- 08/20

$$\begin{aligned}
\vec{w}^2 &= (\alpha\vec{r}+\beta\vec{b})^2 \\
&= \alpha^2 r^2 + \beta^2 b^2 + 2\alpha\beta\vec{r}\cdot\vec{b} \\
&= \alpha^2 r^2 + (1-\alpha\frac{\vec{r}\cdot\vec{b}}{b^2})^2 b^2 + 2\alpha(1-\alpha\frac{\vec{r}\cdot\vec{b}}{b^2})\vec{r}\cdot\vec{b} \\
&= \alpha^2 r^2 + (1+\alpha^2\frac{(\vec{r}\cdot\vec{b})^2}{b^4} - 2\alpha\frac{\vec{r}\cdot\vec{b}}{b^2})b^2 + 2\alpha(1-\alpha\frac{\vec{r}\cdot\vec{b}}{b^2})\vec{r}\cdot\vec{b} \\
&= \alpha^2 r^2 + b^2 - \alpha^2\frac{(\vec{r}\cdot\vec{b})^2}{b^2} \\
&= b^2 + \frac{|\alpha|^2}{b^2}(r^2 b^2 - (\vec{r}\cdot\vec{b})^2)
\end{aligned}$$

- 08/26

In our calculations, the standard deviation of temperature in a certain slab m is expressed as

$$\sigma_{m,s} = \sqrt{\frac{\sum_{i=1}^{\mathcal{N}}\left(T_{m,i}-\overline{T}_m\right)}{\mathcal{N}-1}} \tag{1}$$

where $\overline{T}_m$ is the average value for measurements $T_{m,i}$ and $\mathcal{N}$ represents the total number of measurements.The standard deviation of the averaged value $\overline{T}_m$, therefore, is given by

$$\begin{aligned}
\sigma_m &= \frac{\sigma_{m,s}}{\sqrt{\mathcal{N}}} \qquad (2) \\
&= \sqrt{\frac{\sum_{i=1}^{\mathcal{N}}\left(T_{m,i}-\overline{T}_m\right)}{\mathcal{N}(\mathcal{N}-1)}} \qquad (3)
\end{aligned}$$

With a set of data $(\overline{T}_m, \sigma_m)$ where m goes from 0 to N-1 in our model, we do the fit to the cosine function to determine and fitting parameter of amplitude, which is ΔT in Eq.(1). The standard deviation of ΔT is determined at the same time.Then by using Eq.(2) we can get a relation between $\sigma_{\Delta T}$ and $\sigma_{\kappa_{\text{eff}}}$, which is

$$\frac{\sigma_\kappa}{\kappa_{\text{eff}}} = \frac{\sigma_{\Delta T}}{\Delta T} \tag{4}$$

Thus $\sigma_{\kappa_{\text{eff}}} = \kappa_{\text{eff}}\sigma_{\Delta T}/\Delta T$ gives the standard deviation of κ.

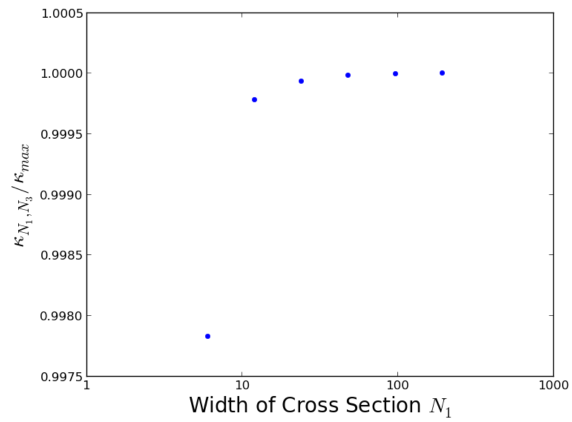
Liquid

Crystal

- 08/09
  Temperature approximately 80K, 0.66 in LJ unit, with the scaling $\epsilon/k_B = 119.6K$, I keep the temperature variance 0.03 during the simulation(LJ unit) to keep my system efficient.We run those systems at constant temperature.

Extrapolation

- 08/23 correction
  summing over Brillouin Zone, the length of the sample is 500a=500d, the ratio is devided by



the kappa(192)

Appendix A

$$\begin{aligned}
\kappa(q) &= \frac{3\kappa_{D,0}}{7\lambda^2}[o(\lambda^3)+1+2\lambda^2-(1-\frac{1}{3}\lambda^2)-\frac{\lambda^{\frac{5}{2}}}{\sqrt{2}}(o(\sqrt{\lambda})+\pi)] \\
&= \kappa_{D,0}-\frac{3\pi\sqrt{\lambda}}{7\sqrt{2}}\kappa_{D,0} \\
&= \kappa_{D,0}-\frac{3\pi}{7}\kappa_{D,0}\sqrt{\frac{\pi l_{min}}{L}}
\end{aligned}$$

Here $o(\lambda^3)$ means terms that have a order lower than or equal to λ^3 in $\lambda \longrightarrow 0$ limit, I am guessing that in summing the $\frac{1}{3}\lambda^2$, the appendix A wrongly subtracted it.

