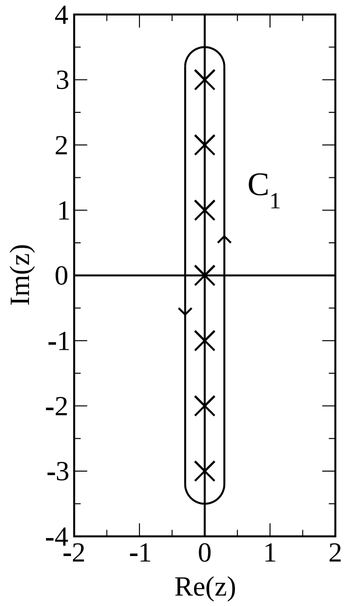

Figure 1: Contour C_1. $\times$'s mark the poles of $1/(e^{2\pi z}-1)$.

Poisson Sum Formula

Suppose we wish to evaluate a sum over all integers (positive, negative, and zero), that is, we want to evaluate something particular like

$$F(x)=\sum_{n=-\infty}^{\infty}\frac{1}{x^2+n^2} \tag{1}$$

The answer happens to be $F(x)=(\pi/x)\coth(\pi x)$ as will be proved below. The general form of the problem is

$$F=\sum_{n=-\infty}^{\infty}f(n)=\sum_{n=-\infty}^{\infty}g(in) \tag{2}$$

where $f(n)=1/(x^2+n^2)$ or $g(in)=1/(x^2-(in)^2)$ in the particular case of eq.(1). The Poisson sum formula is

$$\sum_{n=-\infty}^{\infty}g(in)=-i\oint_{C_1}dz\frac{e^{2\pi mz}}{e^{2\pi z}-1}g(z). \tag{3}$$

where the contour C_1 is shown in fig. 1. The formula holds for any integer m and any $g(z)$ provided the function $g(z)$ is analytic in a neighborhood of the imaginary z axis where the contour runs.

To prove the Poisson sum formula, note that the function $e^{2\pi mz}/(e^{2\pi z}-1)$ which appears in the integrand of eq.(3) has simple poles of residue $1/2\pi$ at $z=in$ for all integers n. Then the Cauchy theorem tells us that if $g(z)$ is analytic inside the contour C_1, the integral is just $2\pi i$ times the sum of the residues $g(in)/2\pi$. The integer m can be chosen at will according to the problem at hand.

Now let us return to our example where $g(z)=1/(x^2-z^2)$. This is analytic as required, having simple poles at $z=\pm x$. The positions of the poles of the integrand are shown in fig. 2 for the case $x=2$. The contour C_1 can be deformed in regions of analytic behavior, and is equivalent to the path shown in fig. 2. This path has three circuits, C_2 which recedes to $|z|\to\infty$, and C_3 and C_4 which surround the poles of $g(z)$. It also contains the double straight segments L and R which can be chosen so that the forward and reverse paths lie on top of each other and cancel. Now the aim will be to argue that the large circular contour C_2 contributes nothing, so that the answer is found from the simple contours C_3

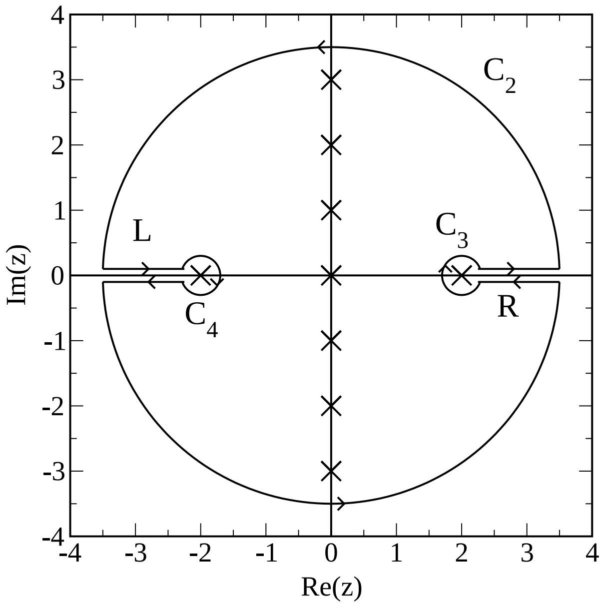

Figure 2: The equivalent contours C_2 + C_3 + C_4. Two new poles denoted by additional ×'s are shown from the function $g(z) = -1/(z^2 - x^2)$.

