2020-08-27 Derivation of Dipolar Fields in NiO

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The temperature scaling of the effective anisotropy constant of dipole anisotropy in NiO was calculated numerically. A scaling exponent of 2 was obtained which is consistent with shape anisotropy in a ferromagnet. Analytic calculations of dipole fields on a 2D lattice elucidate the temperature scaling and agree with the numerical model. It is hoped this result will help the design of room temperature spintronics devices using the prototypical antiferromagnet NiO.

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I. INTRODUCTION

Antiferromagnets are expected to be used in future generations of spintronics devices. They exhibit ultrafast dynamics [1], produce no stray field and have large magnetoresistive effects [2]. Prototype memory devices have been created using antiferromagnetic materials [3] which are compatible with current microelectronic devices. NiO can be used as an enhancer of a spin current [4, 5]. The degree of enhancement is sensitive to the value of the anisotropy. To make a functional device using this material, the size of the free energy barrier between hard and easy directions at finite temperatures must be known. Numerical calculations of the finite temperature anisotropy of NiO have been carried out to obtain the anisotropy constant at finite temperature.

The free energy barrier between the hard and easy directions is reduced at finite temperatures due to fluctuations in the spin direction. This can be implemented into phenomenological equations for anisotropic magnetic materials by introducing a temperature dependent anisotropy constant, $K(T)$. Classical theory from Zener and Callen-Callen [6, 7] states that this is given by a scaling exponent

$$\frac{K(T)}{K(T=0\mathrm{K})} \propto M(T)^{\alpha} \tag{1}$$

Where $M(T)$ is the magnetic order parameter at finite temperature and α is the scaling exponent. The finite temperature energy barrier for single-ion magnetocrystalline anisotropies is trivial and given by Callen-Callen theory [7] at low temperature when nonlinear effects are negligible. Long range dipole-dipole interactions are the largest source of anisotropy in NiO and

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leads to an easy-plane ground state of ferromagnetically aligned (111) planes of spins which are antiparallel to neighbour planes (see Fig3).

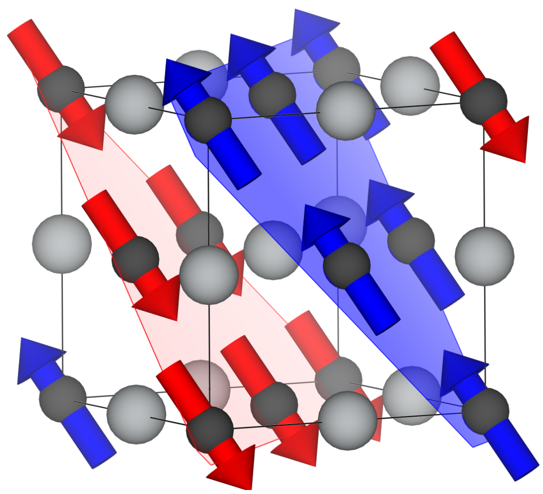

FIG. 1: The conventional unit cell of NiO. Ni sites are represented by small grey spheres with a spin vector which is either blue or red, O sites are lighter spheres. Ferromagnetically aligned (111) planes are highlighted.

Long range anisotropies usually cannot be calculated analytically and their scaling exponents can be non-integer [8]. Often long range anisotropies are mapped to a local anisotropy to simplify calculations but this is insufficient for reproducing finite temperature behaviour [9, 10]. Therefore numerical methods were employed. A scaling exponent of two was calculated, and further analytic equations show that this is primarily due to a magnetostatic (shape) anisotropy within a ferromagnetically aligned (111) plane.

II. METHODS

To model finite temperature anisotropy in NiO a specialist Monte Carlo method - constrained Monte Carlo - was used on an atomistic spin model including only magnetic Ni sites [11]. The magnetic Hamiltonian included nearest neighbour and next-nearest neighbour exchange interactions, magnetic dipole-dipole interactions and a second order cubic anisotropy

$$\mathcal{H} = -\frac{1}{2}\sum_{\langle ij\rangle} \mathbf{S}_i \mathbb{J}_{ij} \mathbf{S}_j - \frac{1}{2}\sum_{i\neq j} \mathbf{S}_i \mathbb{D}_{ij} \mathbf{S}_j - \sum_i K_2 (\mathrm{S}_{ix}\mathrm{S}_{iy}\mathrm{S}_{iz})^2 \tag{2}$$

$\mathbb{J}_{ij}$ is the exchange tensor with exchange constants $J_{1+} = 1.39\mathrm{meV}$, $J_{1-} = 1.35\mathrm{meV}$ and $J_2 = -19.06\mathrm{meV}$ where J_{1+} is the coupling between parallel nearest neighbours, J_{1-} is the coupling between antiparallel nearest neighbours and J_2 is between next-nearest neighbours [12] - the broken degeneracy of nearest-neighbour exchange interactions gives eight distinct magnetic sublattices [13]. $\mathbf{S}_{i,j}$ are classical spin vectors of unit length and $\mathbb{D}_{ij}$ is the magnetic dipole-dipole tensor given by

$$\mathbb{D}_{ij} = \frac{\mu_0 \mu_i \mu_j}{4\pi} \frac{3\hat{\mathbf{r}}_{ij}\hat{\mathbf{r}}_{ij} - 1}{|\mathbf{r}_{ij}|^3} \tag{3}$$

Where μ_0 is the vacuum permeability, μ_i, μ_j are the spin magnetic moments of sites i and j - $1.65\mu_B$ for Ni sites [14], $\mathbf{r}_{ij}$ is the displacement vector between sites i and j, and $\hat{\mathbf{r}}_{ij}$ is the corresponding unit vector. The final term is a second order cubic magnetocrystalline anisotropy of strength $K_2 = 2.27\mu\mathrm{eV}$ [13].

The constrained Monte Carlo method fixes the direction of the order parameter of a magnetic site by altering the Metropolis algorithm to include two spins in each trial move. This doesn't require the use of a fictitious Zeeman energy to impose the constraint unlike other methods. By allowing other magnetic sites to equilibrate by the Metropolis algorithm, the free energy of the system can be reconstructed by the following result [11]

$$\mathcal{F}(\hat{\mathbf{M}}) = \mathcal{F}(\hat{\mathbf{M}}_0) + \int_{\hat{\mathbf{M}}_0}^{\hat{\mathbf{M}}} (\hat{\mathbf{M}}' \times \mathbf{T}) \ d\hat{\mathbf{M}}' \tag{4}$$

Where $\mathcal{F}$ is the free energy, $\hat{\mathbf{M}}$ is the unit vector of the magnetisation and $\mathbf{T}$ is the macroscopic torque on the magnetisation vector. This method can be used at any temperature allowing the effective anisotropy constant to be calculated. In the magnetic system considered, there are eight distinct magnetic sites [13] and four order parameters (Néel vectors). One of these Néel vectors is constrained while allowing other sites to be sampled using the Metropolis algorithm.

Analytic calculations were carried out which show that the energy of the dipole-dipole interactions can be written as $E \propto \mathrm{M}(T)^2$ where $\mathrm{M}(T)$ is the magnetisation of a single (111) plane at finite temperature. The total dipole anisotropy of a single magnetic site in the centre of bulk NiO was split into two contributions; intraplane dipole interactions (ferromagnetic film one atom thick) and interplane dipole interactions. The former result is well known from magnetostatics - shape anisotropy, the latter was calculated by applying a Fourier transformation to the dipolar field from an infinite 2D triangular magnetic lattice, similar to the work of *Tsymbal et al* [15].

In contrast to Tsymbal's work which assumes the total contribution from intraplane dipole interactions and the sum of a few neighbour layers gives the result from magnetostatics, here the atomically thin ferromagnetic film is treated as a true 2D film in which the ratio of the lateral dimension R and thickness L is $\frac{R}{L} = \infty$ and neighbour layers act as a deviation from this. In this case, the intraplane contribution to the anisotropy energy is given by the following equation in units of J/magnetic site

$$\begin{aligned} \mathrm{E}^0_{\mathrm{IP}}(T) &= -\frac{1}{3}\left(\frac{1}{2}\mu_0\langle M\rangle^2 V\right) \\ \mathrm{E}^0_{\mathrm{OOP}}(T) &= \frac{2}{3}\left(\frac{1}{2}\mu_0\langle M\rangle^2 V\right) \end{aligned} \tag{5}$$

Where the superscript denotes the neighbour layer number from the magnetic site, the subscript denotes an in-plane (IP) or out-of-plane (OOP) magnetisation direction, $\langle M\rangle$ denotes the thermal average of the layer magnetisation and V is taken to be the volume of the Wigner-Sietz cell for Ni sites in NiO and is taken as 18.181Å^3. This gives $E^0_{\mathrm{IP}}(T = 0K) = -2.69710^{-24}$J/site and $E^0_{\mathrm{OOP}}(T = 0K) = 5.39510^{-24}$J/site. Interplane contributions are calculated from the magnetic potential on a triangular 2D lattice (see Fig 2). [does this need to be explicitly a NiO (111) plane?]

