I. EWALD SUMMATION

The magnetostatic energy of an infinite lattice of dipoles is

$$U = \sum_{i<j}^{\infty} \boldsymbol{S}_i \cdot \boldsymbol{J}(\boldsymbol{r}_{ij}) \cdot \boldsymbol{S}_j \tag{1}$$

where

$$\boldsymbol{J}_{\mu\nu}(\boldsymbol{r}) = -\partial_\mu \partial_\nu \frac{1}{r} \tag{2}$$

Is the coupling matrix which has no dependence on the orientation of spins. To approximate an infinite lattice sum we set periodic boundary conditions on a finite-sized system to unlimited range.

$$U = \sum_{\boldsymbol{n}}^{\infty} \sum_{i<j}^{N} \boldsymbol{S}_i \cdot \boldsymbol{J}(\boldsymbol{r}_{ij} + \boldsymbol{n}L) \cdot \boldsymbol{S}_j \tag{3}$$

$$= \sum_{i<j}^{N} \boldsymbol{S}_i \cdot \left(\sum_{\boldsymbol{n}}^{\infty} \boldsymbol{J}(\boldsymbol{r}_{ij} + \boldsymbol{n}L) \right) \cdot \boldsymbol{S}_j \tag{4}$$

where L is the linear size of the lattice containing N dipoles in the direction of cubic translation vectors and $\boldsymbol{n}$ is a translation vector of the simulation box which contains the lattice. The inner sum is conditionally convergent and can't be approximated by truncation. Ewald summation replaces this sum with two fast converging sums.

We use the identity,

$$\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-t^2 r^2} dt \tag{5}$$

Now the integral is split into two parts

$$\frac{1}{r} = \frac{2}{\sqrt{\pi}} \int_0^{\alpha} e^{-t^2 r^2} dt + \frac{1}{r} \mathrm{erfc}(\alpha r) \tag{6}$$

where erfc is the complimentary error function. The new parameter α is called the splitting parameter. So the energy may be decomposed as

$$U = U_{\mathrm{SR}} + U_{\mathrm{LR}} \tag{7}$$

The first term in (A6) contributes to the long range part of the total energy, U_{LR}, and is summed in reciprocal space. The second term in (A6) contributes to the short range part, U_{SR}, which is summed in position space.

We have,

$$U_{\mathrm{LR}} = \sum_{i<j}^{N} \boldsymbol{S}_i \cdot \boldsymbol{A}_{ij} \cdot \boldsymbol{S}_j \tag{8}$$

where

$$A_{ij}^{\mu\nu} = -\sum_{\boldsymbol{n}}^{\infty} \frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \int_0^{\alpha} e^{-t^2 |\boldsymbol{r}_{ij} + \boldsymbol{n}L|^2} dt \tag{9}$$

$$= -\frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu M(\boldsymbol{r}_{ij}) \tag{10}$$

where

$$M(\boldsymbol{r}) = \sum_{\boldsymbol{n}}^{\infty} \int_0^{\alpha} e^{-t^2 |\boldsymbol{r} + \boldsymbol{n}L|^2} dt \tag{11}$$

$$= \int \left[\sum_{\boldsymbol{n}}^{\infty} \delta(\boldsymbol{r}' - \boldsymbol{n}L) \int_0^{\alpha} e^{-t^2 |\boldsymbol{r} + \boldsymbol{r}'|^2} dt \right] d^3 r' \tag{12}$$

$$= \int \left[\frac{1}{V} \sum_{\boldsymbol{G}}^{\infty} e^{i\boldsymbol{G} \cdot \boldsymbol{r}'} \int_0^{\alpha} e^{-t^2 |\boldsymbol{r} + \boldsymbol{r}'|^2} dt \right] d^3 r' \tag{13}$$

$$= \frac{2\pi\sqrt{\pi}}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{1}{G^2} e^{-G^2/4\alpha^2} e^{-i\boldsymbol{G} \cdot \boldsymbol{r}} \tag{14}$$

So the long-range part of the coupling matrix is

$$A_{ij}^{\mu\nu} = -\frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \frac{2\pi\sqrt{\pi}}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{1}{G^2} e^{-G^2/4\alpha^2} e^{-i\boldsymbol{G} \cdot \boldsymbol{r}_{ij}} \tag{15}$$

$$= \frac{4\pi}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{G_\mu G_\nu}{G^2} e^{-G^2/4\alpha^2} e^{-i\boldsymbol{G} \cdot \boldsymbol{r}_{ij}} \tag{16}$$

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

$$-\frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \int_0^{\alpha} e^{-t^2 r^2} dt \bigg|_{\boldsymbol{r}=\boldsymbol{0}} = \frac{4\alpha^3}{3\sqrt{\pi}} \delta_{\mu\nu} \tag{17}$$

The short range contribution to the energy is

$$U_{\mathrm{SR}} = \frac{1}{2} \sum_{ij}^{N} \boldsymbol{S}_i \cdot \boldsymbol{B}_{ij} \cdot \boldsymbol{S}_j \tag{18}$$

where $\boldsymbol{B}$ is the short range part of the coupling matrix

$$B_{ij}^{\mu\nu} = -\sum_{\boldsymbol{n}}^{\infty} \frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \int_{\alpha}^{\infty} e^{-t^2 |\boldsymbol{r}_{ij} + \boldsymbol{n}L|^2} dt \tag{19}$$

$$= \sum_{\boldsymbol{n}}^{\infty} \frac{1}{|\boldsymbol{r}_{ij} + \boldsymbol{n}L|^5} \Big(|\boldsymbol{r}_{ij} + \boldsymbol{n}L|^2 X(|\boldsymbol{r}_{ij} + \boldsymbol{n}L|) \delta_{\mu\nu} \tag{20}$$

$$+ (\boldsymbol{r}_{ij} + \boldsymbol{n}L)_\mu (\boldsymbol{r}_{ij} + \boldsymbol{n}L)_\nu Y(|\boldsymbol{r}_{ij} + \boldsymbol{n}L|) \Big) \tag{21}$$

where

$$X(r) = \mathrm{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r e^{-\alpha^2 r^2} \tag{22}$$

$$Y(r) = 3\mathrm{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r (3 + 2\alpha^2 r^2) e^{-\alpha^2 r^2} \tag{23}$$

So we may decompose the total coupling strength as

$$\sum_{\boldsymbol{n}}^{\infty} \boldsymbol{J}(\boldsymbol{r}_{ij} + \boldsymbol{n}L) = \boldsymbol{A}_{ij} + \boldsymbol{B}_{ij} - \frac{4\alpha^3}{3\sqrt{\pi}} \mathbf{1} \delta_{ij} \tag{24}$$

Thus the conditionally convergent sum may be written as two fast converging sums for an appropriate choice of the splitting parameter, α. Typically Ewald summation will converge well when α is of the order of one inverse lattice spacing. Convergence in this region may be easily checked by varying α.