Two defect Dzyaloshinskii approximation

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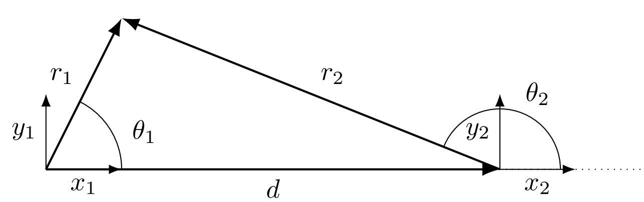
1 Expression of director around one defect from interaction with another (isotropic)

The configuration is as below: Here we consider the director angle as a function of θ_1 and r_1. Note



that the director angle ϕ is given by:

$$\phi(x, y) = q_1\theta_1(x, y) + q_2\theta_2(x, y) \tag{1}$$

If we call coordinates (x_2, y_2) centered on q_2 then we get:

$$\theta_2(x_2, y_2) = \arctan\left(\frac{y_2}{x_2}\right) \tag{2}$$

Writing these in terms of (x_1, y_1) coordinates centered at q_1 we get:

$$\begin{aligned} x_1 &= x_2 + d \\ y_1 &= y_2 \end{aligned} \tag{3}$$

Substituting in yields:

$$\theta_2(x_1, y_1) = \arctan\left(\frac{y_1}{x_1 - d}\right) \tag{4}$$

Then, considering polar coordinates (θ_1, r_1) we get that:

$$\begin{aligned} x_1 &= r_1\cos(\theta_1) \\ y_1 &= r_1\sin(\theta_1) \end{aligned} \tag{5}$$

Substituting yields:

$$\theta_2(\theta_1, r_1) = \arctan\left(\frac{r_1\sin(\theta_1)}{r_1\cos(\theta_1) - d}\right) \tag{6}$$

Hence, the isotropic contribution to the director field at the location of q_1 from the defect pair is:

$$\phi_{\text{iso}}(\theta_1, r_1) = q_1\theta_1 + q_2\arctan\left(\frac{r_1\sin(\theta_1)}{r_1\cos(\theta_1) - d}\right) \tag{7}$$

If we consider isomorph (a), then add $\pi/2$, otherwise don't add anything.

Finally, if we would like to write out the isotropic director field from two defects at q_2, everything is the same except d changes sign:

$$\phi_{\text{iso}}(\theta_2, r_2) = q_1\arctan\left(\frac{r_2\sin(\theta_2)}{r_2\cos(\theta_2) + d}\right) + q_2\theta_2 \tag{8}$$

2 Checking Fourier series

We need to check that the analysis of the director Fourier modes is correct. To do this, we note that the director ϕ as a function of θ for a $-1/2$ in isomorph (a) is given by:

$$\phi(\theta) = -\frac{1}{2}\theta + \frac{\pi}{2} \tag{9}$$

on the interval $[0, 2\pi]$. We would like to find the Fourier series of this. This is given by:

$$s(\theta) = A_0 + \sum_{n=1}^{\infty} A_n\cos(n\theta) + B_n\sin(n\theta) \tag{10}$$

We calculate these coefficients as follows:

$$\begin{aligned} A_0 &= \frac{1}{2\pi}\int_0^{2\pi}\phi(\theta)d\theta \\ &= \frac{1}{2\pi}\left[-\frac{1}{4}\theta^2 + \frac{\pi}{2}\theta\right]_0^{2\pi} \\ &= 0 \end{aligned} \tag{11}$$

$$\begin{aligned} B_n &= \frac{1}{\pi}\int_0^{2\pi}\phi(\theta)\sin(n\theta)\,d\theta \\ &= -\frac{1}{2\pi}\left[\frac{-2\pi}{n}\right] \\ &= \frac{1}{n} \end{aligned} \tag{12}$$

3 Verifying DFT identities

From the numpy documentation, we have that the inverse DFT is given by:

$$a_m = \frac{1}{n}\sum_{k=0}^{n-1} A_k \exp\left\{2\pi i\frac{mk}{n}\right\} \tag{13}$$

Here a_m is a set of values of our function f taken at some discrete points x_m. If $x \in [0, L)$ then:

$$\frac{x_m}{L} = \frac{m}{n} \implies m = \frac{x_m n}{L} \tag{14}$$

Substituting, we get:

$$f(x_m) = \frac{1}{n} \sum_{k=0}^{n-1} A_k \exp\left\{\frac{2\pi}{L} ikx_m\right\} \tag{15}$$