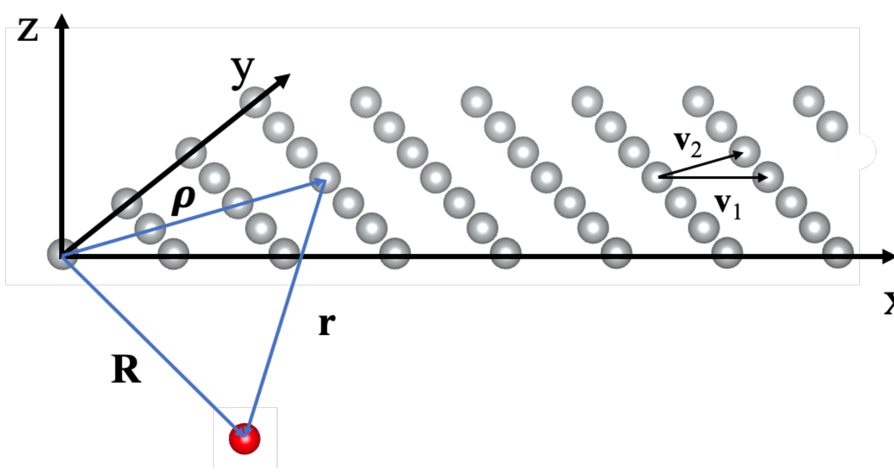

FIG. 2: A single plane of (111) textured NiO with Ni sites represented as grey spheres. Oxygen sites have been removed for clarity. Primitive intraplane vectors are denoted $\mathbf{v}_1$ and $\mathbf{v}_2$.

The magnetic potential at some point in space $\mathbf{x} = (x, y, z)$ for a system of discrete dipoles at positions $\mathbf{s}_i$ is given as

$$\Phi(x, y, z) = \frac{1}{4\pi}\sum_i \frac{\boldsymbol{\mu}_i \cdot \mathbf{r}_i}{|\mathbf{r}_i|^3} \tag{6}$$

Where the sum is over all dipole moments $\boldsymbol{\mu}_i$ and the vector $\mathbf{r}_i = \mathbf{x} - \mathbf{s}_i$. For the 2D magnetic film of NiO, $\mu = 1.65\mu_B$, $\mathbf{s}_i = n_i\mathbf{v}_1 + m_i\mathbf{v}_2$ with n, m are integers and $\mathbf{v}_1 = (\frac{1}{2}, 0, 0)a$, $\mathbf{v}_2 = (-\frac{1}{4}, \frac{\sqrt{3}}{4}, 0)a$ and $a = 5.90298\text{Å}$ is the lattice parameter.

III. INTRODUCING THE ANALYTIC DERIVATION

A. Discrete Dipole-Dipole Interactions

Magnetic dipole-dipole interactions in an atomistic formalism are pairwise interactions between magnetic moments. In a lattice this can lead to an intrinsic anisotropy of magnetostatic origin which reflects the symmetry of the magnetic lattice and can be mapped to the phenomenological equations for magnetocrystalline anisotropy. The dipole B-field due to a magnetic moment $\boldsymbol{\mu}$ is

$$\mathbf{B} = -\frac{\mu_0}{4\pi}\frac{3(\boldsymbol{\mu}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}} - \boldsymbol{\mu}}{|\mathbf{r}|^3} \tag{7}$$

Where μ_0 is the permeability of free space, $\mathbf{r}$ is the displacement between the magnetic moment and a point in space and $\hat{\mathbf{r}}$ is its unit vector.

For analytical calculations, it is convenient to work directly with the potential, Φ. This is related to the field by

$$\mathbf{B}(\mathbf{r}) = -\mu_0\nabla\Phi \tag{8}$$

Dropping the factor $\frac{1}{4\pi}$ (to be reintroduced later), the magnetic potential due to a single atom is therefore

$$\Phi(\mathbf{r}) = \frac{\boldsymbol{\mu}\cdot\mathbf{r}}{|\mathbf{r}|^3} \tag{9}$$

B. Dipole Anisotropy in NiO

NiO is a antiferromagnetic insulator with a (111) easy-plane dipole anisotropy which can be mapped to a uniaxial magnetocrystalline anisotropy. The scaling exponent of the effective anisotropy constant has been modelled to be 2. This can be expressed as

$$K_{\text{dip}}(T) \propto M_{AF}(T)^2 \tag{10}$$

Where $K_{\text{dip}}(T)$ is the anisotropy constant at finite temperature and $M_{AF}(T)$ is the staggered magnetisation. This differs from the temperature scaling of a magnetocrystalline uniaxial anisotropy, but coincides with the value for shape anisotropy - another magnetostatic anisotropy in ***ferromagnets*** dependent on the geometry of the system (thin film, ellipsoidal, etc). This is because the magnetic ground state of NiO is ferromagnetically aligned (111) sheets of spins which are aligned antiparallel to nearest neighbour sheets. This is similar to atomically thin ferromangetic films stacked antiparallel with each film having a shape anisotropy. In this case, the anisotropy is intrinsic to the magnetic structure and independent of geometry of the superlattice.

C. Motivation for the Calculation

To give a convincing argument that this is the case, for a given atom, the dipolar field of each sheet of atoms must be calculated for both the easy plane (in-plane) and hard axis (out-of-plane). Consider an atom in NiO. The magnetisation of that layer is given as $\langle\mathbf{M}_0\rangle$ where $\langle...\rangle$ denotes a thermodynamic average. The magnetisation of the *n*th neighbour sheet is given as $\langle\mathbf{M}_n\rangle = (-1)^{n+1}\langle\mathbf{M}_0\rangle$. Since all magnetic atoms are equivalent, $|\langle\mathbf{M}_n\rangle| = |\langle\mathbf{M}_0\rangle| = |\langle\mathbf{M}_{AF}\rangle|$. If the dipole anisotropy can be recast in this way, the anisotropy constant can be shown to take the form

$$K_{\text{dip}}(T) \propto |\langle\mathbf{M}_{AF}\rangle|^2 \tag{11}$$

Giving the simulated scaling exponent.

IV. REQUIRED KNOWLEDGE

A. The Magnetic Lattice

Below, the magnetic structure of NiO is given (Fig 3)

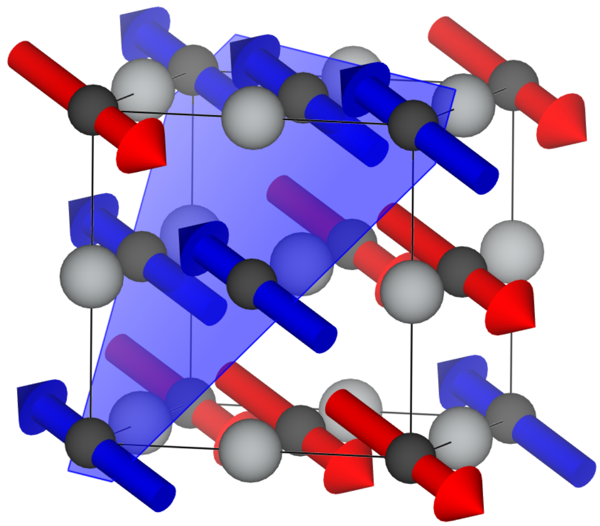

FIG. 3: Magnetic unit cell of NiO. Blue plane is a (111) plane of ferromagnetically aligned spins

