Simple isotropic crystal.-

Toy model of a crystal : $E = \frac{c}{2} \int d^3x \, (\nabla \cdot \vec{u})^2$ (only dilatation, no shear).

Introduce Fourier Transform: $\vec{u}(\vec{r}) = \int \frac{d^3k}{(2\pi)^3} \, \hat{u}(\vec{k}) \, e^{i\vec{k}\cdot\vec{r}}$

$$\rightarrow \quad \nabla \cdot \vec{u} = \int \frac{d^3k}{(2\pi)^3} \, (i\vec{k}\cdot\hat{u}(\vec{k})) \, e^{i\vec{k}\cdot\vec{r}}$$

As shown in class, (cf. Parseval's identity).

$$\int d^3x \, (\nabla\cdot\vec{u})^2 = \int \frac{d^3k}{(2\pi)^3} \, |i\vec{k}\cdot\hat{u}(\vec{k})|^2$$

(using the fact that $\vec{k}$ is real and $\hat{u}(-\vec{k}) = \hat{u}^*(\vec{k})$)

$$\Rightarrow \quad E = \frac{c}{2} \int \frac{d^3k}{(2\pi)^3} \, k^2 \, |\hat{u}_\ell(\vec{k})|^2 \quad \text{with } \hat{u}_\ell = \hat{k}\cdot\hat{u}(\vec{k})$$

the "longitudinal" projection of $\hat{u}$.

We next evaluate $|\hat{u}_\ell(\vec{k})|^2$ as shown in the notes. As done there, and for simplicity, we turn to a discrete representation (Fourier Series):

$$E = \frac{c}{2} \frac{1}{L^3} \sum_{\vec{k}} k^2 \, |\hat{u}_\ell(\vec{k})|^2$$

where $\vec{k}$ is now discrete.

The thermal average is defined:

$$\langle |\hat{u}_\ell(\vec{k}_0)|^2 \rangle = \frac{\prod_{k} \int d\hat{u}(\vec{k}) \, |\hat{u}_\ell(\vec{k}_0)|^2 \, e^{-\frac{\beta c}{2L^3} \sum_{\vec{k}} k^2 |\hat{u}_\ell(\vec{k})|^2}}{\prod_{\vec{k}} \int d\hat{u}_\ell(\vec{k}) \, e^{-\frac{\beta c}{2L^3} \sum_{\vec{k}} k^2 |\hat{u}_\ell(\vec{k})|^2}}$$

(*): The integrand is only a function of $u_\ell(\vec{k})$: for a fixed $\vec{k}$, it only depends on the projection of $\hat{u}(\vec{k})$ onto the $\vec{k}$ direction. We therefore write:

$$d\hat{u}(\vec{k}) = d\hat{u}_\ell(\vec{k})\, d\hat{u}_t(\vec{k})$$

where $\hat{u}_t(\vec{k})$ spans the two dimensional plane perpendicular to $\vec{k}$.

Since the integrand does not depend on $\hat{u}_t(\vec{k})$ the integrals for each $\vec{k}$ in numerator and denominator cancel. We are left with:

$$\langle |\hat{u}_\ell(\vec{k}_0)|^2 \rangle = \frac{\prod_{\vec{k}} \int d\hat{u}_\ell(\vec{k})\, |\hat{u}_\ell(\vec{k}_0)|^2\, e^{-\frac{\beta C}{2L^3} \sum_{\vec{k}} k^2 |\hat{u}_\ell(\vec{k})|^2}}{\prod_{\vec{k}} \int d\hat{u}_\ell(\vec{k})\, e^{-\frac{\beta C}{2L^3} \sum_{\vec{k}} k^2 |\hat{u}_\ell(\vec{k})|^2}}$$