and C_4. The large z behavior of $g(z)$ is favorable, decreasing as $1/z^2$ which is sufficiently fast to make the contour C_2 contribute nothing provided the remaining factor $e^{2\pi mz}/(e^{2\pi z} - 1)$ does not diverge along C_2. If m is negative, it diverges for large negative z and for m greater than 1 it diverges for large positive z, so there are two choices that work, $m = 0$ and $m = 1$. Writing $g(z)$ as the sum of two simple poles $2xg(z) = 1/(z + x) - 1/(z - x)$, one can verify using Cauchy's theorem that the contours C_3 plus C_4 generate the answer $F = (\pi/x)\coth(\pi x)$ for both choices $m = 0$ and $m = 1$.

Now let us apply this to "temperature Green's functions" found in lattice dynamics. A modified version of eq.(3) with new variables appropriate to such problems is

$$\frac{1}{\beta}\sum_{\mu} f(i\omega_\mu) = \frac{1}{2\pi i}\oint_{C_1} dz \frac{e^{m\beta z}}{e^{\beta z} - 1} f(z). \tag{4}$$

where $i\omega_\mu$ is the Matsubara frequency $2\pi i\mu/\beta$ and μ runs over all integers. For example, the temperature Green's function of a harmonic lattice is

$$G(\vec{k}, i\omega_\mu) = \frac{\hbar}{2M\Omega_k}\left[\frac{1}{i\omega_\mu - \hbar\Omega_k} - \frac{1}{i\omega_\mu + \hbar\Omega_k}\right] \tag{5}$$

while the value at the "imaginary time" σ is given by the Fourier transform

$$G(\vec{k}, \sigma) = \frac{1}{\beta}\sum_{\mu} e^{-i\omega_\mu \sigma} G(\vec{k}, i\omega_\mu). \tag{6}$$

We evaluate this Fourier transform using the Poisson sum eq.(4). Therefore, $f(z)$ is

$$f(z) = \frac{\hbar}{2M\Omega_k} e^{-\sigma z}\left[\frac{1}{z - \hbar\Omega_k} - \frac{1}{z + \hbar\Omega_k}\right]. \tag{7}$$

Like our simple example above, this has two simple poles, at $z = \pm\hbar\Omega_k$, and (apart from the dangerous factor $\exp(-\sigma z)$) it behaves as $1/z^2$ for large $|z|$. The contour C_1 is thus replaced by C_2 + C_3 + C_4, and we enquire whether we can ignore the difficult contour C_2. The dangerous factor $\exp(-\sigma z)$ comes in

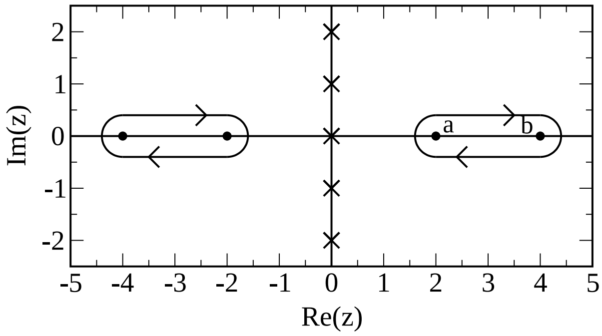

Figure 3: The contour surrounding the poles on the imaginary axis has been deformed to two new contours surrounding the branch cuts of the function $g(z) = \log((b^2 - z^2)/(a^2 - z^2))$ where the points a and b lie on the real axis as shown.