The JAMS config file for (111) textured NiO is as follows

```
materials = (
{ name      = "Ni+";
  moment    = 1.65;
  alpha     = 0.01;
  spin      =[0.0, 0.0, 1.0];},
{ name      = "Ni-";
  moment    = 1.65;
  alpha     = 0.01;
  spin      =[-0.0, -0.0, -1.0];}
);
unitcell: {
   coordinate_format = "fractional";
   calculate_interaction_vectors = 1.01;
   parameter = 4.17404e-10
   basis = (
    [1.4142136, -0.7071068, 0.0],
    [0.0, 1.2247449, 0.0],
    [0.0, 0.0, 3.4641016]);
positions = (
     ("Ni+", [0.000000000,         0.000000000,         0.000000000]),
     ("Ni+", [0.333333333,         0.666666667,         0.333333333]),
     ("Ni+", [0.666666667,         0.333333333,         0.666666667]),
     ("Ni+", [0.833333333,         0.166666667,         0.333333333]),
     ("Ni+", [0.166666667,         0.833333333,         0.666666667]),
     ("Ni+", [0.500000000,         0.500000000,         0.000000000]),
     ("Ni+", [0.833333333,         0.666666667,         0.333333333]),
     ("Ni+", [0.166666667,         0.333333333,         0.666666667]),
     ("Ni+", [0.500000000,         0.000000000,         0.000000000]),
     ("Ni+", [0.333333333,         0.166666667,         0.333333333]),
```

```
    ("Ni+", [0.666666667,          0.833333333,          0.666666667]),
    ("Ni+", [0.000000000,          0.500000000,          0.000000000]),
    ("Ni-", [0.666666667,          0.333333333,          0.166666667]),
    ("Ni-", [0.000000000,          0.000000000,          0.500000000]),
    ("Ni-", [0.333333333,          0.666666667,          0.833333333]),
    ("Ni-", [0.166666667,          0.833333333,          0.166666667]),
    ("Ni-", [0.500000000,          0.500000000,          0.500000000]),
    ("Ni-", [0.833333333,          0.166666667,          0.833333333]),
    ("Ni-", [0.666666667,          0.833333333,          0.166666667]),
    ("Ni-", [0.000000000,          0.500000000,          0.500000000]),
    ("Ni-", [0.333333333,          0.166666667,          0.833333333]),
    ("Ni-", [0.166666667,          0.333333333,          0.166666667]),
    ("Ni-", [0.500000000,          0.000000000,          0.500000000]),
    ("Ni-", [0.833333333,          0.666666667,          0.833333333])
    );
};
```

This gives the expected 12 nearest neighbours separated by a distance $\frac{\sqrt{2}}{2} \times 4.17404\text{Å}$ and 6 next nearest neighbours separated by 4.17404Å. In fractional coordinates, the intraplane vectors are $\mathbf{v}_{1frac} = \left(\frac{1}{2}, 0, 0\right)$ and $\mathbf{v}_{2frac} = \left(0, \frac{1}{2}, 0\right)$, and the interplane vector is $\mathbf{v}_{3frac} = \left(\frac{1}{6}, \frac{1}{3}, \frac{1}{6}\right)$. If we move to cartesian coordinates and change the basis so the lattice parameter is $\sqrt{2}\times 4.17404\text{Å}$, we obtain

$$
\begin{aligned}
\mathbf{v}_1 &= \left(\frac{1}{2}, 0, 0\right) a \\
\mathbf{v}_2 &= \left(-\frac{1}{4}, \frac{\sqrt{3}}{4}, 0\right) a \\
\mathbf{v}_3 &= \left(0, \frac{\sqrt{3}}{6}, \frac{\sqrt{6}}{6}\right) a
\end{aligned}
\tag{12}
$$

Where $a = 5.90434\text{Å}$. This is the infinite film we wish to calculate the dipole field from at some point in space. We will later need the reciprocal lattice vectors so we will calculate those now. Let $\mathbb{X} = (\mathbf{v}_1 \mathbf{v}_2)$, suppose $\mathbf{b}_1$, $\mathbf{b}_2$ be the intraplane reciprocal lattice vectors and let $\mathbb{B} = (\mathbf{b}_1 \mathbf{b}_2)$ A standard result from solid state physics is that

$$
\mathbb{B}^{\mathrm{T}} \mathbb{X} = 2\pi \mathbb{I} \tag{13}
$$

Where $\mathbb{I}$ is the identity matrix. If we multiple right by $\mathbb{X}^{-1}$ this becomes

$$
\mathbb{B}^{\mathrm{T}} = 2\pi \mathbb{X}^{-1} \tag{14}
$$

$$
\mathbb{B}^{T} = \frac{2\pi}{\det(\mathbb{X})} \begin{bmatrix} \frac{1}{2}a & -\frac{1}{4}a \\ 0 & \frac{\sqrt{3}}{4}a \end{bmatrix}^{-1} \tag{15}
$$

The inverse of a 2×2 matrix is given by the following

$$
\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} \tag{16}
$$

This gives

$$
\mathbb{B}^{\mathrm{T}} = \frac{4\pi}{a} \begin{bmatrix} 1 & \frac{1}{\sqrt{3}} \\ 0 & \frac{2}{\sqrt{3}} \end{bmatrix} \tag{17}
$$

So the reciprocal lattice vectors are

$$\begin{aligned}\mathbf{b}_1 &= \frac{4\pi}{a}\left(1, \frac{1}{\sqrt{3}}\right)\\ \mathbf{b}_2 &= \frac{4\pi}{a}\left(0, \frac{2}{\sqrt{3}}\right)\end{aligned} \tag{18}$$

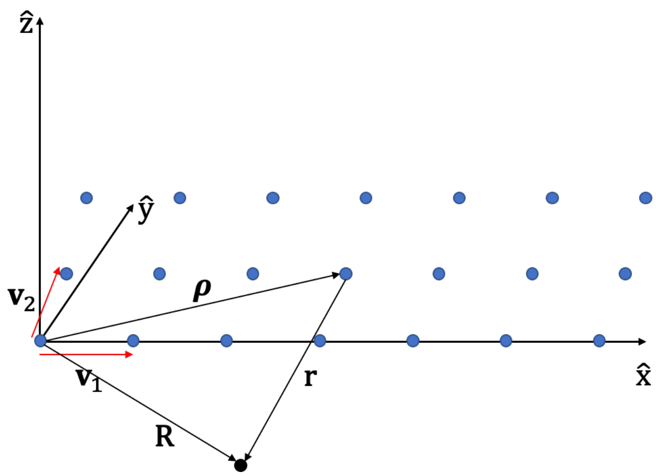

FIG. 4: Single layer of (111) textured NiO lying at $z = 0$

For a given point in space

$$\mathbf{R} = (x, y, z) \tag{19}$$

And a given atomic site

$$\boldsymbol{\rho}_{nm} = n\mathbf{v}_1 + m\mathbf{v}_2 = \left(\frac{1}{2}na - \frac{1}{4}ma, \frac{\sqrt{3}}{4}ma, 0\right) \tag{20}$$

The displacement vector is given by

$$\mathbf{r}_{nm} = \mathbf{R} - \boldsymbol{\rho}_{nm} = \left(x - \frac{1}{2}na + \frac{1}{4}ma,\ y - \frac{\sqrt{3}}{4}ma,\ z\right) \tag{21}$$

Assuming spins lie in the *y*-direction and are in thermal equilibrium

$$\boldsymbol{\mu}_{nm} = \langle\boldsymbol{\mu}\rangle = \mu\,\hat{\mathbf{y}}, \quad \forall\,(n, m) \tag{22}$$

Recalling equation 9, this gives a total magnetic potential due to the film of

$$\Phi(x, y, z) = \sum_{n,m=-\infty}^{\infty} \frac{\mu\left(y - \frac{\sqrt{3}}{4}ma\right)}{\left[\left(x - \frac{1}{2}na + \frac{1}{4}ma\right)^2 + \left(y - \frac{\sqrt{3}}{4}ma\right)^2 + z^2\right]^{\frac{3}{2}}} \tag{23}$$

Summing over many individual atoms converges slowly. Instead it is more efficient to work in *k*-space by use of a Fourier transform which sums over the harmonics of the interaction - this converges quickly.