All products over $\vec{k}$ in the numerator cancel the denominator, except for $\vec{k} = \vec{k}_0$. ~~and $\{\vec{k} = -\vec{k}_0\}$, with the~~. As shown in the notes, there are two terms in

$$\sum_{\vec{k}} k^2 |\hat{u}_\ell(\vec{k})|^2$$

that contribute to the integral for $\vec{k}_0$ as the energy of $\vec{k}_0$ is the same as the energy of $-\vec{k}_0$:

$$\langle |\hat{u}_\ell(\vec{k}_0)|^2 \rangle = \frac{\int d\hat{u}_\ell(\vec{k}_0)\, |\hat{u}_\ell(k_0)|^2\, e^{-\frac{\beta C}{L^3} k_0^2 |\hat{u}_\ell(\vec{k}_0)|^2}}{\int d\hat{u}_\ell(\vec{k}_0)\, e^{-\frac{\beta C}{L^3} k_0^2 |\hat{u}_\ell(\vec{k}_0)|^2}}$$

Since $\hat{u}_\ell(\vec{k}_0)$ is a complex variable, the integral remaining is a two dimensional integral over the complex plane. However, the integrand only depends on the modulus $|\hat{u}_\ell(\vec{k}_0)|^2$, but not on the phase. Therefore the integral over the phase angle in the numerator cancels the

Same integral in the denominator. ~~Let the sample~~ Therefore:

$$\langle |\hat{u}_\ell(\vec{k}_0)|^2 \rangle = \frac{\int |\hat{u}_\ell(\vec{k}_0)|\, d|\hat{u}_\ell(k_0)|\; |\hat{u}_\ell(\vec{k}_0)|^2 e^{-\frac{\beta C}{L^3} k_0^2 |\hat{u}_\ell(k_0)|^2}}{\int |\hat{u}_\ell(k_0)|\, d|\hat{u}_\ell(k_0)| \cdot e^{-\frac{\beta C}{L^3} k_0^2 |\hat{u}_\ell(\vec{k}_0)|^2}}$$

We have an integral of the form: $(x \equiv |\hat{u}_\ell(\vec{k}_0)|)$

$$\int_0^\infty x^3 dx\, e^{-ax^2} \quad \left(a = \frac{\beta C}{L^3} k_0^2 \right)$$ in the numerator and

~~We use the~~

$$\int_0^\infty x\, dx\, e^{-ax^2}$$ in the denominator.

By using the result: $$\int_0^\infty x^m e^{-ax^2} dx = \frac{\Gamma((m+1)/2)}{2a^{(m+1)/2}}$$

where Γ is the Gamma function,
we find:

$$\int_0^\infty x^3 dx\, e^{-ax^2} = \frac{\Gamma(2)}{2a^2} \qquad \int_0^\infty x\, dx\, e^{-ax^2} = \frac{\Gamma(1)}{2a}$$

Then:

$$\langle |\hat{u}_\ell(\vec{k}_0)|^2 \rangle = \frac{\Gamma(2)/\cancel{2}a^{\cancel{2}}}{\Gamma(1)/\cancel{2a}} = \frac{\Gamma(2)}{\Gamma(1)} \frac{1}{a}$$

and $\Gamma(1) = 1$, $\Gamma(2) = 1$

$$\Rightarrow \langle |\hat{u}_\ell(\vec{k}_0)|^2 \rangle = \frac{k_B T}{C} L^3 \frac{1}{k_0^2}$$

As shown in class, the correlation function $G(\vec{k})$ is defined:

$$\langle |\hat{u}_\ell(\vec{k})|^2 \rangle = G(\vec{k}) L^3 \Rightarrow \boxed{G(\vec{k}) = \frac{k_B T}{C k^2}}$$

We finally use the result : (u_ℓ is a scalar at this stage)

$$\langle u_\ell(0)\, u_\ell(\vec{r}) \rangle = \int \frac{d^3k}{(2\pi)^3}\, G(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}$$

and in particular: (equal position $\vec{r}=0$)

$$\langle u_\ell(\vec{r})^2 \rangle \qquad \langle u_\ell^2 \rangle = \int \frac{d^3k}{(2\pi)^3}\, G(\vec{k}) = \int \frac{d^3k}{(2\pi)^3}\, \frac{k_B T}{c k^2}$$

$$= \int \frac{4\pi \cancel{k^2} dk}{(2\pi)^3}\, \frac{k_B T}{c \cancel{k^2}} = \frac{1}{2\pi^2} \int_0^{q_c} \frac{k_B T}{c}\, dk \Rightarrow$$

no cut-off needed for low k as there is no divergence in the integrand.

