I. EWALD SUMMATION

A. Computation of Dipolar Lattice Sums

The total energy of an infinite lattice of dipoles is

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

where

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

is the coupling matrix for dipoles separated by a distance, $\boldsymbol{r}$. To approximate an infinite lattice sum we set periodic boundary conditions on a finite-sized system to unlimited range.

$$\begin{aligned} U &= \sum_{\boldsymbol{n}}^{\infty} \sum_{i<j}^{N} \boldsymbol{\mu}_i \cdot \boldsymbol{J}(\boldsymbol{r}_{ij} + \boldsymbol{n}L) \cdot \boldsymbol{\mu}_j & (3) \\ &= \sum_{i<j}^{N} \boldsymbol{\mu}_i \cdot \left(\sum_{\boldsymbol{n}}^{\infty} \boldsymbol{J}(\boldsymbol{r}_{ij} + \boldsymbol{n}L) \right) \cdot \boldsymbol{\mu}_j & (4) \end{aligned}$$

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.

The long range contribution to the energy is

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

where $\boldsymbol{A}_{ij}$ is the long range part of the coupling matrix

$$\begin{aligned} A_{ij}^{\mu\nu} &= \sum_{\boldsymbol{n}}^{\infty} \frac{2}{\sqrt{\pi}} \left[-\partial_\mu \partial_\nu \int_0^{\alpha} e^{-t^2 r^2} dt \right]_{\boldsymbol{r}=\boldsymbol{r}_{ij}+\boldsymbol{n}L} & (9) \\ &= \frac{2}{\sqrt{\pi}} \int \sum_{\boldsymbol{n}}^{\infty} \delta(\boldsymbol{r}' - \boldsymbol{n}L) \left[-\partial_\mu \partial_\nu \int_0^{\alpha} e^{-t^2 r^2} dt \right]_{\boldsymbol{r}=\boldsymbol{r}_{ij}+\boldsymbol{r}'} d^3 r' & (10) \\ &= \frac{2}{\sqrt{\pi}} \int \frac{1}{V} \sum_{\boldsymbol{G}}^{\infty} e^{-i\boldsymbol{G}\cdot\boldsymbol{r}'} \left[-\partial_\mu \partial_\nu \int_0^{\alpha} e^{-t^2 r^2} dt \right]_{\boldsymbol{r}=\boldsymbol{r}_{ij}+\boldsymbol{r}'} d^3 r' & (11) \\ &= \frac{\sqrt{2}\, 4\pi}{V} \sum_{\boldsymbol{G}} \mathcal{F}_{(\boldsymbol{G})} \left(-\partial_\mu \partial_\nu \int_0^{\alpha} e^{-t^2 r^2} dt \right) e^{i\boldsymbol{G}\cdot\boldsymbol{r}_{ij}} & (12) \\ &= -\frac{\sqrt{2}\, 4\pi}{V} \sum_{\boldsymbol{G}} G_\mu G_\nu \int_0^{\alpha} \mathcal{F}_{(\boldsymbol{G})} \left(e^{-t^2 r^2} \right) dt \; e^{i\boldsymbol{G}\cdot\boldsymbol{r}_{ij}} & (13) \\ &= \frac{4\pi}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{G_\mu G_\nu}{G^2} e^{-G^2/4\alpha^2} e^{i\boldsymbol{G}\cdot\boldsymbol{r}_{ij}} & (14) \end{aligned}$$

where V is the volume of the simulation box and $\mathcal{F}_{(\boldsymbol{G})}$ is the 3D Fourier transform evaluated at $\boldsymbol{G}$.