V. THE ANALYTIC DERIVATION OF THE DIPOLAR FIELD

A. In-Plane Spin Configuration

Since the potential is applied to a discretised space, we make use of Poisson's summation formula to apply a Fourier transform. For a function $f(na)$ in 1D this takes the form

$$\sum_{n=-\infty}^{\infty} f(na) = \frac{1}{a} \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) \mathrm{e}^{-\mathrm{i}\frac{2\pi}{a}kx} dx \tag{24}$$

Where $\frac{2\pi}{a}$ is the reciprocal lattice vector. This can easily be generalised to 2-dimensional space:

$$\sum_{n,m=-\infty}^{\infty} f(na, ma) = \frac{1}{a^2} \sum_{k,l=-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y)\, \mathrm{e}^{-\mathrm{i}\frac{2\pi}{a}kx}\, \mathrm{e}^{-\mathrm{i}\frac{2\pi}{a}ly} dxdy \tag{25}$$

Our function is not strictly a function of na, ma. Instead we have $f \equiv f(x - \frac{1}{2}na + \frac{1}{4}ma, y - \frac{\sqrt{3}}{4}ma)$. The position variables x, y acts as a translation in the Fourier transform. For a function $g(na - x)$ this takes the form

$$\sum_{n=-\infty}^{\infty} g(na - x) = \frac{1}{a} \sum_{k=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\frac{2\pi}{a}kx} \int_{-\infty}^{\infty} g(x')\, \mathrm{e}^{\mathrm{i}\frac{2\pi}{a}kx'} dx' \tag{26}$$

A dummy variable x' has been introduced. This is the shift theorem for Fourier analysis (see here for a brief proof of the shift theorem). There is another consideration for the magnetic potential as the lattice vectors $\mathbf{v}_1$, $\mathbf{v}_2$ are non-orthogonal. In Eq 25 the coefficient $\frac{1}{a^2}$ must be replaced with the area subtended by the in-plane vectors $|\mathbf{v}_1 \times \mathbf{v}_2|$. The Fourier transform of Φ is

$$\Phi(x, y, z) = \frac{1}{|\mathbf{v}_1 \times \mathbf{v}_2|} \sum_{k,l=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}(k\mathbf{b}_1\cdot\mathbf{R} + l\mathbf{b}_2\cdot\mathbf{R})} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx'dy' \frac{\mu y'}{[x'^2 + y'^2 + z^2]^{\frac{3}{2}}} \mathrm{e}^{\mathrm{i}\left(k\mathbf{b}_1\cdot\mathbf{R}' + l\mathbf{b}_2\cdot\mathbf{R}'\right)} \tag{27}$$

Where $\mathbf{b}_1$, $\mathbf{b}_2$ are the reciprocal lattice vectors. Substituting the reciprocal lattice vectors and the area of the Wigner-Seitz cell into the potential, we have

$$\Phi(x, y, z) = \frac{8\mu}{\sqrt{3}a^2} \sum_{k,l=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx + \frac{1}{\sqrt{3}}ky + \frac{2}{\sqrt{3}}ly\right)} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx'dy' \frac{y'}{[x'^2 + y'^2 + z^2]^{\frac{3}{2}}} \mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx' + \frac{1}{\sqrt{3}}ky' + \frac{2}{\sqrt{3}}ly'\right)} \tag{28}$$

The double integral in the above equation can be calculated analytically. Taking the result from Tsymbal

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dxdy \frac{y}{(x^2 + y^2 + z^2)^{\frac{3}{2}}} \exp\left(\mathrm{i}\frac{2\pi}{a}Ax\right) \exp\left(\mathrm{i}\frac{2\pi}{a}By\right) = 2\pi\mathrm{i}\frac{B}{\sqrt{A^2 + B^2}} \exp\left(-\frac{2\pi}{a}\sqrt{A^2 + B^2}|z|\right) \tag{29}$$

with $A = 2k$ and $B = \frac{2\sqrt{3}}{3}(k + 2l)$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx'dy' \frac{y'}{[x'^2+y'^2+z^2]^{\frac{3}{2}}} \mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx'+\frac{1}{\sqrt{3}}ky'+\frac{2}{\sqrt{3}}ly'\right)} = \frac{4\sqrt{3}\pi\mathrm{i}}{3}\frac{(k+2l)}{\sqrt{4k^2+\frac{4}{3}(k+2l)^2}}\exp\left(-\frac{2\pi}{a}\sqrt{4k^2+\tfrac{4}{3}(k+2l)^2}|z|\right) \tag{30}$$

$$= \frac{2\sqrt{3}\pi\mathrm{i}}{3}\frac{(k+2l)}{\sqrt{k^2+\frac{1}{3}(k+2l)^2}}\exp\left(-\frac{4\pi}{a}\sqrt{k^2+\tfrac{1}{3}(k+2l)^2}|z|\right) \tag{31}$$

$$= 2\pi\mathrm{i}\frac{(k+2l)}{\sqrt{3k^2+(k+2l)^2}}\exp\left(-\frac{4\sqrt{3}\pi}{3a}\sqrt{3k^2+(k+2l)^2}|z|\right) \tag{32}$$

$$= \pi\mathrm{i}\frac{(k+2l)}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right) \tag{33}$$

Substituting this into the potential and tidying coefficients we have

$$\Phi(x,y,z) = \frac{8}{\sqrt{3}}\frac{\mu\pi}{a^2}\sum_{k,l=-\infty}^{\infty}\mathrm{i}\frac{(k+2l)}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right) \tag{34}$$

The summations can be simplified to run over the positive infinite range by identifying terms with negative and positive arguments in the exponentials which form trigonometric functions. First evaluating the series with the k prefactor

$$\begin{aligned}
&\sum_{k=-\infty}^{\infty}\sum_{l=-\infty}^{\infty}\mathrm{i}\frac{k}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right) = \\
&\quad\sum_{k=-\infty}^{\infty}\left\{\sum_{l=1}^{\infty}\mathrm{i}\left[\frac{k}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\right.\right.\\
&\qquad\left.+\frac{k}{\sqrt{k^2-kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\right]\\
&\qquad\left.+\frac{k}{|k|}\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\right\}
\end{aligned} \tag{35}$$

$$\sum_{k=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} \mathrm{i}\frac{k}{\sqrt{k^2+kl+l^2}}\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)=$$
$$\begin{aligned}\sum_{k=1}^{\infty}\Bigg\{\sum_{l=1}^{\infty}\mathrm{i}\Bigg[&\frac{k}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\\ &+\frac{k}{\sqrt{k^2-kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\Bigg]\\ &+\frac{k}{|k|}\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\\ -\sum_{l=1}^{\infty}\mathrm{i}\Bigg[&\frac{k}{\sqrt{k^2-kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(-kx-\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\\ &+\frac{k}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(-kx-\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\Bigg]\\ &-\frac{k}{|k|}\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(-kx-\tfrac{1}{\sqrt{3}}ky\right)\right)\Bigg\}\end{aligned} \tag{36}$$

$$\sum_{k=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} \mathrm{i}\frac{k}{\sqrt{k^2+kl+l^2}}\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)=$$
$$\begin{aligned}&2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{k}{\sqrt{k^2-kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\\ &+2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{k}{\sqrt{k^2+kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\\ &+2\sum_{k=1}^{\infty}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\end{aligned} \tag{37}$$

Now evaluating the $2l$ series

$$\sum_{k=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} \mathrm{i}\frac{2l}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)=$$
$$\begin{aligned}\sum_{k=-\infty}^{\infty}\Bigg\{\sum_{l=1}^{\infty}\mathrm{i}\Bigg[&\frac{2l}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\\ &-\frac{2l}{\sqrt{k^2-kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\Bigg]\Bigg\}\end{aligned} \tag{38}$$

$$
\begin{aligned}
&\sum_{k=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} \mathrm{i}\frac{2l}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)= \\
&\quad\sum_{k=1}^{\infty}\Bigg\{\sum_{l=1}^{\infty}\mathrm{i}\Bigg[\frac{2l}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right) \\
&\qquad-\frac{2l}{\sqrt{k^2-kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\Bigg] \\
&\quad+\sum_{l=1}^{\infty}\mathrm{i}\Bigg[\frac{2l}{\sqrt{k^2-kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(-kx-\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right) \\
&\qquad-\frac{2l}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(-kx-\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\Bigg]\Bigg\} \\
&\quad+\sum_{l=1}^{\infty}\mathrm{i}\Bigg[\frac{2l}{|l|}\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\tfrac{2}{\sqrt{3}}ly\right) \\
&\qquad-\frac{2l}{|l|}\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)\exp\left(\mathrm{i}\frac{4\pi}{a}\tfrac{2}{\sqrt{3}}ly\right)\Bigg]
\end{aligned}
\tag{39}
$$

$$
\begin{aligned}
&\sum_{k=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} \mathrm{i}\frac{2l}{\sqrt{k^2+kl+l^2}}\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\exp\left(-\mathrm{i}\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)= \\
&\quad-2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{2l}{\sqrt{k^2-kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right) \\
&\quad+2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{2l}{\sqrt{k^2+kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right) \\
&\quad+4\sum_{l=1}^{\infty}\sin\left(\frac{8\sqrt{3}\pi}{3a}ly\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)
\end{aligned}
\tag{40}
$$