$$\boxed{\langle u_\ell^2 \rangle = \frac{k_B T}{2\pi^2 c} \cdot q_c}$$

Columnar phase

Now $\vec{u}_\perp = (u_x, u_y, 0)$ is a two dimensional displacement field. Order only along x and y. Note, however, that $u_x = u_x(x,y,z)$, $u_y = u_y(x,y,z)$, functions of three dimensional space.

The energy of a configuration of a columnar phase is:

$$E = \frac{c}{2} \int d^3x \left[(\nabla_\perp \vec{u}_\perp)^2 + \lambda^2 \left(\partial_z^2 \vec{u}_\perp \right)^2 \right]$$

We again introduce the Fourier transform:

$$\vec{u}_\perp(\vec{r}) = \int \frac{d^3k}{(2\pi)^3}\, \hat{u}_\perp(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}$$

this is a two dimensional vector, of complex components.

We now take the divergence in 2D space:

$$\nabla_\perp \cdot \vec{u}_\perp = \int \frac{d^3k}{(2\pi)^3} \left(i\vec{k}_\perp \cdot \hat{u}_\perp(\vec{k}) \right) e^{i\vec{k}\cdot\vec{r}} \qquad \vec{k}_\perp = (k_x, k_y, 0)$$

$$\vec{u}_\perp = (u_x, u_y, 0)$$

As in the former case, with Parseval's identity:

$$\int d^3x \left(\nabla_\perp \cdot \vec{u}_\perp \right)^2 = \int \frac{d^3k}{(2\pi)^3} \left| i\vec{k}_\perp \cdot \hat{u}_\perp(\vec{k}) \right|^2$$ again, using that $\hat{u}_\perp(-\vec{k}) = \hat{u}_\perp^*(\vec{k})$

and $\vec{k} = (k_x, k_y, k_z)$ remains a three dimensional vector.

The new term can be treated similarly:

$$\partial_z \vec{u}_\perp = \int \frac{d^3k}{(2\pi)^3} \hat{u}_\perp(\vec{k})(ik_z) e^{i\vec{k}\cdot\vec{r}} \quad ; \quad \partial_z^2 \vec{u}_\perp = \int \frac{d^3k}{(2\pi)^3} \hat{u}_\perp(\vec{k})(-k_z^2) e^{i\vec{k}\cdot\vec{r}}$$

Therefore:

$$\frac{c\lambda^2}{2} \int d^3x \left(\partial_z^2 \vec{u}_\perp \right)^2 = \frac{c\lambda^2}{2} \int d^3x \int \frac{d^3k}{(2\pi)^3} \hat{u}_\perp(\vec{k})(-k_z^2) e^{i\vec{k}\cdot\vec{r}} \int \frac{d^3k'}{(2\pi)^3} \hat{u}_\perp(\vec{k}')(-k_z'^2) e^{i\vec{k}'\cdot\vec{r}}$$

$$= \frac{c\lambda^2}{2} \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} (-k_z^2)(-k_z'^2)\, \hat{u}_\perp(\vec{k})\, \hat{u}_\perp(\vec{k}') \underbrace{\int d^3x\, e^{i(\vec{k}+\vec{k}')\cdot\vec{r}}}_{(2\pi)^3 \delta(\vec{k}+\vec{k}')}$$

$$= \frac{c\lambda^2}{2} \int \frac{d^3k}{(2\pi)^3} (-k_z^2)(-k_z^2)\, \hat{u}_\perp(\vec{k})\, \hat{u}_\perp(-\vec{k})$$

$$= \frac{c\lambda^2}{2} \int \frac{d^3k}{(2\pi)^3} k_z^4 \left| \hat{u}_\perp(\vec{k}) \right|^2$$

