1 (10 points)

Given the form of the Matsubara Green's function in frequency and momentum space

$$\mathcal{G}_k(\omega_n) = \frac{1}{\beta M} \frac{1}{\omega_n^2 + \Omega_k^2}$$

we want to evaluate the following sum over Matsubara frequencies $\omega_n = 2\pi n/\beta$, $n \in \mathbb{Z}$. We first convert the sum into a contour integral by multiplying with the term $\frac{\beta}{e^{\beta\omega}-1}$ which has first order poles at $i\omega_m$, each with residue 1. The integration is performed over the contour C that encloses all its poles. We get

$$
\begin{aligned}
C_{kk'} &= \frac{1}{\beta}\sum_m \mathcal{G}_k(\omega_m)\mathcal{G}_{k'}(\omega_n - \omega_m) = \frac{1}{\beta}\frac{1}{2\pi i}\oint_{\gamma_1}\frac{\beta}{e^{\beta\omega}-1}\mathcal{G}_k(i\omega)\mathcal{G}_{k'}(\omega_n - i\omega)d\omega \\
&= \frac{1}{\beta^2 M^2}\frac{1}{2\pi i}\oint_{\gamma_1}\frac{1}{e^{\beta\omega}-1}\frac{1}{(i\omega)^2+\Omega_k^2}\frac{1}{(\omega_n - i\omega)^2+\Omega_{k'}^2}d\omega \\
&= \frac{1}{\beta^2 M^2}\frac{1}{2\pi i}\oint_{\gamma_1}d\omega \underbrace{\frac{1}{e^{\beta\omega}-1}\frac{1}{(\omega-\Omega_k)(\omega+\Omega_k)(\omega-\Omega_{k'}+i\omega_n)(\omega+\Omega_{k'}+i\omega_n)}}_{f(\omega)}
\end{aligned}
$$

We see that the integrand has poles at

$$\omega = \pm\Omega_k \tag{1}$$

$$\omega = \pm\Omega_{k'} - i\omega_n \tag{2}$$

in addition to the infinite number of poles at $\omega = i\omega_m = i2\pi m/\beta$.

Below is an illustration of the general strategy, taken from Altland and Simons. Following the definition, we would have to integrate along the contour that encloses the infinite number of points at $\omega = 2\pi n/\beta$, $n \in \mathbb{Z}$. We instead try to deform the contour into a circle of infinite radius.

Deforming the contour does not change the value of the integral as long the contour does not cross a pole in the process. Since our Green's function may have poles on its own (4 in our case, 2 poles are illustrated in the figure), we actually cannot just push the contour all the way to infinity.

The next best thing is shown in the right panel. We see that we now have a contour of infinite radius and some smaller contours that encircle the poles of the Green's function. Since the Green's function decays sufficiently fast, the integral along the large circle vanishes. The remainig contour integrals are easily evalued using the Residue theorem.

Note that the orientation of these new contours is now in the opposite sense. We have to take this into account by multiplying with a minus sign!

(a)   (b)
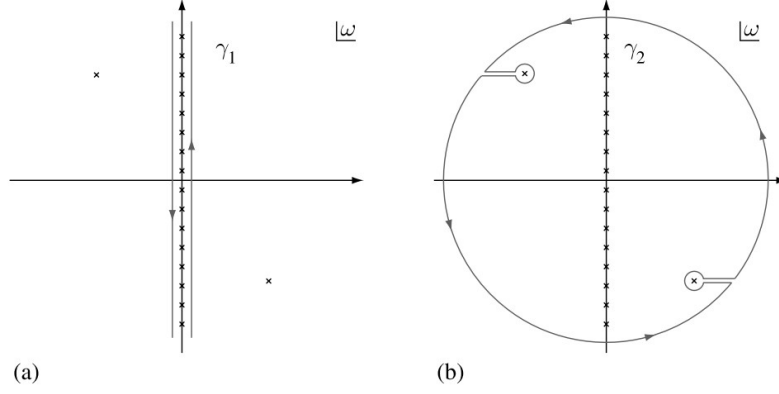
We thus get

$$C_{kk'} = \frac{1}{\beta^2 M^2} \frac{1}{2\pi i} \oint_{\gamma_2} f(\omega) d\omega = -\frac{1}{\beta^2 M^2} \sum_k \mathrm{Res}(f, \omega_k)$$

where the sum is over the four poles listed in Eqs. (1-2).