Combining everything

$$
\begin{aligned}
\Phi(x,y,z)=\frac{8}{\sqrt{3}}\frac{\mu\pi}{a^2}\Bigg[&2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{k}{\sqrt{k^2-kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right) \\
&+2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{k}{\sqrt{k^2+kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right) \\
&+2\sum_{k=1}^{\infty}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right) \\
&-2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{2l}{\sqrt{k^2-kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right) \\
&+2\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{2l}{\sqrt{k^2+kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right) \\
&+4\sum_{l=1}^{\infty}\sin\left(\frac{8\sqrt{3}\pi}{3a}ly\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)\Bigg]
\end{aligned}
\tag{41}
$$

$$\begin{aligned}\Phi(x,y,z) = \frac{16}{\sqrt{3}}\frac{\mu\pi}{a^2}\Bigg[&\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k-2l)}{\sqrt{k^2-kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\\ &+\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k+2l)}{\sqrt{k^2+kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\\ &+\sum_{k=1}^{\infty}\sin\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\\ &+2\sum_{l=1}^{\infty}\sin\left(\frac{8\sqrt{3}\pi}{3a}ly\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)\Bigg]\end{aligned} \tag{42}$$

Now it is best to transform the potential back into a magnetic field so that it can be used. Recalling equation 8

$$\mathbf{B}(x,y,z) = -\frac{\mu_0}{4\pi}\nabla\Phi(x,y,z) \tag{43}$$

$$\begin{pmatrix} B_x(\mathbf{R})\\ B_y(\mathbf{R})\\ B_z(\mathbf{R})\end{pmatrix} = -\frac{\mu_0}{4\pi}\begin{pmatrix}\frac{\partial\Phi(\mathbf{R})}{\partial x}\\ \frac{\partial\Phi(\mathbf{R})}{\partial y}\\ \frac{\partial\Phi(\mathbf{R})}{\partial z}\end{pmatrix} \tag{44}$$

For $\partial/\partial x$ we get

$$\begin{aligned}\frac{\partial\Phi}{\partial x} = \frac{16}{\sqrt{3}}\frac{\mu\pi}{a^2}\Bigg[&\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k-2l)}{\sqrt{k^2-kl+l^2}}\left(\frac{4\pi}{a}k\right)\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\\ &+\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k+2l)}{\sqrt{k^2+kl+l^2}}\left(\frac{4\pi}{a}k\right)\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\\ &+\sum_{k=1}^{\infty}\left(\frac{4\pi}{a}k\right)\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\Bigg]\end{aligned} \tag{45}$$

$$\begin{aligned}\frac{\partial\Phi}{\partial x} = \frac{64}{\sqrt{3}}\frac{\mu\pi^2}{a^3}\Bigg[&\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k-2l)k}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\\ &+\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k+2l)k}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\\ &+\sum_{k=1}^{\infty}k\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\Bigg]\end{aligned} \tag{46}$$

Then $\partial/\partial y$ we get

$$\frac{\partial\Phi}{\partial y} = \frac{16}{\sqrt{3}}\frac{\mu\pi}{a^2}\Bigg[\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k-2l)}{\sqrt{k^2-kl+l^2}}\left(\frac{4\pi}{a}(\tfrac{1}{\sqrt{3}}k-\tfrac{2}{\sqrt{3}}l)\right)\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)$$
$$+\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k+2l)}{\sqrt{k^2+kl+l^2}}\left(\frac{4\pi}{a}(\tfrac{1}{\sqrt{3}}k+\tfrac{2}{\sqrt{3}}l)\right)\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)$$
$$+\sum_{k=1}^{\infty}\left(\frac{4\sqrt{3}\pi}{3a}k\right)\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)$$
$$+2\sum_{l=1}^{\infty}\left(\frac{8\sqrt{3}}{3a}l\right)\cos\left(\frac{8\sqrt{3}\pi}{3a}ly\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)\Bigg] \tag{47}$$

$$\begin{aligned}\frac{\partial\Phi}{\partial y} = \frac{64}{3}\frac{\mu\pi^2}{a^3}\Bigg[&\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k-2l)^2}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\\
&+\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k+2l)^2}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\\
&+\sum_{k=1}^{\infty}k\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\\
&+2\sum_{l=1}^{\infty}2l\cos\left(\frac{8\sqrt{3}\pi}{3a}ly\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)\Bigg]\end{aligned} \tag{48}$$

We'll be considering the field in the y direction so

$$\begin{aligned}B_y = -\frac{16}{3}\frac{\mu\mu_0\pi}{a^3}\Bigg[&\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k-2l)^2}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2-kl+l^2}|z|\right)\\
&+\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k+2l)^2}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right)\\
&+\sum_{k=1}^{\infty}k\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|k||z|\right)\\
&+2\sum_{l=1}^{\infty}2l\cos\left(\frac{8\sqrt{3}\pi}{3a}ly\right)\exp\left(-\frac{8\sqrt{3}\pi}{3a}|l||z|\right)\Bigg]\end{aligned} \tag{49}$$

We can write this a bit more succinctly (and make implementing numerically a bit cleaner) by defining

$$\xi_{kl}(z) = \exp\left(-\frac{8\sqrt{3}\pi}{3a}\sqrt{k^2+kl+l^2}|z|\right) \tag{50}$$

$$
\begin{aligned}
B_y = -\frac{16}{3}\frac{\mu\mu_0\pi}{a^3}\Bigg[&\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k-2l)^2}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky-\tfrac{2}{\sqrt{3}}ly\right)\right)\xi_{-kl}(z)\\
&+\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{(k+2l)^2}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky+\tfrac{2}{\sqrt{3}}ly\right)\right)\xi_{kl}(z)\\
&+\sum_{k=1}^{\infty}k\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{1}{\sqrt{3}}ky\right)\right)\xi_{k0}(z)\\
&+2\sum_{l=1}^{\infty}2l\cos\left(\frac{8\sqrt{3}\pi}{3a}ly\right)\xi_{0l}(z)\Bigg]
\end{aligned}
\tag{51}
$$

For B_y we must employ the chain rule giving

$$
\begin{aligned}
\mathrm{B}_y = -\frac{4\mu_0\mu}{\sqrt{3}a^2}\Bigg[&\sum_{k=1}^{\infty}\left(\frac{4\pi}{\sqrt{3}a}k\right)\cos\left(\frac{4\pi}{a}k\left(x+\tfrac{y}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|}+\sum_{l=1}^{\infty}\left(\frac{16\pi}{\sqrt{3}a}l\right)\cos\left(\frac{8\pi}{\sqrt{3}a}ly\right)\\
&\times\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}+\sum_{k,l,=1}^{\infty}\Bigg\{\left(\frac{4\pi}{\sqrt{3}a}\right)\frac{(k+2l)^2}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{ky}{\sqrt{3}}+\tfrac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|}\\
&+\left(\frac{4\pi}{\sqrt{3}a}\right)\frac{(k-2l)^2}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{ky}{\sqrt{3}}-\tfrac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\Bigg]
\end{aligned}
\tag{52}
$$

A factor $\frac{4\pi}{\sqrt{3}a}$ can be collected, giving

$$
\begin{aligned}
\mathrm{B}_y = -\frac{16\pi\mu_0\mu}{3a^3}\Bigg[&\sum_{k=1}^{\infty}k\cos\left(\frac{4\pi}{a}k\left(x+\tfrac{y}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|}+4\sum_{l=1}^{\infty}l\cos\left(\frac{8\pi}{\sqrt{3}a}ly\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}\\
&+\sum_{k,l,=1}^{\infty}\Bigg\{\frac{(k+2l)^2}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}k\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|}\\
&+\frac{(k-2l)^2}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}k\left(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\Bigg\}\Bigg]
\end{aligned}
\tag{53}
$$