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.

$$-\frac{2}{\sqrt{\pi}} \partial_\mu \partial_\nu \int_0^{\alpha} e^{-t^2 r^2} dt \bigg|_{\boldsymbol{r}=\boldsymbol{0}} = \frac{4\alpha^3}{3\sqrt{\pi}} \delta_{\mu\nu} \tag{15}$$

The short range contribution to the energy is

$$U_{\mathrm{SR}} = \frac{1}{2} \sum_{ij}^{N} \boldsymbol{\mu}_i \cdot \boldsymbol{B}_{ij} \cdot \boldsymbol{\mu}_j \tag{16}$$

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

$$\begin{aligned} B_{ij}^{\mu\nu} &= \sum_{\boldsymbol{n}}^{\infty} \left[-\partial_\mu \partial_\nu \left(\frac{\mathrm{erfc}(\alpha r)}{r} \right) \right]_{\boldsymbol{r}=\boldsymbol{r}_{ij}+\boldsymbol{n}L} & (17) \\ &= \sum_{\boldsymbol{n}}^{\infty} \left[\frac{1}{r^3} X(r) \delta_{\mu\nu} + \frac{r_\mu r_\nu}{r^5} Y(r) \right]_{\boldsymbol{r}=\boldsymbol{r}_{ij}+\boldsymbol{n}L} & (18) \end{aligned}$$

where

$$X(r) = \mathrm{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r e^{-\alpha^2 r^2} \tag{19}$$

$$Y(r) = 3\mathrm{erfc}(\alpha r) + \frac{2}{\sqrt{\pi}} \alpha r (3 + 2\alpha^2 r^2) e^{-\alpha^2 r^2} \tag{20}$$

So we may decompose the total coupling strength as

$$\boxed{\sum_{\boldsymbol{n}}^{\infty} \boldsymbol{J}(\boldsymbol{r}_{ij} + \boldsymbol{n}L) = \boldsymbol{A}_{ij} + \boldsymbol{B}_{ij} - \frac{4\alpha^3}{3\sqrt{\pi}} \boldsymbol{1} \delta_{ij}} \tag{21}$$

Thus the conditionally convergent sum may be written as two fast converging sums which may be approximated by truncation 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.

For lattice systems of dipoles, the matrices, $\boldsymbol{A}$ and $\boldsymbol{B}$, may be computed once at the initialization stage of a Monte Carlo simulation. This reduces the computational cost of each Monte Carlo step to $O(N)$.

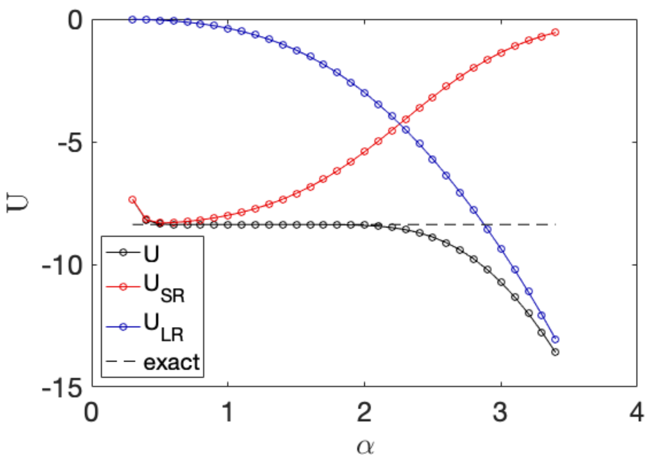

FIG. 1. Convergence of the Ewald sum with splitting parameter, α, for an FCC lattice in the ferromagnetic state. The energy converges to the exact value in the range $\alpha \in [1,2]$. The summation has bad convergence for a poor choice of α. The Ewald summation was performed with a length constraint 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).

B. The Fourier Transform of J

The derivation of the Fourier transform of the coupling strength, $\boldsymbol{J}(\boldsymbol{q})$, parallels the derivation of the lattice sum in (A21). For simplicity, we present a calculation of $\boldsymbol{J}(\boldsymbol{q})$ for Bravais lattices only. A more general derivation is given in Ref.[1,2].