Appendix B

$$\begin{aligned}
\frac{\kappa_{00}(q)}{\kappa_{D,0}} &= \frac{n^{\frac{1}{3}}}{2N_xN_y}\int_{\epsilon}^{1}dx\frac{x^2}{x^4+\lambda^4} \\
&= \frac{n^{\frac{1}{3}}}{2N_xN_y}\times\frac{1}{\sqrt{\lambda}}[\frac{\sqrt{2}}{8}\ln\frac{1+\lambda+\sqrt{2\lambda}}{1+\lambda-\sqrt{2\lambda}}+\frac{\sqrt{2}}{4}\arctan(\sqrt{\frac{2}{\lambda}}+1)+\frac{\sqrt{2}}{4}\arctan(\sqrt{\frac{2}{\lambda}}-1) \\
&-\frac{\sqrt{2}}{8}\ln\frac{1+\frac{\epsilon^2}{\lambda}-\sqrt{\frac{2}{\lambda}}\epsilon}{1+\frac{\epsilon^2}{\lambda}+\sqrt{\frac{2}{\lambda}}\epsilon}-\frac{\sqrt{2}}{4}\arctan(\sqrt{\frac{2}{\lambda}}\epsilon+1)-\frac{\sqrt{2}}{4}\arctan(\sqrt{\frac{2}{\lambda}}\epsilon-1)] \\
&= \frac{n^{\frac{1}{3}}}{2N_xN_y}\times\frac{1}{\sqrt{\lambda}}(\frac{\sqrt{2}}{8}\ln\frac{1+\lambda+\sqrt{2\lambda}}{1+\lambda-\sqrt{2\lambda}}+\frac{\sqrt{2}}{4}\pi) \\
&= \frac{n^{\frac{1}{3}}}{2N_xN_y}\times\frac{1}{\sqrt{\lambda}}(-\frac{1}{2}\sqrt{\lambda}+\frac{\sqrt{2}}{4}\pi) \\
&= \frac{n^{\frac{1}{3}}}{2N_xN_y}\times(\frac{\sqrt{2}}{4}\frac{\pi}{\sqrt{\lambda}}-\frac{1}{2}) \\
&= \frac{n^{\frac{1}{3}}}{2N_xN_y}\times(\frac{1}{4}\sqrt{\frac{\pi L}{\ell_m}}-\frac{1}{2})
\end{aligned}$$

Q

For a crystal of a $N_1\times N_2\times N_3$ cell in the real space:
The wave vector we are summing over is in the form$\vec{Q}=\frac{2\pi}{a}(\frac{n_1}{N_1},\frac{n_2}{N_2},\frac{n_3}{N_3})$
where n_1, N_2, n_3 are to be decided.

There are 8 constraints on n_1, n_2, n_3,because by the property of BZ, the BZ is enclosed by the bi-sector of wave vector:

$$\frac{2\pi}{a}(1,1,1),\ \frac{2\pi}{a}(\bar{1},\bar{1},\bar{1});\ \frac{2\pi}{a}(\bar{1},1,1),\ \frac{2\pi}{a}(1,\bar{1},\bar{1});$$
$$\frac{2\pi}{a}(1,\bar{1},1),\ \frac{2\pi}{a}(\bar{1},1,\bar{1})\text{ and }\frac{2\pi}{a}(1,1,\bar{1}),\ \frac{2\pi}{a}(\bar{1},\bar{1},1);$$

For $\frac{2\pi}{a}(1,1,1)$, $\frac{2\pi}{a}(\bar{1},\bar{1},\bar{1})$:

$$-\frac{\sqrt{3}}{2}<\frac{\frac{n_1}{N_1}+\frac{n_2}{N_2}+\frac{n_3}{N_3}}{\sqrt{3}}\le\frac{\sqrt{3}}{2}$$

$\Longleftrightarrow$

$$-3N_1N_2N_3<2n_1N_2N_3+2N_12_2N_3+2N_1n_2N_3+2N_1N_2n_3<3N_1N_2N_3+1$$

For $\frac{2\pi}{a}(\bar{1},1,1)$, $\frac{2\pi}{a}(1,\bar{1},\bar{1})$:

$$-3N_1N_2N_3<-2n_1N_2N_3+2N_12_2N_3+2N_1n_2N_3+2N_1N_2n_3<3N_1N_2N_3+1$$

$(1,\bar{1},1)$, $(1,1,\bar{1})$ are similar.

we can use a triple-loops to search these wave vectors:

$$n_1:-N_1+1\to N_1$$
$$n_2:-N_2+1\to N_2$$
$$n_3:-N_3+1\to N_3$$