I. EWALD SUMMATION

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

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

So that the total electrostatic energy of the lattice is

$$U = \sum_i E_i. \tag{2}$$

The electric field produced by a dipole is[1]

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

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

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

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

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

Then equation (2) becomes

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

Where

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

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

$$U = \sum_{\boldsymbol{n}}^{\infty}\sum_{i<j}^{N}\boldsymbol{S}_i\cdot\boldsymbol{J}(\boldsymbol{r}_{ij}+\boldsymbol{n}L)\cdot\boldsymbol{S}_j \qquad i,j\in\{1,2\dots N\} \tag{8}$$

$$= \sum_{i<j}^{N}\boldsymbol{S}_i\cdot\left(\sum_{\boldsymbol{n}}^{\infty}\boldsymbol{J}(\boldsymbol{r}_{ij}+\boldsymbol{n}L)\right)\cdot\boldsymbol{S}_j \tag{9}$$

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

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

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

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

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

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

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

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

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

So the energy can be decomposed as

$$U = U_{\mathrm{SR}} + U_{\mathrm{LR}} \tag{16}$$

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.

$$U_{\mathrm{LR}} = \sum_{i<j}^{N}\boldsymbol{S}_i\cdot\boldsymbol{A}_{ij}\cdot\boldsymbol{S}_j \tag{17}$$

$$A_{ij}^{\mu\nu} = -\sum_{\boldsymbol{n}}^{\infty}\frac{2}{\sqrt{\pi}}\partial_\mu\partial_\nu\int_0^\alpha e^{-t^2|\boldsymbol{r}_{ij}+\boldsymbol{n}L|^2}dt \tag{18}$$

$$= -\frac{2}{\sqrt{\pi}}\partial_\mu\partial_\nu\sum_{\boldsymbol{n}}^{\infty}\int_0^\alpha e^{-t^2|\boldsymbol{r}_{ij}+\boldsymbol{n}L|^2}dt \tag{19}$$

$$= -\frac{2}{\sqrt{\pi}}\partial_\mu\partial_\nu M(\boldsymbol{r})\bigg|_{\boldsymbol{r}=\boldsymbol{r}_{ij}} \tag{20}$$

Where

$$M(\boldsymbol{r}) = \sum_{\boldsymbol{n}}^{\infty}\int_0^\alpha e^{-t^2|\boldsymbol{r}+\boldsymbol{n}L|^2}dt \tag{21}$$

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

$$= \int\left[\frac{1}{V}\sum_{\boldsymbol{G}}^{\infty}e^{i\boldsymbol{G}\cdot\boldsymbol{r}'}\int_0^\alpha e^{-t^2|\boldsymbol{r}+\boldsymbol{r}'|^2}dt\right]d^3r' \tag{23}$$

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

$$= \frac{1}{V}\sum_{\boldsymbol{G}}^{\infty}e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}\mathcal{F}\left[\int_0^\alpha e^{-t^2\boldsymbol{r}^2}dt\right](\boldsymbol{G}) \tag{25}$$

$$= \frac{2\pi\sqrt{2\pi}}{V}\sum_{\boldsymbol{G}}^{\infty}e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}\int_0^\alpha\frac{1}{2\sqrt{2}t^3}e^{-G^2/4t^2}dt \tag{26}$$

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

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

$$= \frac{2\pi\sqrt{\pi}}{V}\sum_{\boldsymbol{G}}^{\infty}\frac{1}{G^2}e^{-G^2/4\alpha^2}e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} \tag{29}$$

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]

$$\sum_{\boldsymbol{n}}^{\infty} \delta(\boldsymbol{r} - \boldsymbol{n}L) = \frac{1}{V} \sum_{\boldsymbol{G}}^{\infty} e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} \tag{30}$$

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

$$\begin{aligned}
\int L \sum_{n}^{\infty} \delta(x - nL)dx &= \sum_{n}^{\infty} \int_{(x-nL)/2}^{(x+nL)/2} \delta(x - nL)dx && (31)\\
&= \sum_{n}^{\infty} \int_{(x-nL)/2}^{(x+nL)/2} \sum_{G}^{\infty} e^{-iG(x-nL)}dx && (32)\\
&= \int \sum_{G}^{\infty} e^{-iGx}dx && (33)
\end{aligned}$$

which can be easily generalized to the 3D case.