The residues are

$$\mathrm{Res}(f, \pm\Omega_k) = \mp \frac{1}{2\Omega_k} \frac{1}{e^{\pm\beta\Omega_k} - 1} \frac{1}{\Omega_{k'}^2 + (\omega_n \mp i\Omega_k)^2}$$

$$\mathrm{Res}(f, \pm\Omega_{k'} - i\omega_n) = \mp \frac{1}{2\Omega_{k'}} \frac{1}{e^{\pm\beta\Omega_{k'} - i\beta\omega_n} - 1} \frac{1}{\Omega_k^2 + (\omega_n \pm i\Omega_{k'})^2}$$

and they sum up to yield the result

$$\beta^2 M^2 C_{kk'} = \frac{1}{2\Omega_k} \left[\frac{1}{e^{\beta\Omega_k} - 1} \frac{1}{\Omega_{k'}^2 + (\omega_n - i\Omega_k)^2} - \frac{1}{e^{-\beta\Omega_k} - 1} \frac{1}{\Omega_{k'}^2 + (\omega_n + i\Omega_k)^2} \right]$$
$$+ \frac{1}{2\Omega_{k'}} \left[\frac{1}{e^{\beta\Omega_{k'}} - 1} \frac{1}{\Omega_k^2 + (\omega_n + i\Omega_{k'})^2} - \frac{1}{e^{-\beta\Omega_{k'}} - 1} \frac{1}{\Omega_k^2 + (\omega_n - i\Omega_{k'})^2} \right],$$

where we used the fact that $e^{\pm i\beta\omega_n} = 1$.

2   (10 points)

From the imaginary part of the retarded Green's function, we can obtain the spectral density function

$$A(\omega) = -\frac{2}{1 - e^{-\beta\omega}} \mathrm{Im} G^R(\omega).$$

The time-ordered Green's function can be expressed in terms of $A(\omega)$ in the following way:

$$G(\omega) = \int_{-\infty}^{\infty} A(\omega') \left\{ \frac{1}{\omega - \omega' + i\eta} - \frac{e^{-\beta\omega'}}{\omega - \omega' - i\eta} \right\} \frac{d\omega'}{2\pi}$$

The strategy is now straightforward. Given G^R, we compute A, and use it to compute G. The retarded Green's function for the phonon problem was derived in DS Eq. (2.3.10),

$$G_{\mathbf{k}}^R(\omega) = \frac{1}{2M\Omega_{\mathbf{k}}} \left\{ \frac{1}{\omega - \Omega_{\mathbf{k}} + i\eta} - \frac{1}{\omega + \Omega_{\mathbf{k}} + i\eta} \right\}$$

We can extract the imaginary part by making use if the SokhotskiPlemelj identity (prove it as an exercise)

$$\frac{f(x)}{x \pm i\eta} = \mp i\pi f(x)\delta(x) + \mathcal{P}\frac{f(x)}{x}.$$

We find

$$\text{Im}G_{\mathbf{k}}^R = -\frac{\pi}{2M\Omega_{\mathbf{k}}}\left(\delta\left(\omega - \Omega_{\mathbf{k}}\right) - \delta\left(\omega + \Omega_{\mathbf{k}}\right)\right)$$

and

$$A(\omega) = \frac{2\pi}{1 - e^{-\beta\omega}}\frac{1}{2M\Omega_{\mathbf{k}}}\left(\delta\left(\omega - \Omega_{\mathbf{k}}\right) - \delta\left(\omega + \Omega_{\mathbf{k}}\right)\right).$$

