$

So the final expression for the lattice sum is

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

<sup>1</sup> Landau and Lifshitz, *The Classical Theory of Fields*.

<sup>2</sup> Chaikin and Lubensky, *Principles of Condensed Matter Physics*.

<sup>3</sup> J. M. Luttinger and L. Tisza, *Phys. Rev.* **70**, 954 (1946).

<sup>4</sup> D. Litvin, *Physica* **77**, 205 (1974).

<sup>5</sup> D. C. Johnston, *Phys. Rev. B* **93**, 014421 (2016).

<sup>6</sup> M. Enjalran and M. J. P. Gingras, *Phys. Rev. B* **70**, 174426 (2004).

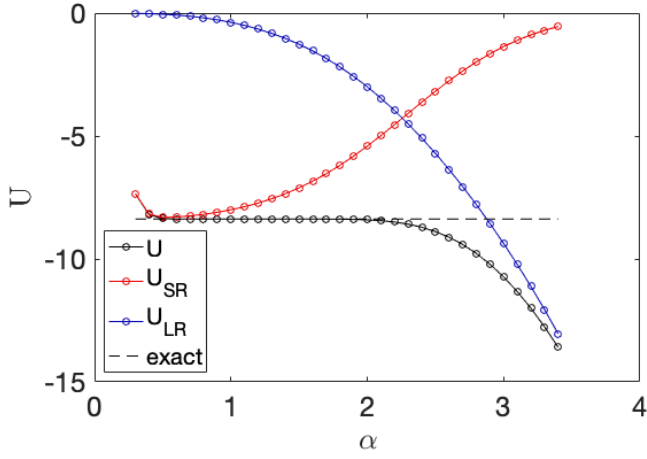


FIG. 1. Convergence of the Ewald summation with splitting parameter,  $\alpha$ , for an FCC lattice in the ferromagnetic state. The energy converges to the exact value in the range  $\alpha \in [1, 2]$ . The summation has bad convergence for a poor choice of  $\alpha$ . The Ewald summation was performed 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  $\alpha$  is chosen to be large (as expected).

- <sup>7</sup> Stasiak, Pawel, “Theoretical studies of frustrated magnets with dipolar interactions,” (2009).  
<sup>8</sup> A. Del Maestro and M. Gingras, *Journal of Physics: Condensed Matter* **16**, 3339 (2004).