Expanding into trigonometric functions using Euler's formula, and splitting A_k into real and imaginary components, we get:

$$\begin{aligned}
f(x_m) &= \frac{1}{n} \sum_{k=0}^{n-1} (B_k + iC_k) \left[\cos\left(\frac{2\pi}{L} kx_m\right) + i \sin\left(\frac{2\pi}{L} kx_m\right)\right] \\
&= \frac{1}{n} \sum_{k=0}^{n-1} B_k \cos\left(\frac{2\pi}{L} kx_m\right) - C_k \sin\left(\frac{2\pi}{L} kx_m\right) + i \left[B_k \sin\left(\frac{2\pi}{L} kx_m\right) + C_k \cos\left(\frac{2\pi}{L} kx_m\right)\right] \\
&= \frac{1}{n} \sum_{k=0}^{n-1} B_k \cos\left(\frac{2\pi}{L} kx_m\right) - C_k \sin\left(\frac{2\pi}{L} kx_m\right)
\end{aligned} \tag{16}$$

Where the last line follows from the fact that $f(x)$ is real. Hence, the trigonometric Fourier coefficients should correspond with B_k/n and $-C_k/n$ respectively.

4 Verifying DFT identities a different way

Suppose $f(x) = \sin(2\pi qx)$, and call $x_m = 2\pi m/n$. Then, its Discrete Fourier Transform is given by:

$$\begin{aligned}
A_k &= \sum_{m=0}^{n-1} \sin(2\pi q x_m) e^{-2\pi imk/n} \\
&= \sum_{m=0}^{n-1} \frac{1}{2i} \left(e^{i2\pi qm/n} - e^{-i2\pi qm/n}\right) e^{-2\pi imk/n} \\
&= \frac{1}{2i} \sum_{m=0}^{n-1} \left(e^{i2\pi(q-k)/n}\right)^m - \frac{1}{2i} \sum_{m=0}^{n-1} \left(e^{-i2\pi(q+k)/n}\right)^m
\end{aligned} \tag{17}$$

Now note that:

$$\frac{1}{2i} \sum_{m=0}^{n-1} \left(e^{i2\pi(q-k)/n}\right)^m = \begin{cases} \frac{1}{2i}\left(\frac{1-e^{i2\pi(q-k)}}{1-e^{i2\pi(q-k)/n}}\right) = 0 & (k-q) \mod n \neq 0 \\ \frac{n}{2i} & (k-q) \mod n = 0 \end{cases} \tag{18}$$

And similarly:

$$\frac{1}{2i} \sum_{m=0}^{n-1} e^{-i2\pi m/n(q+k)} = \begin{cases} \frac{1}{2i}\left(\frac{1+e^{-i2\pi m(q+k)}}{1-e^{-i2\pi m/n(q+k)}}\right) = 0 & (k+q) \mod n \neq 0 \\ \frac{n}{2i} & (k+q) \mod n = 0 \end{cases} \tag{19}$$

Hence, we get:

$$A_k = \begin{cases} \frac{n}{2i} & (k-q) \mod n = 0 \\ -\frac{n}{2i} & (k+q) \mod n = 0 \\ 0 & \text{otherwise} \end{cases} \tag{20}$$

Hence, to get the sin coefficient we must take $-\frac{2}{n}\mathrm{Im}(A_k)$. Similarly we should take $\frac{2}{n}\mathrm{Re}(A_k)$ to get the cos coefficient.

5 Verifying inverse DFT

Here we will just explicitly take the Inverse Discrete Fourier Transform of the sin coefficients:

$$
\begin{aligned}
f(x_m) &= \frac{1}{n}\sum_{k=0}^{n-1} A_k e^{2\pi imk/n} \\
&= \frac{1}{n}\left(\frac{n}{2i}e^{2\pi imq/n} - \frac{n}{2i}e^{2\pi im(n-q)/n}\right) \\
&= \sin(2\pi mq/n) \\
&= \sin(qx_m)
\end{aligned}
\tag{21}
$$

6 Identifying the issue

There is an issue in Eq. (16). The formula is entirely correct, but the conclusion one might draw is incorrect. Indeed, note that:

$$
\begin{aligned}
\cos\left(\frac{2\pi}{L}(n-k)x_m\right) &= \cos\left(\frac{2\pi}{L}nx_m\right)\cos\left(\frac{2\pi}{L}kx_m\right) + \sin\left(\frac{2\pi}{L}nx_m\right)\sin\left(\frac{2\pi}{L}kx_m\right) \\
&= \cos\left(2\pi m\right)\cos\left(\frac{2\pi}{L}kx_m\right) + \sin\left(2\pi m\right)\sin\left(\frac{2\pi}{L}kx_m\right) \\
&= \cos\left(\frac{2\pi}{L}kx_m\right)
\end{aligned}
\tag{22}
$$

Hence, you get two terms of the form $\cos\left(\frac{2\pi}{L}kx_m\right)$, one which essentially corresponds to the negative frequency component. This is where the factor of 2 comes from.