combination with $\exp(m\beta z)$, that is, we have $\exp((m\beta - \sigma)z)$. If σ is positive, then to prevent a problem at negative z it is necessary to choose the integer m positive to make $m\beta - \sigma$ positive. But then there will be a problem at positive z unless the exponent βz in the denominator is larger than $(m\beta - \sigma)z$ in the numerator. Thus a unique choice of m is dictated which makes $m\beta - \sigma$ lie in the interval $(-\beta, 0)$. Since this exponent is the only place where the variable σ occurs, it is clear that choosing m in this way makes $G(\vec{k}, \sigma)$ periodic in σ with period β, a result which agrees with the Fourier representation eq.(5). Thus it is sufficient to evaluate for σ in the range $(0, \beta)$ in which interval m must be chosen as 1. Using this choice, and using Cauchy's theorem on the circuits C_3 and C_4, one finds

$$G(\vec{k}, \sigma) = -\frac{\hbar}{2M\Omega_k}\left[(n_k + 1)e^{-\sigma\hbar\Omega_k} + n_k e^{\sigma\hbar\Omega_k}\right], \tag{8}$$

where n_k is the Bose-Einstein occupation function $n_k = 1/(\exp(\beta\hbar\Omega_k) - 1)$. It is important to remember that this formula must be evaluated for σ *modulo* β, such that $0 < \sigma < \beta$.

Now let us evaluate a different sort of sum,

$$S = \sum_{n=-\infty}^{\infty} \log\left(\frac{b^2 + n^2}{a^2 + n^2}\right) = -i \oint_{C_1} dz \frac{e^{2\pi m z}}{e^{2\pi z} - 1} \log\left(\frac{b^2 - z^2}{a^2 - z^2}\right). \tag{9}$$

We assume $b > a$. The deformed contour is shown in fig. 3. For large $|z|$, the logarithm gets small as $1/z^2$, so the piece of the contour at infinity can be neglected, provided the choice $m = 0$ or $m = 1$ for the free integer m is taken. The function $\log(z) = \log(|z| \exp(i\phi)) = \log(|z|) + i\phi$ has multiple branches corresponding to the possible choices of the phase ϕ differing by multiples of 2π. By choosing $|\phi| \leq \pi$, the logarithm becomes single-valued, at the price of having to make the discontinuous switch from $-\pi$ to π. For our function $g(z)$, this discontinuity occurs as we cross the real axis for $a < |\Re z| < b$. Approaching the real axis from above on the positive $\Re z$ side, the phase increases to π. After crossing the axis, the phase continues to increase, but we agreed to keep $|\phi|$ less than π so we have to subtract 2π. The logarithm is $\log|(b^2 - z^2)/(a^2 - z^2)|$ with zero imaginary part except for in $a < |\Re z| < b$ where the imaginary part is $+i\pi$ above the axis on the positive side, $-i\pi$ below the axis on the positive side, and opposite on the negative side of the real axis. The log part of the integrand is analytic except on these two lines of discontinuity, so the deformed contour circulates around the branch cuts as shown. The real part of the log cancels as we integrate forward and back from a to b, and the imaginary part is twice the value in the forward direction.

The integral (9) thus becomes

$$S = 2\pi \int_a^b dz \frac{e^{2\pi m z}}{e^{2\pi z} - 1} - 2\pi \int_{-b}^{-a} dz \frac{e^{2\pi m z}}{e^{2\pi z} - 1}. \tag{10}$$

Since $m = 0$ and $m = 1$ are equally valid, the simplest proceedure is to use the average of the two,

$$\frac{1}{2}\left[\frac{1}{e^{2\pi z}-1}+\frac{e^{2\pi z}}{e^{2\pi z}-1}\right]=\frac{1}{2}\coth(\pi z)=\frac{1}{2\pi}\frac{d}{dz}\log[\sinh(\pi z)]. \tag{11}$$

The two integrals of eq.(10) are equal, and the answer is

$$S = 2\log\left[\frac{\sinh(\pi b)}{\sinh(\pi a)}\right] \tag{12}$$