Inserting this into Eq. (3) yields

$$G_{\mathbf{k}}^T(\omega) = -\frac{n_{\mathbf{k}} + 1}{2M\Omega_{\mathbf{k}}}\left(\frac{1}{\omega + \Omega_{\mathbf{k}} - i\eta} - \frac{1}{\omega - \Omega_{\mathbf{k}} + i\eta}\right) - \frac{n_{\mathbf{k}}}{2M\Omega_{\mathbf{k}}}\left(\frac{1}{\omega - \Omega_{\mathbf{k}} - i\eta} - \frac{1}{\omega + \Omega_{\mathbf{k}} + i\eta}\right)$$

Here we have used that the Bose-Einstein distribution is $n_{\mathbf{k}} = (e^{\beta\Omega_{\mathbf{k}}} - 1)^{-1}$ and $n_{\mathbf{k}} + 1 = (1 - e^{-\beta\Omega_{\mathbf{k}}})^{-1}$.

3   (20 points)

The ensemble average $\langle u_j^2 \rangle$ can be obtained from the Matsubara Green's function in the limit $\tau \to 0^+$:

$$\langle u_j^2 \rangle = \lim_{\tau \to 0^+}\langle \mathcal{T}u_j(\tau)u_j(0)\rangle = \mathcal{G}_{jj}(0^+) = \frac{1}{N}\sum_{\mathbf{k} \in BZ}\mathcal{G}_{\mathbf{k}}(0^+)e^{i\mathbf{k}(R_j - R_j)} = \frac{1}{N}\sum_{\mathbf{k} \in BZ}\mathcal{G}_{\mathbf{k}}(0^+)$$

Here, we assume a d-dimensional crystal with N lattice sites. In class, we derived

$$\mathcal{G}_{\mathbf{k}}(\tau = 0^+) = \frac{1}{2\Omega_{\mathbf{k}}M}\coth\frac{1}{2}\beta\Omega_{\mathbf{k}} = \frac{1}{2\Omega_{\mathbf{k}}M}\left(\frac{2}{e^{\beta\Omega_{\mathbf{k}}} - 1} + 1\right)$$

and we are given the acoustic phonon dispersion

$$\Omega_{\mathbf{k}} = 2\sqrt{\frac{K}{M}}\left[\sum_{i=1}^d \sin^2(ak_i/2)\right]^{\frac{1}{2}}.$$

Thus, we next have to perform the $\mathbf{k}$-sum

$$\langle u_j^2 \rangle = \frac{1}{N}\sum_{\mathbf{k} \in BZ}\frac{1}{2\Omega_{\mathbf{k}}M}\left(\frac{2}{e^{\beta\Omega_{\mathbf{k}}} - 1} + 1\right). \tag{3}$$

Unfortunately, a solution to this sum (or integral in the thermodynamic limit) in closed form is not known. We will instead compute it in the Debye approximation. This approximation assumes a linear dispersion, i.e.

$$\Omega_{\mathbf{k}} = \Omega_k = \sqrt{\frac{K}{M}}a|\mathbf{k}| = ck$$

Of course, in this case we cannot define a Brillouin zone anymore. What region of $\mathbf{k}$-space should we then integrate over? In the Debye approximation one integrates over a sphere in $\mathbf{k}$-space of the same volume as the Brillouin zone. This criterion allows for a definition of the Debye frequency Ω_D by $\int_0^{\Omega_D} D(\Omega)d\Omega = N$, where N is the number of lattice sites of the d-dimensional crystal.

The density of states is defined by:

$$D(\Omega) = \frac{g}{V}\sum_k \delta(\Omega - \Omega_{\mathbf{k}})$$

where g is the degeneracy due to different polarizations. In the limit of long wavelengths and assuming a linear dispersion we can approximate this as

$$D(\Omega) = \frac{g}{V}\sum_q \delta(\Omega - c\,|\mathbf{k}|) = g\int\frac{d^d\mathbf{k}}{(2\pi)^d}\delta(\Omega - c\,|\mathbf{k}|) = \frac{g}{(2\pi)^d}\Phi(d)\int dk\,k^{d-1}\delta(\Omega - ck)$$

$$= \frac{g}{(2\pi)^d}\Phi(d)\frac{\Omega^{d-1}}{c^d} = \frac{g}{2^{d-1}\pi^{d/2}\Gamma(d/2)}\frac{\Omega^{d-1}}{c^d}$$

where the function $\Phi(d)$ is just the angular integral, i.e, the volume of the unit sphere in d dimensions.