The long-range coupling matrix is

$$\begin{aligned}
A_{ij}^{\mu\nu} &= -\frac{2}{\sqrt{\pi}}\partial_\mu\partial_\nu \frac{2\pi\sqrt{\pi}}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{1}{G^2} e^{-G^2/4\alpha^2} e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_{ij}} && (34)\\
&= -\frac{4\pi}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{1}{G^2} e^{-G^2/4\alpha^2} \left(\partial_\mu\partial_\nu e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_{ij}}\right) && (35)\\
&= \frac{4\pi}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{G_\mu G_\nu}{G^2} e^{-G^2/4\alpha^2} e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_{ij}} && (36)
\end{aligned}$$

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.

$$\begin{aligned}
&-\frac{2}{\sqrt{\pi}}\partial_\mu\partial_\nu \int_0^\alpha e^{-t^2r^2}dt\Big|_{\boldsymbol{r}=\boldsymbol{0}} && (37)\\
&= -\int_0^\alpha \left(\frac{8}{\sqrt{\pi}}t^4 r_\mu r_\nu e^{-r^2t^2} - \frac{4}{\sqrt{\pi}}t^2\delta_{\mu\nu}e^{-r^2t^2}\right)\Big|_{\boldsymbol{r}=\boldsymbol{0}} dt && (38)\\
&= \frac{4\alpha^3}{3\sqrt{\pi}}\delta_{\mu\nu} && (39)
\end{aligned}$$

So we have the correction to (17)

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

The short range contribution to the energy is

$$U_{\mathrm{SR}} = \frac{1}{2}\sum_{ij}^{N} \boldsymbol{S}_i \cdot \boldsymbol{B}_{ij} \cdot \boldsymbol{S}_j \tag{41}$$

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

$$\begin{aligned}
B_{ij}^{\mu\nu} &= -\sum_{\boldsymbol{n}}^{\infty} \frac{2}{\sqrt{\pi}}\partial_\mu\partial_\nu \int_\alpha^\infty e^{-t^2r_{ij}^2}dt && (42)\\
&= -\sum_{\boldsymbol{n}}^{\infty} \int_\alpha^\infty \left(\frac{8}{\sqrt{\pi}}t^4 r_{ij}^\mu r_{ij}^\nu e^{-r_{ij}^2t^2} - \frac{4}{\sqrt{\pi}}t^2\delta_{\mu\nu}e^{-r_{ij}^2t^2}\right)dt && (43)
\end{aligned}$$

Computing the first integral

$$\begin{aligned}
&\frac{8}{\sqrt{\pi}}r^\mu r^\nu \int_\alpha^\infty t^4 e^{-r^2t^2}dt && (44)\\
&= \frac{8}{\sqrt{\pi}}\frac{r^\mu r^\nu}{r^5}\int_{(\alpha r)^2}^\infty u^2 e^{-u}\frac{du}{2\sqrt{u}}, \quad u = t^2r^2 && (45)
\end{aligned}$$

Integrating by parts twice

$$\begin{aligned}
&\frac{4}{\sqrt{\pi}}\frac{r^\mu r^\nu}{r^5}\int_{(\alpha r)^2}^\infty u^{3/2}e^{-u}du && (46)\\
&= \frac{4}{\sqrt{\pi}}\frac{r^\mu r^\nu}{r^5}\left[\int_{(\alpha r)^2}^\infty \frac{3}{2}u^{1/2}e^{u}du + \alpha^3r^3e^{-\alpha^2r^2}\right] && (47)\\
&= \frac{4}{\sqrt{\pi}}\frac{r^\mu r^\nu}{r^5}\left[\frac{3}{2}\left[\int_{(\alpha r)^2}^\infty e^{u}\frac{du}{2\sqrt{u}} + \alpha r e^{-\alpha^2r^2}\right] + \alpha^3r^3e^{-\alpha^2r^2}\right] && (48)\\
&= \frac{r^\mu r^\nu}{r^5}\left[3\mathrm{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}}\alpha r(3 + 2\alpha^2r^2)e^{-\alpha^2r^2}\right] && (49)
\end{aligned}$$