Putting both results together:

$$\boxed{E = \frac{c}{2} \int \frac{d^3k}{(2\pi)^3} \left[\left| \vec{k}_\perp \cdot \hat{u}_\perp(\vec{k}) \right|^2 + \lambda^2 k_z^4 \left| \hat{u}_\perp(\vec{k}) \right|^2 \right]}$$

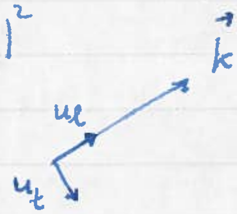
In analogy to the case of a crystal, we define:

$$\hat{u}_\ell = \hat{k}_\perp \cdot \vec{u}_\perp(\vec{k})$$

$\uparrow$ unit vector. Given $\vec{k}$, $\hat{k}_\perp$ points in the (x,y) direction, and $\hat{u}_\ell$ is the projection on this two dimensional plane.

$$\rightarrow \quad |\vec{k}_\perp \cdot \hat{u}_\perp(\vec{k})|^2 = k_\perp^2 \, |\hat{u}_\ell(k)|^2 \quad \text{by definition.}$$

$$\rightarrow \quad |\hat{u}_\perp(\vec{k})|^2 = |\hat{u}_\ell(\vec{k})|^2 + |\hat{u}_t(\vec{k})|^2$$



this is a vector $(\hat{u}_x, \hat{u}_y, 0)$

So that it will have a projection along $\vec{k}$ (u_ℓ) and a projection perpendicular to $\vec{k}$ (u_t).

Therefore, the energy in $\vec{k}$ space is written as:

$$E = \frac{c}{2} \int \frac{d^3k}{(2\pi)^3} \left\{ k_\perp^2 \, |\hat{u}_\ell(\vec{k})|^2 + \lambda^2 k_z^4 \, |\hat{u}_\ell(\vec{k})|^2 + \lambda^2 k_z^4 \, |\hat{u}_t(\vec{k})|^2 \right\}$$

We now proceed to calculate $\langle |\hat{u}_\ell(\vec{k})|^2 \rangle$ as in the previous case. Note that the energy has two additive terms, one proportional to $|\hat{u}_\ell|^2$, the other proportional to $\langle |\hat{u}_t|^2 \rangle$, therefore the two decouple and do not contribute cross correlations.

In analogy to the case of a crystal, we have:

$$\boxed{G(\vec{k}) = \frac{k_B T}{c(k_\perp^2 + \lambda^2 k_z^4)}}$$

We finally compute $\langle u_\ell^2 \rangle$ as the inverse Fourier transform of $\langle |\hat{u}_\ell(k)|^2 \rangle$:

$$\langle u_\ell^2 \rangle = \int \frac{d^3k}{(2\pi)^3} \frac{k_B T}{C\left(k_\perp^2 + \lambda^2 k_z^4\right)}$$

Consider now the change of variables:
$$\begin{cases} \vec{q} = \left(k_x, k_y, \lambda k_z^2\right) \rightarrow q^2 = k_\perp^2 + \lambda^2 k_z^4 \\ d^3q = dk_x\, dk_y\, 2\lambda k_z\, dk_z \end{cases}$$

Therefore: $d^3q = d^3k\,(2\lambda k_z)$ and we need k_z in terms of the new $\vec{q} = (q_x, q_y, q_z)$

$$\rightarrow q_z = \lambda k_z^2 \quad \rightarrow 2\lambda k_z = 2\sqrt{\lambda q_z}$$

We find:

$$\langle u_\ell^2 \rangle = \int \frac{d^3q / 2\sqrt{\lambda q_z}}{(2\pi)^3} \frac{k_B T}{C q^2}$$

We now use spherical coordinates in q-space:
$$\begin{cases} d^3q = q^2 \sin\theta \, dq\, d\theta\, d\varphi \\ q_z = q\cos\theta \end{cases}$$