For this to be useful, the harmonics must be summed over, and the coordinates of an atom in another film by inputted as $\mathbf{R} = (x, y, z)$. This gives the dipole field due to a (111) sheet of NiO at arbitrary distance. The same procedure needs to be undertaken for a film magnetised out-of-plane. Again dropping a factor $\frac{1}{4\pi}$, the potential for an out-of-plane spin configuration is given by

$$
\Phi(x,y,z) = \sum_{n,m=-\infty}^{\infty}\frac{\mu z}{\left[\left(x-\frac{1}{2}na+\frac{1}{4}ma)\right)^2+\left(y-\frac{\sqrt{3}}{4}ma\right)^2+z^2\right]^{\frac{3}{2}}}
\tag{54}
$$

Upon applying a Fourier transform this becomes

$$
\Phi = \frac{8\mu}{\sqrt{3}a^2}\sum_{k,l=-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx'dy'\frac{z}{[x'^2+y'^2+z^2]^{\frac{3}{2}}}\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}
\tag{55}
$$

The double integral can be simplified by letting the exponential function take the form $\mathrm{e}^{i(ax+by)}$ where a and b are now dummy coefficients. The following integral can be calculated analytically

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy\ \frac{z\ \mathrm{e}^{iax}\ \mathrm{e}^{iby}}{[x^2+y^2+z^2]^{\frac{3}{2}}} \tag{56}$$

Rewriting in cylindrical polar coordinates this becomes

$$\int_{0}^{\infty}\int_{0}^{2\pi} d\theta dr\ \frac{z\ r\ \mathrm{e}^{ir(a\sin\theta+b\cos\theta)}}{[r^2+z^2]^{\frac{3}{2}}} \tag{57}$$

The integral over θ can be separated into just the exponential given by

$$\int_{0}^{2\pi} \mathrm{e}^{ir(a\sin\theta+b\cos\theta)}\ d\theta \tag{58}$$

To compute this integral, we need the following result from the definition of the zeroth order Bessel function of the first kind

$$2\pi J_0(x) = \int_0^{2\pi} e^{ix\sin\theta}\ d\theta = \int_0^{2\pi} e^{ix\cos\theta}\ d\theta \tag{59}$$

This comes from the definition of the Bessel function and the definition of the exponential function

$$J_n(x) = \sum_{s=0}^{\infty} \frac{(-1)^s}{(n+s)!s!}\left(\frac{x}{2}\right)^{n+2s} \tag{60}$$

$$e^x = \sum_{s=0}^{\infty} \frac{x^s}{s!} \tag{61}$$

To show this is true, we will show the first few terms agree with this result. The integral can be written as

$$\int_0^{2\pi} e^{ix\sin\theta}\ d\theta = \int_0^{2\pi}\sum_{n=0}^{\infty}\frac{(ir\sin\theta)^n}{n!}d\theta \tag{62}$$

Notice that for n odd, the function in the integral is zero due to the symmetry of $\sin\theta$. For $n = 0$ we have

$$\int_0^{2\pi} d\theta = 2\pi \tag{63}$$

For $n = 2$

$$\begin{aligned}\int_0^{2\pi}\frac{(ir\sin\theta)^2}{2!}d\theta &= -\frac{r^2}{2!}\int_0^{2\pi}\sin^2\theta\ d\theta \\ &= -\frac{r^2}{2!}\left[\theta-\sin\theta\cos\theta\right]_0^{2\pi} \\ &= -2\pi\frac{r^2}{2} \\ &= 2\pi\frac{(-1)^1}{(1!)^2}\left(\frac{r^2}{2}\right)^1\end{aligned} \tag{64}$$

For $n = 4$

$$\int_0^{2\pi} \frac{(ir\sin\theta)^4}{4!} d\theta = \frac{r^4}{32(4!)}\left[12\theta - 8\sin 2\theta + \sin 4\theta\right]_0^{2\pi}$$
$$= 2\pi \frac{r^4}{64} \tag{65}$$
$$= 2\pi \frac{(-1)^2}{(2!)^2}\left(\frac{r^2}{2}\right)^2$$

This is not a rigorous derivation but shows the result is true. We can now write this as a generalised expression for all terms

$$\int_0^{2\pi} \mathrm{e}^{ir\sin\theta}\, d\theta = 2\pi \sum_{n=0, n\text{ even}}^{\infty} \left(\frac{r^2}{2}\right)^{n/2} \frac{(-1)^{\frac{n}{2}}}{\left[\left(\frac{n}{2}\right)!\right]^{\frac{n}{2}}} \tag{66}$$

We can make a transformation to a new summation variable $n_{\text{even}} \to s = \frac{n}{2}$ giving

$$2\pi \sum_{s=0}^{\infty} \left(\frac{r}{2}\right)^s \frac{(-1)^s}{(s!)^s} = 2\pi J_0(r) \tag{67}$$

Extending this to the case when the exponent is a superposition of trigonometric functions

$$\int_0^{2\pi} e^{ix(a\sin\theta + b\cos\theta)}\, d\theta = 2\pi J_0(x\sqrt{a^2+b^2}) \tag{68}$$

Our simplified integral is therefore

$$\int_0^{\infty}\int_0^{2\pi} d\theta dr \frac{z\ r\ \mathrm{e}^{ir(a\sin\theta + b\cos\theta)}}{\left[r^2+z^2\right]^{\frac{3}{2}}} = \int_0^{\infty} \frac{z\ r}{\left[r^2+z^2\right]^{\frac{3}{2}}}\left[2\pi J_0(r\ \sqrt{a^2+b^2})\right]\ dr \tag{69}$$

The integral over r is a standard result in mathematics, but its derivation is more detailed than required for this calculation. The result is

$$2\pi \int_0^{\infty} \frac{z\ r\ J_0\left(r\sqrt{a^2+b^2}\right)}{\left[r^2+z^2\right]^{\frac{3}{2}}} dr = 2\pi \frac{z\ \mathrm{e}^{-\sqrt{a^2+b^2}|z|}}{|z|} \tag{70}$$

Now we can return to the potential, upon substitution this yields

$$\Phi(x,y,z) = \frac{16\pi\mu}{\sqrt{3}a^2}\ \mathrm{sign}(z) \sum_{k,l=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx + \frac{1}{\sqrt{3}}ky + \frac{2}{\sqrt{3}}ly\right)} \mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} \tag{71}$$

As with the IP calculation, the sum can be split into trigonometric functions. Explicitly for the case when $l = 0$, we have a term

$$\sum_{k=-\infty}^{\infty}\Bigg|_{l=0} \mathrm{e}^{-\frac{4\pi}{a}(kx + \frac{1}{\sqrt{3}}ky)}\ \mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}|k||z|} = 2\sum_{k=1}^{\infty} \cos\left(\frac{4\pi}{a}\left(kx + \tfrac{1}{\sqrt{3}}ky\right)\right) \mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|} \tag{72}$$

Expanding the sums we obtain

$$\begin{aligned}\Phi = \frac{16\pi\mu}{\sqrt{3}a^2}\mathrm{sign}(z)\Bigg[&\sum_{k=1}^{\infty}\left(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}k\left(x+\frac{y}{\sqrt{3}}\right)} + \mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}k\left(x+\frac{y}{\sqrt{3}}\right)}\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{l=1}^{\infty}\left(\mathrm{e}^{\mathrm{i}\frac{8\pi}{\sqrt{3}a}ly} + \mathrm{e}^{-\mathrm{i}\frac{8\pi}{\sqrt{3}a}ly}\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}\\ &+ \left[\sum_{k=1}^{\infty} + \sum_{k=-1}^{-\infty}\right]\left[\sum_{l=1}^{\infty} + \sum_{l=-1}^{-\infty}\right]\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|}\Bigg]\end{aligned} \tag{73}$$

The final term inside the double summation can be rewritten as

$$\sum_{k,l,=1}^{\infty}\left\{\left(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}+\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}\sqrt{k^2+kl+l^2}|z|}+\left(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}+\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\right)\right.$$
$$\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}\sqrt{k^2+kl+l^2}|z|}\right\} \tag{74}$$