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

$$\begin{aligned}
&-\frac{4}{\sqrt{\pi}}\delta_{\mu\nu}\int_\alpha^\infty t^2e^{-t^2r_{ij}^2}dt && (50)\\
&= -\frac{4}{\sqrt{\pi}}\frac{\delta_{\mu\nu}}{r_{ij}^3}\int_{(\alpha r_{ij})^2}^\infty ue^{-u}\frac{du}{2\sqrt{u}} && (51)\\
&= -\frac{4}{\sqrt{\pi}}\frac{\delta_{\mu\nu}}{r_{ij}^3}\left[\int_{(\alpha r_{ij})^2}^\infty e^{-u}\frac{du}{2\sqrt{u}} + \frac{1}{2}\alpha r_{ij}e^{-\alpha^2r_{ij}^2}\right] && (52)\\
&= -\frac{\delta_{\mu\nu}}{r_{ij}^3}\left[\mathrm{erfc}(\alpha r_{ij}) + \frac{2}{\sqrt{\pi}}\alpha r_{ij}e^{-\alpha^2r_{ij}^2}\right] && (53)
\end{aligned}$$

So the final expression for the lattice sum is

$$\boxed{\begin{aligned}
\sum_{\boldsymbol{n}}^{\infty}\boldsymbol{J}(\boldsymbol{r}_{ij} + \boldsymbol{n}L) &= \boldsymbol{A}_{ij} + \boldsymbol{B}_{ij} - \frac{4\alpha^3}{3\sqrt{\pi}}\delta_{ij}\boldsymbol{1}\\
\boldsymbol{A}_{ij} &= \frac{4\pi}{V}\sum_{\boldsymbol{G}}^{\infty}\frac{\boldsymbol{G}\otimes\boldsymbol{G}}{G^2}e^{-G^2/4\alpha^2}e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_{ij}}\\
B_{ij} &= \sum_{\boldsymbol{n}}^{\infty}\frac{1}{|\boldsymbol{r}_{ij} + \boldsymbol{n}L|^5}\Big(|\boldsymbol{r}_{ij} + \boldsymbol{n}L|^2X(|\boldsymbol{r}_{ij} + \boldsymbol{n}L|)\boldsymbol{1}\\
&\quad + (\boldsymbol{r}_{ij} + \boldsymbol{n}L)\otimes(\boldsymbol{r}_{ij} + \boldsymbol{n}L)Y(|\boldsymbol{r}_{ij} + \boldsymbol{n}L|)\Big)\\
X(r) &= \mathrm{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}}\alpha r e^{-\alpha^2r^2}\\
Y(r) &= 3\mathrm{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}}\alpha r(3 + 2\alpha^2r^2)e^{-\alpha^2r^2}
\end{aligned}}$$

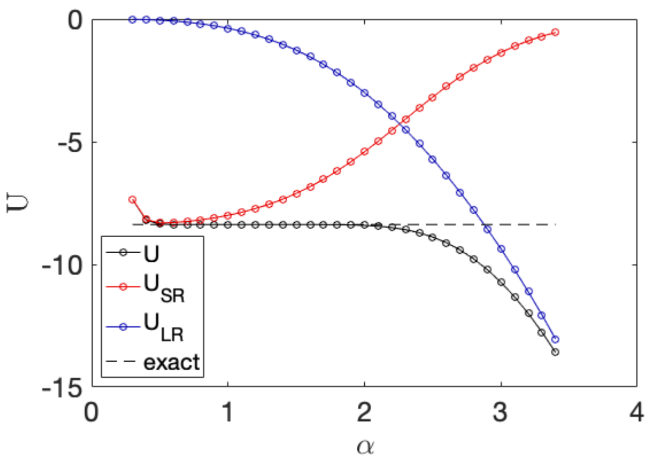

FIG. 1. Convergence of the Ewald summation with splitting parameter, α, for an FCC lattice in the ferromagnetic state. The energy converges to the exact value in the range $\alpha \in [1, 2]$. The summation has bad convergence for a poor choice of α. The Ewald summation was performed with a length constraint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

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