The discrete Fourier transform of the coupling strength is

$$\tilde{\boldsymbol{J}}(\boldsymbol{q}) = \sum_{\boldsymbol{n}}^{\infty} \boldsymbol{J}(\boldsymbol{n}a) e^{i\boldsymbol{q}\cdot\boldsymbol{n}a} = \tilde{\boldsymbol{A}}_{\boldsymbol{q}} + \tilde{\boldsymbol{B}}_{\boldsymbol{q}} - \frac{4\alpha^3}{3\sqrt{\pi}} \mathbf{1}\delta_{ij} \tag{22}$$

where $\tilde{\boldsymbol{A}}_{\boldsymbol{q}}$ is computed in a reciprocal space sum

$$\tilde{A}^{\mu\nu}_{\boldsymbol{q}} = \sum_{\boldsymbol{n}}^{\infty} \frac{2}{\sqrt{\pi}} \left[-\partial_\mu \partial_\nu \int_0^\alpha e^{-t^2 r^2} dt \right]_{r=\boldsymbol{n}a} e^{i\boldsymbol{q}\cdot\boldsymbol{n}a} \tag{23}$$

$$= \frac{2}{\sqrt{\pi}} \int \sum_{\boldsymbol{n}}^{\infty} \delta(\boldsymbol{r}' - \boldsymbol{n}a) \left[-\partial_\mu \partial_\nu \int_0^\alpha e^{-t^2 r^2} dt \right]_{r=\boldsymbol{r}'} e^{i\boldsymbol{q}\cdot\boldsymbol{r}'} d^3 r' \tag{24}$$

$$= \frac{2}{\sqrt{\pi}} \int \frac{1}{V} \sum_{\boldsymbol{G}}^{\infty} e^{-i(\boldsymbol{G}-\boldsymbol{q})\cdot\boldsymbol{r}'} \left[-\partial_\mu \partial_\nu \int_0^\alpha e^{-t^2 r^2} dt \right]_{r=\boldsymbol{r}'} d^3 r' \tag{25}$$

$$= \frac{\sqrt{2}\, 4\pi}{V} \sum_{\boldsymbol{G}} \mathcal{F}_{(\boldsymbol{G}-\boldsymbol{q})} \left(-\partial_\mu \partial_\nu \int_0^\alpha e^{-t^2 r^2} dt \right) \tag{26}$$

$$= -\frac{\sqrt{2}\, 4\pi}{V} \sum_{\boldsymbol{G}} (\boldsymbol{q}-\boldsymbol{G})_\mu (\boldsymbol{q}-\boldsymbol{G})_\nu \int_0^\alpha \mathcal{F}_{(\boldsymbol{G}-\boldsymbol{q})} \left(e^{-t^2 r^2} \right) dt \tag{27}$$

$$= \frac{4\pi}{V} \sum_{\boldsymbol{G}}^{\infty} \frac{(\boldsymbol{q}-\boldsymbol{G})_\mu (\boldsymbol{q}-\boldsymbol{G})_\nu}{|\boldsymbol{q}-\boldsymbol{G}|^2} e^{-|\boldsymbol{q}-\boldsymbol{G}|^2/4\alpha^2} \tag{28}$$

and $\tilde{\boldsymbol{B}}_{\boldsymbol{q}}$ is computed straightforwardly in a position space sum

$$\tilde{B}^{\mu\nu}_{\boldsymbol{q}} = \sum_{\boldsymbol{n}}^{\infty} \left[\frac{1}{r^3} X(r) \delta_{\mu\nu} + \frac{r_\mu r_\nu}{r^5} Y(r) \right]_{r=\boldsymbol{n}a} e^{i\boldsymbol{q}\cdot\boldsymbol{n}a} \tag{29}$$

where X and Y are the functions defined in (A19) and (A20) respectively.

[1] M. Enjalran and M. J. P. Gingras, Phys. Rev. B **70**, 174426 (2004).
[2] Huang and Born, *Dynamical theory of crystal lattices* (1954).
[3] Landau and Lifshitz, *The Classical Theory of Fields*.
[4] Chaikin and Lubensky, *Principles of Condensed Matter Physics*.