Plugging the density of states into

$$\int_0^{\Omega_D} D(\Omega)d\Omega = gN$$

we find

$$\frac{gV}{2^{d-1}\pi^{d/2}\Gamma(d/2)}\frac{\Omega_D^d}{dc^d} = gN, \qquad \Omega_D = 2\sqrt{\pi}\sqrt{\frac{K}{M}}a\left(\frac{dN}{2V}\Gamma(d/2)\right)^{1/d}$$

Replacing the sum in Eq. (3) by an integral and writing it in terms of $D(\Omega)$ we find

$$\langle u_j^2\rangle = \frac{V}{2MN}\int_0^{\Omega_D} d\Omega \frac{D(\Omega)}{\Omega}\left(\frac{2}{e^{\beta\Omega}-1}+1\right).$$

The first term represents thermal fluctuations while the second represents quantum fluctuations (zero-point motion) of the ions. We now substitute the long wavelength form $D(\Omega) = A_d\Omega^{d-1}/c^d$ found above and perform the integral. We find

$$\langle u_j^2\rangle = \frac{V}{2MNc^d}A_d\left[2b_d(k_BT)^{d-1}+\frac{(\Omega_D)^{d-1}}{d-1}\right]$$

with

$$b_d = \int_0^{\beta\Omega_D} dx\frac{x^{d-2}}{e^x-1}.$$

Clearly this last integral is infrared divergent for $d \leq 2$, implying that, according to the Lindemann criterion, lattices are unstable in lower dimensions: the melting temperature, which is inversely proportional to the above integral, is zero. In $d = 2$ the lattice is stable at $T = 0$. In $d = 1$ quantum fluctuation destroy the lattice even at $T = 0$. These results can be understood as consequences of a general theorem due to Mermin and Wagner.

In $d = 3$ (where $g = 3$) the integral converges and we will evaluate it approximately as follows. For high temperatures such that $\beta\Omega_D \gg 1$ we may consider extending the upper integral boundary to ∞. This is motivated from the fact that the integrand decays exponentially. We get:

$$b_3 \approx \int_0^\infty dx\frac{x}{e^x-1} = \frac{\pi^2}{6}.$$

However we observe that typical Debye temperatures in crystalline solids range from $T_D = 170$K (gold) to $T_D = 645$ K (silicon) and melting temperatures are on the order of 1000K. We conclude that in most situations $\beta\Omega_D \lesssim 1$. Consequently, the low temperature limit is more appropriate here. We thus expand the exponential for small x and obtain

$$b_3 \approx \int_0^{\beta\Omega_D} dx\frac{x}{1+x-1} = \beta\Omega_D.$$

We use this to estimate the melting temperature T_M from the Lindemann criterion,

$$T_M = \left[c_L^2\frac{2\pi^2Mc^3}{3k_B^2a\theta_D}-\frac{1}{4}\theta_D\right],$$

with $\theta_D = \Omega_D/k_B$ the Debye temperature.

Note: The results obtained above for $d = 1, 2$ should be regarded as a failure of the Lindemann criterion in dimensions below 3. Clearly solids do exist in $d = 1, 2$ (think e.g. graphene, carbon nanotubes or DNA) and are stable even at room temperature. What the divergences found above indicate is the lack of long-range positional order in dimensions below 3. While in a 3D crystal positions of distant ions are perfectly correlated, in 2D and 1D systems they are not. These low-dimensional 'solids' do retain their mechanical rigidity even though technically we cannot classify them as crystals.