This can be rewritten as trigonometric functions

$$\Phi=\frac{32\pi\mu}{\sqrt{3}a^2}\mathrm{sign}(z)\left[\sum_{k=1}^{\infty}\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|}+\sum_{l=1}^{\infty}\cos\left(\frac{8\pi}{\sqrt{3}a}ly\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}\right.$$
$$\left.+\sum_{k,l=1}^{\infty}\left\{\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|}+\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{75}$$

By reintroducing the factor $\frac{1}{4\pi}$ and differentiating, we again yield the effective field

$$\mathrm{B}_z=-\frac{8\mu_0\mu}{\sqrt{3}a^2}\mathrm{sign}(z)\left[\sum_{k=1}^{\infty}\left(-\frac{8\pi}{\sqrt{3}a}k\ \mathrm{sign}(z)\right)\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|}+\sum_{l=1}^{\infty}\left(-\frac{8\pi}{\sqrt{3}a}l\ \mathrm{sign}(z)\right)\right.$$
$$\times\cos\left(\frac{8\pi}{\sqrt{3}a}ly\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}+\sum_{k,l=1}^{\infty}\left\{\left(-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}\ \mathrm{sign}(z)\right)\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|}\right.$$
$$\left.\left.+\left(-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}\ \mathrm{sign}(z)\right)\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{76}$$

A factor $-\frac{8\pi}{\sqrt{3}a}\mathrm{sign}(z)$ can be factored out giving

$$\mathrm{B}_z=\frac{64\pi\mu_0\mu}{3a^3}\left[\sum_{k=1}^{\infty}k\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|}+\sum_{l=1}^{\infty}l\cos\left(\frac{8\pi}{\sqrt{3}a}ly\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}+\sum_{k,l=1}^{\infty}\left\{\sqrt{k^2+kl+l^2}\right.\right.$$
$$\times\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}})\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|}+\sqrt{k^2-kl+l^2}\cos\left(\frac{4\pi}{a}(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}})\right)$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{77}$$

For consistency, it is important to check for an easy plane anisotropy. We will now derive the dipolar field for spins lying in the x-direction. The relevant magnetic potential takes the form

$$\Phi(x,y,z)=\frac{8\mu}{\sqrt{3}a^2}\sum_{k,l=-\infty}^{\infty}\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{x'}{[x'^2+y'^2+z^2]^{\frac{3}{2}}}\mathrm{e}^{-\frac{4\pi}{\sqrt{3}a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}dx'dy' \tag{78}$$

The integral is identical to the one in 28 upon relabelling x and y giving

$$\Phi=\frac{16\pi\mu}{a^2}\sum_{k,l=-\infty}^{\infty}\frac{k}{\sqrt{(k+2l)^2+3k^2}}\mathrm{i}\mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\mathrm{e}^{-\frac{4\pi}{\sqrt{3}a}\sqrt{(k+2l)^2+3k^2}|z|} \tag{79}$$

Unlike 28, when separated, $k=0$ gives are no terms

$$\Phi = \frac{16\pi\mu}{a^2}\left[\sum_{k=1}^{\infty}\frac{1}{2\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}\right)} - \mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}\right)}\right) + \sum_{k,l,=1}^{\infty}\left\{\frac{k}{2\mathrm{i}\sqrt{k^2+kl+l^2}}\left(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\right.\right.\right.$$
$$\left.- \mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)}\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} + \frac{k}{2\mathrm{i}\sqrt{k^2-kl+l^2}}\left(\mathrm{e}^{\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}}\right)} - \mathrm{e}^{-\mathrm{i}\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}}\right)}\right)$$
$$\times\, \mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|} \tag{80}$$

This can be reduced to

$$\Phi = \frac{16\pi\mu}{a^2}\left[\sum_{k=1}^{\infty}\sin\left(\frac{4\pi}{a}k\left(x+\frac{y}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{k,l,=1}^{\infty}\left\{\frac{k}{\sqrt{k^2+kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)\right)\right.\right.$$
$$\left.\left.\times\, \mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} + \frac{k}{\sqrt{k^2-kl+l^2}}\sin\left(\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{81}$$

As before, reintroduce a factor $\frac{1}{4\pi}$ and differentiate to get the dipolar field

$$\mathrm{B}_x = -\frac{4\mu_0\mu}{a^2}\left[\sum_{k=1}^{\infty}\left(\frac{4\pi}{a}k\right)\cos\left(\frac{4\pi}{a}k\left(x+\frac{y}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{k,l,=1}^{\infty}\left\{\left(\frac{4\pi}{a}k\right)\frac{k}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)\right)\right.\right.$$
$$\left.\left.\times\, \mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} + \left(\frac{4\pi}{a}k\right)\frac{k}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{82}$$

Collecting $\frac{4\pi}{a}$ terms we have

$$\mathrm{B}_x = -\frac{16\mu_0\mu}{a^3}\left[\sum_{k=1}^{\infty}k\cos\left(\frac{4\pi}{a}k\left(x+\frac{y}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{k,l,=1}^{\infty}\left\{\frac{k^2}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}+\frac{2ly}{\sqrt{3}}\right)\right)\right.\right.$$
$$\left.\left.\times\, \mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} + \frac{k^2}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\frac{ky}{\sqrt{3}}-\frac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{83}$$

B. Calculating the Dipole Field

Now both the in-plane and out-of-plane magnetic field from an atomic film of (111) textured NiO have been derived. The above equations are analytic and only the first few (~ 10) harmonics will have to be summed for the field to converge to sufficient precision. The energy can then be calculated by taking the dot product of the field with a spin direction which is parallel, or antiparallel to the spin direction considered.

The position vector (x, y, z) does not have to be close to the origin as all terms are periodic with the reciprocal lattice vectors. One inter-plane translation vector between atoms are given as $\mathbf{v}_1$, $\mathbf{v}_2$. The inter-plane vector will be denoted $\mathbf{v}_3$ and is equal to

$$\mathbf{v}_3 = a\left(0, \frac{\sqrt{3}}{6}, \frac{\sqrt{6}}{6}\right) \tag{84}$$

Where $a = 5.904341623\text{Å}$ as defined at the beginning. The distance to the nth layer is given by substituting $\mathbf{R} = n\mathbf{v}_3$ into the analytic forms of the dipolar field.

$$\mathrm{E} = -\frac{8\mu_0\mu_S^2\langle S\rangle^2}{a^3}\left[\sum_{k=1}^{\infty} k\cos\left(\frac{4\pi}{a}k\left(x+\tfrac{y}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{k,l,=1}^{\infty}\left\{\frac{k^2}{\sqrt{k^2+kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{ky}{\sqrt{3}}+\tfrac{2ly}{\sqrt{3}}\right)\right)\right.\right.$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} + \frac{k^2}{\sqrt{k^2-kl+l^2}}\cos\left(\frac{4\pi}{a}\left(kx+\tfrac{ky}{\sqrt{3}}-\tfrac{2ly}{\sqrt{3}}\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{85}$$

The dipole energy with the spins laying in the x, y-plane is:

$$E_x = -\frac{8\mu_0\mu_S^2}{a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{k,l,=1}^{\infty}\left\{\frac{k^2}{\sqrt{k^2+kl+l^2}}\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right.\right.$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} + \frac{k^2}{\sqrt{k^2-kl+l^2}}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{86}$$

where $\mathbf{R}_n = n\mathbf{v}_3$. We can pick any point on an adjacent plane but it must be on another atom, it's convenient to go along the lattice vector.

$$E_z = \frac{64\pi\mu_0\mu_S^2}{3a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|} + \sum_{l=1}^{\infty} l\cos\left(l\mathbf{b}_2\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|} + \sum_{k,l=1}^{\infty}\left\{\sqrt{k^2+kl+l^2}\right.\right.$$
$$\times\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|} + \sqrt{k^2-kl+l^2}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right))$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{87}$$

Let's define $\varphi_{kl}^{\pm} = \sqrt{k^2 \pm kl + l^2}$
Which gives us

$$E_x = -\frac{8\mu_0\mu_S^2}{a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{k,l,=1}^{\infty}\left\{\frac{k^2}{\varphi_{kl}^{+}}\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right.\right.$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{+}|z|} + \frac{k^2}{\varphi_{kl}^{-}}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{-}|z|}\right\}\right] \tag{88}$$

$$E_z = \frac{64\pi\mu_0\mu_S^2}{3a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|} + \sum_{l=1}^{\infty} l\cos\left(l\mathbf{b}_2\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|} + \sum_{k,l=1}^{\infty}\left\{\varphi_{kl}^{+}\right.\right.$$
$$\times\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{+}|z|} + \varphi_{kl}^{-}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right))$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{-}|z|}\right\}\right] \tag{89}$$