2+ (range in θ halved)

$$= \frac{k_B T}{2(2\pi)^3 C\sqrt{\lambda}} \int_0^\infty dq \int_0^{2\pi} d\varphi \int_0^{\pi/2} d\theta \; \frac{\cancel{q^2} \sin\theta}{\sqrt{q\cos\theta}} \frac{1}{\cancel{q^2}}$$

Original variable k_z^2, so the integrand is zero in the bottom lower half of k space.

$$= \frac{k_B T}{2(2\pi)^2 C\sqrt{\lambda}} \int_0^{q_c} \frac{dq}{\sqrt{q}} \int_0^{\pi/2} d\theta \frac{\sin\theta}{\sqrt{\cos\theta}} =$$

$$= \frac{k_B T}{2(2\pi)^2 C\sqrt{\lambda}} \left[\frac{q^{1/2}}{1/2}\right]_0^{q_c} \cdot \int_0^{\pi/2} d\theta \frac{\sin\theta}{\sqrt{\cos\theta}} =$$

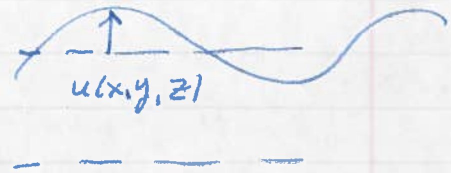
$$= \frac{k_B T}{(2\pi)^2 c} \sqrt{\frac{q_c}{\lambda}} \cdot \Big[-2\sqrt{\cos\theta} \Big]_0^{\pi/2}$$

Finally:

$$\boxed{\langle u_\ell^2 \rangle = \frac{k_B T}{2(\pi)^2 C} \sqrt{\frac{q_c}{\lambda}}}$$

Smectic phase.

The displacement is now a 1-dimensional scalar



and the energy:

$$E = \frac{C}{2} \int d^3x \left[(\partial_z u)^2 + \lambda^2 (\nabla_\perp^2 u)^2 \right]$$

Introducing again: $u(x,y,z) = \int \frac{d^3k}{(2\pi)^3} \hat{u}(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}$

now $\hat{u}$ is a scalar.

- $\frac{C}{2} \int d^3x\, (\partial_z u)^2 =$

$$= \frac{C}{2} \int \frac{d^3k}{(2\pi)^3} k_z^2 \, |\hat{u}(\vec{k})|^2$$ as we have done earlier.

- $\frac{C\lambda^2}{2} \int d^3x \, (\nabla_\perp^2 u)^2 = \frac{C\lambda^2}{2} \int \frac{d^3k}{(2\pi)^3} k_\perp^4 \, |\hat{u}(\vec{k})|^2$ again, standard calculation.

$$\Rightarrow \quad E = \frac{C}{2} \int \frac{d^3k}{(2\pi)^3} \left[k_z^2 + \lambda^2 k_\perp^4 \right] |\hat{u}(\vec{k})|^2$$

and repeating the steps above:

$$\boxed{G(\vec{k}) = \frac{k_B T}{C} \frac{1}{k_z^2 + \lambda^2 k_\perp^4}}$$

u is now a scalar, so we can directly compute:

$$\langle u^2 \rangle = \int \frac{d^3k}{(2\pi)^3} \; G(\vec{k}) = \frac{k_B T}{c} \int \frac{d^3k}{(2\pi)^3} \frac{1}{k_z^2 + \lambda^2 k_\perp^4} \rightarrow k_\perp^4 = (k_x^2 + k_y^2)^2$$

We perform the same change of variables as in the case of the columnar phase:

$$\vec{q} = (\lambda k_x^2 , \lambda k_y^2 , k_z) \quad (\text{of course } k_\perp = (k_x, k_y, 0))$$

The Jacobian of the transformation follows:

$$d^3q = (2\lambda k_x dk_x)(2\lambda k_y dk_y)\, dk_z = 4\lambda^2 k_x k_y \, d^3k$$

and using $q_x = \lambda k_x^2$ and $q_y = \lambda k_y^2$

we find:

$$d^3q = 4\lambda^2 \sqrt{q_x/\lambda} \sqrt{q_y/\lambda} \, d^3k = 4\lambda \sqrt{q_x q_y} \, d^3k$$