Let's calculate the energy difference $\Delta E = E_z - E_x$

$$E_x = -\frac{8\mu_0\mu_S^2}{a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}}k|z|} + \sum_{k,l,=1}^{\infty}\left\{\frac{k^2}{\varphi_{kl}^{+}}\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right.\right.$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{+}|z|} + \frac{k^2}{\varphi_{kl}^{-}}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{-}|z|}\right\}\right] \tag{90}$$

$$E_z = \frac{64\pi\mu_0\mu_S^2}{3a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|} + \sum_{l=1}^{\infty} l\cos\left(l\mathbf{b}_2\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|} + \sum_{k,l=1}^{\infty}\left\{\varphi_{kl}^{+}\right.\right.$$
$$\times\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{+}|z|} + \varphi_{kl}^{-}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right)$$
$$\left.\left.\times\,\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{-}|z|}\right\}\right] \tag{91}$$

$$\Delta E = \frac{88\pi\mu_0\mu_S^2}{3a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|} + \frac{64}{88}\sum_{l=1}^{\infty} l\cos\left(l\mathbf{b}_2\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}\right.$$
$$+\sum_{k,l=1}^{\infty}\left\{\left(\varphi_{kl}^{+}+\frac{k^2}{\varphi_{kl}^{+}}\right)\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{+}|z|}\right.$$
$$\left.\left.+\left(\varphi_{kl}^{-}+\frac{k^2}{\varphi_{kl}^{-}}\right)\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\varphi_{kl}^{-}|z|}\right\}\right] \tag{92}$$

Using

$$\varphi_{kl}^{+}+\frac{k^2}{\varphi_{kl}^{+}} = \frac{k^2+(\varphi_{kl}^{+})^2}{\varphi_{kl}^{+}} = \frac{k^2+k^2+kl+l^2}{\sqrt{k^2+kl+l^2}} = \frac{2k^2+kl+l^2}{\sqrt{k^2+kl+l^2}} \tag{93}$$

and

$$\varphi_{kl}^{-}+\frac{k^2}{\varphi_{kl}^{-}} = \frac{k^2+(\varphi_{kl}^{-})^2}{\varphi_{kl}^{-}} = \frac{k^2+k^2-kl+l^2}{\sqrt{k^2-kl+l^2}} = \frac{2k^2-kl+l^2}{\sqrt{k^2-kl+l^2}} \tag{94}$$

$$\Delta E = \frac{88\pi\mu_0\mu_S^2}{3a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}k|z|} + \frac{64}{88}\sum_{l=1}^{\infty} l\cos\left(l\mathbf{b}_2\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}l|z|}\right.$$
$$+\sum_{k,l=1}^{\infty}\left\{\frac{2k^2+kl+l^2}{\sqrt{k^2+kl+l^2}}\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2+kl+l^2}|z|}\right.$$
$$\left.\left.+\frac{2k^2-kl+l^2}{\sqrt{k^2-kl+l^2}}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right)\mathrm{e}^{-\frac{8\pi}{\sqrt{3}a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{95}$$

Remembering that a has actually been changed from the cubic lattice parameter (4.17404Å) so $a = a_{\mathrm{cubic}}/\sqrt{2}$ so redefining a

$$\Delta E = \frac{176\sqrt{2}\pi\mu_0\mu_S^2}{3a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}k|z|} + \frac{64}{88}\sum_{l=1}^{\infty} l\cos\left(l\mathbf{b}_2\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}l|z|}\right.$$
$$+\sum_{k,l=1}^{\infty}\left\{\frac{2k^2+kl+l^2}{\sqrt{k^2+kl+l^2}}\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}\sqrt{k^2+kl+l^2}|z|}\right.$$
$$\left.\left.+\frac{2k^2-kl+l^2}{\sqrt{k^2-kl+l^2}}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}\sqrt{k^2-kl+l^2}|z|}\right\}\right] \tag{96}$$

Fixing z to be dependent on n

$$\Delta E = \frac{176\sqrt{2}\pi\mu_0\mu_S^2}{3a^3}\sum_{n=-\infty}^{\infty}\left[\sum_{k=1}^{\infty} k\cos\left(k\mathbf{b}_1\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}k|\mathbf{R}_n\cdot\hat{\mathbf{z}}|} + \frac{64}{88}\sum_{l=1}^{\infty} l\cos\left(l\mathbf{b}_2\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}l|\mathbf{R}_n\cdot\hat{\mathbf{z}}|}\right.$$
$$+\sum_{k,l=1}^{\infty}\left\{\frac{2k^2+kl+l^2}{\sqrt{k^2+kl+l^2}}\cos\left(\left(k\mathbf{b}_1+l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}\sqrt{k^2+kl+l^2}|\mathbf{R}_n\cdot\hat{\mathbf{z}}|}\right.$$
$$\left.\left.+\frac{2k^2-kl+l^2}{\sqrt{k^2-kl+l^2}}\cos\left(\left(k\mathbf{b}_1-l\mathbf{b}_2\right)\cdot\mathbf{R}_n\right)\right)\mathrm{e}^{-\frac{8\sqrt{6}\pi}{3a}\sqrt{k^2-kl+l^2}|\mathbf{R}_n\cdot\hat{\mathbf{z}}|}\right\}\right] \tag{97}$$

A factor of $(-1)^n$ must be added to the above equation to account for the anti-parallel alignment of neighbouring planes of spins.

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[1] J. Ubbink, J. A. Poulis, H. J. Gerritsen, and C. J. Gorter, Physica **18**, 361 (1952).
[2] Z. Qiu, D. Hou, J. Barker, K. Yamamoto, O. Gomonay, and E. Saitoh, Nat. Mater. **17**, 577 (2018), arXiv:1804.04516.
[3] K. Olejník, V. Schuler, X. Marti, V. Novák, Z. Kašpar, P. Wadley, R. P. Campion, K. W. Edmonds, B. L. Gallagher, J. Garces, M. Baumgartner, P. Gambardella, and T. Jungwirth, Nat. Commun. **8** (2017), 10.1038/ncomms15434.
[4] R. Khymyn, I. Lisenkov, V. S. Tiberkevich, A. N. Slavin, and B. A. Ivanov, Phys. Rev. B **93**, 1 (2016), arXiv:1511.05785.
[5] M. Dabrowski, T. Nakano, D. M. Burn, A. Frisk, D. G. Newman, C. Klewe, Q. Li, M. Yang, P. Shafer, E. Arenholz, T. Hesjedal, G. van der Laan, Z. Q. Qiu, and R. J. Hicken, , 1 (2019), arXiv:1912.05621.
[6] C. Zener, Phys. Rev. **96**, 1335 (1954).
[7] H. B. Callen and E. Callen, J. Phys. Chem. Solids **27**, 1271 (1966).
[8] R. F. Evans, L. Rózsa, S. Jenkins, and U. Atxitia, Phys. Rev. B **102**, 1 (2020), arXiv:2002.02548.
[9] A. Latiff Awang and M. G. Cottam, J. Phys. C Solid State Phys. **12**, 121 (1979).
[10] A. Stevens, J. Phys. C Solid State Phys. **5**, 1859 (1972).
[11] P. Asselin, R. F. Evans, J. Barker, R. W. Chantrell, R. Yanes, O. Chubykalo-Fesenko, D. Hinzke, and U. Nowak, Phys. Rev. B - Condens. Matter Mater. Phys. **82**, 1 (2010), arXiv:1006.3507.
[12] M. T. Hutchings and E. J. Samuelsen, Phys. Rev. B **6**, 3447 (1972).
[13] J. Milano, L. B. Steren, and M. Grimsditch, Phys. Rev. Lett. **93**, 077601 (2004).
[14] S. Kwon and B. Min, Phys. Rev. B - Condens. Matter Mater. Phys. **62**, 73 (2000), arXiv:0003371 [cond-mat].
[15] E. Tsymbal, J. Magn. Magn. Mater. **130**, L6 (1994).