In the new coordinate system:

$$\langle u^2 \rangle = \frac{k_B T}{c} \frac{1}{(2\pi)^3} \frac{1}{4\lambda} \int \frac{d^3q}{\sqrt{q_x q_y}} \frac{1}{q^2}$$

Introduce again ~~polar~~ spherical coordinates: $d^3q = q^2 \sin\theta \, dq \, d\theta \, d\varphi$

$$q_x = q \sin\theta \cos\varphi$$
$$q_y = q \sin\theta \sin\varphi$$

$$\langle u^2 \rangle = \frac{k_B T}{c} \frac{1}{(2\pi)^3} \frac{1}{4\lambda} \int \frac{\cancel{q^2} \cancel{\sin\theta} \, dq \, d\theta \, d\varphi}{\sqrt{q^2 \sin^2\theta \cos\varphi \sin\varphi}} \frac{1}{\cancel{q^2}}$$

$$= \frac{k_B T}{c} \frac{1}{(2\pi)^3} \frac{1}{4\lambda} \int \frac{dq}{q} \cdot \underbrace{\int_0^{\pi} d\theta}_{\text{no restriction in } k_z} \cdot \underbrace{\int_0^{\pi/2} \frac{d\varphi}{\sqrt{\sin\varphi \cos\varphi}}}_{\text{only first quadrant: both } k_x^2 \text{ and } k_y^2 \text{ are positive.}}$$

Now: $\displaystyle\int_{1/L}^{q_c} \frac{dq}{q} = \ln(q_c L)$ we need both cut-offs in this case.

$$\Rightarrow \quad \langle u^2 \rangle = \frac{k_B T}{c} \frac{\pi}{4\lambda} \frac{1}{(2\pi)^3} \ln(q_c L) \underbrace{\int_0^{\pi/2} \frac{d\varphi}{\sqrt{\sin\varphi \cos\varphi}}}_{\simeq 3.7081 \,=\, 2 K(\sqrt{2}/2)}$$

(Maple).

$$= \frac{k_B T}{c} \frac{1}{4\lambda} \frac{1}{8\pi^2} \ln(q_c L)\, 3.7081$$

$$\langle u^2 \rangle = \int \frac{d^3 k}{(2\pi)^3} \frac{k_B T}{c\left(k_z^2 + \lambda^2 (k_x^2 + k_y^2)^2\right)} \qquad \begin{aligned} k_x &= r\cos\theta \\ k_y &= r\sin\theta \end{aligned}$$

$$= \frac{k_B T}{(2\pi)^3 c} \int_0^{2\pi} d\theta \int_{1/L}^{q_r} r\,dr \int_{-\infty}^{\infty} dk_z \frac{1}{k_z^2 + \lambda^2 r^4} =$$

$$= \frac{k_B T}{(2\pi)^3} \frac{1}{c} 2\pi \int_{\frac{1}{L}}^{q_c} r\,dr \left[\frac{1}{\lambda r^2} \tan^{-1}\left(\frac{k_z}{\lambda r^2}\right)\right]_{-\infty}^{\infty}$$

$$= \frac{k_B T}{(2\pi)^2 c} \int_{\frac{1}{L}}^{q_c} r\,dr \left[\frac{1}{\lambda r^2} \frac{\pi}{2} - \frac{1}{\lambda r^2}\left(-\frac{\pi}{2}\right)\right] = \frac{k_B T}{(2\pi)^2 c} \int_{\frac{1}{L}}^{q_c} r \cdot \frac{1}{\lambda r^2} \pi\,dr =$$

$$= \frac{k_B T}{4\pi c \lambda} \int_{1/L}^{q_c} \frac{1}{r}\,dr = \frac{k_B T}{4\pi c \lambda} \ln(q_c L)$$

See de Gennes - Prost, p. 31