Chapter 3

Contour Integration and the Calculus of Residues

3.1 A Useful Example

Consider the following integral:

$$I = \int_0^\infty dx \, \frac{x^\alpha}{(1+x^2)^2} \tag{3.1}$$

where $\alpha \in (-1, +3)$. We turn this into a contour integral by noting that

$$e^{i\pi\alpha} \, I = \int_{-\infty}^0 dx \, \frac{x^\alpha}{(1+x^2)^2} \ , \tag{3.2}$$

and hence

$$I = \frac{1}{(1+e^{i\pi\alpha})} \int_{-\infty}^\infty dx \, \frac{x^\alpha}{(1+x^2)^2} \ . \tag{3.3}$$

Closing in the upper half plane, we obtain

$$I = \frac{2\pi i}{(1+e^{i\pi\alpha})} \, \mathrm{Res}\bigg|_{z=i} \left\{ \frac{z^\alpha}{(z-i)^2 \, (z+i)^2} \right\} \ . \tag{3.4}$$

To compute the residue, let $z = i + \epsilon$ and expand in ϵ. The residue is the $\mathcal{O}(\epsilon^{-1})$ term:

$$
\begin{aligned}
\frac{z^\alpha}{(z-i)^2\,(z+i)^2} &= \frac{1}{\epsilon^2}\,\frac{(i+\epsilon)^\alpha}{(2i+\epsilon)^2} \\
&= \frac{e^{i\pi\alpha/2}}{4i^2\epsilon^2}\,(1-i\epsilon)^\alpha\,(1-\tfrac{1}{2}i\epsilon)^{-2} \\
&= \tfrac{1}{4}\,e^{i\pi\alpha/2}\bigg\{-\frac{1}{\epsilon^2}+\frac{(1-\alpha)}{i\epsilon}+\mathcal{O}\big(\epsilon^0\big)\bigg\}\ , \qquad (3.5)
\end{aligned}
$$

and the residue is thus $(1-\alpha)\,e^{i\pi\alpha/2}/4i$. We therefore find

$$
I = \int\limits_0^\infty\!dx\,\frac{x^\alpha}{(1+x^2)^2} = \frac{\pi}{4}\,\frac{1-\alpha}{\cos\big(\frac{1}{2}\pi\alpha\big)}\ . \qquad (3.6)
$$

3.2 Matsubara Sums

Perturbative expansions in finite temperature field theory generally require the computation of sums of the following form:

$$
M(\tau) = k_{\mathrm{B}}T\sum_{\omega_n}\hat{M}(i\omega_n)\,e^{i\omega_n\tau}\ , \qquad (3.7)
$$

where T is temperature, $\omega_n = 2\pi n k_{\mathrm{B}}T/\hbar$ is a "bosonic Matsubara frequency" and $\hat{M}(i\omega_n)$ is some function. For fermions, one obtains a similar expression except that the sum is over fermionic Matsubara frequencies $\nu_n = 2\pi(n+\frac{1}{2})k_{\mathrm{B}}T/\hbar$. The sums are over all integers n.

For our mathematical study, we'll set $\hbar = k_{\mathrm{B}}T = 1$ and focus on computing the expressions

$$
\begin{aligned}
H_{\mathrm{B}}(s) &= \sum_{\omega_n}\hat{H}(i\omega_n)\,e^{i\omega_n s} \qquad (3.8)\\
H_{\mathrm{F}}(s) &= \sum_{\nu_n}\hat{H}(i\nu_n)\,e^{i\nu_n s}\ , \qquad (3.9)
\end{aligned}
$$

with 'Matsubara frequencies' $\omega_n = 2\pi n$ and $\nu_n = 2\pi(n+\frac{1}{2})$. Note that the bosonic and fermionic functions $H_{\mathrm{B}}(s)$ and $H_{\mathrm{F}}(s)$ are respectively periodic and antiperiodic with period 1:

$$
\begin{aligned}
H_{\mathrm{B}}(s+1) &= +H_{\mathrm{B}}(s) \qquad (3.10)\\
H_{\mathrm{F}}(s+1) &= -H_{\mathrm{F}}(s)\ . \qquad (3.11)
\end{aligned}
$$

Without loss of generality, then, we may restrict s to the interval $s \in [0, 1)$.

To convert these sums into contour integrals, we need to find functions $n(\omega)$ and $f(\nu)$ which have each have poles only at the appropriate Matsubara frequencies ($\omega = i\omega_n$ and $\nu = i\nu_n$), and with the same residue at each pole. These functions are the familiar bosonic and fermionic occupation functions:

$$n(\omega) = \frac{1}{\exp(\omega) - 1} \tag{3.12}$$

$$f(\nu) = \frac{1}{\exp(\nu) + 1} \; . \tag{3.13}$$

To see this, consider first $n(\omega)$, which has poles whenever $\exp(\omega) = 1$, *i.e.* at $\omega = i\omega_n$. Let $\omega = i\omega_n + \epsilon)$ and find

$$n(i\omega_n + \epsilon) = \frac{1}{\exp(\epsilon) - 1} = \frac{1}{\epsilon} + \mathcal{O}(\epsilon^0) \; . \tag{3.14}$$

Thus, $n(\omega)$ has simple poles with residue $+1$ at $\omega = i\omega_n$, for all n. In the fermionic case, poles occur for $\exp(\nu) = -1$ which says $\nu = i\nu_n$, and setting $\nu = i\nu_n + \epsilon$ we find

$$f(i\nu_n + \epsilon) = \frac{1}{-\exp(\epsilon) + 1} = -\frac{1}{\epsilon} + \mathcal{O}(\epsilon^0) \; . \tag{3.15}$$

Thus, $f(\nu)$ has simple poles with residue -1 at $\nu = i\nu_n$, for all n.

Therefore, we may write

$$\sum_{\omega_n} \hat{H}(i\omega_n)\, e^{i\omega_n s} = +\oint_{\mathcal{C}} \frac{d\omega}{2\pi i}\, n(\omega)\, H(\omega)\, e^{\omega s} \tag{3.16}$$

$$\sum_{\nu_n} \hat{H}(i\nu_n)\, e^{i\nu_n s} = -\oint_{\mathcal{C}} \frac{d\nu}{2\pi i}\, f(\nu)\, H(\nu)\, e^{\nu s} \; , \tag{3.17}$$

where the contour $\mathcal{C}$ runs from $\epsilon - i\infty$ up to $\epsilon + i\infty$ and from $-\epsilon + i\infty$ down to $-\epsilon - i\infty$, where ϵ is a positive infinitesimal. *I.e.* the contour runs parallel to the imaginary axis, headed 'up' just to the right of the axis and 'down' just to the left of the axis. If the function $\hat{H}(u)$ has only poles and no branch cuts in the right and left half planes, we may close the contours

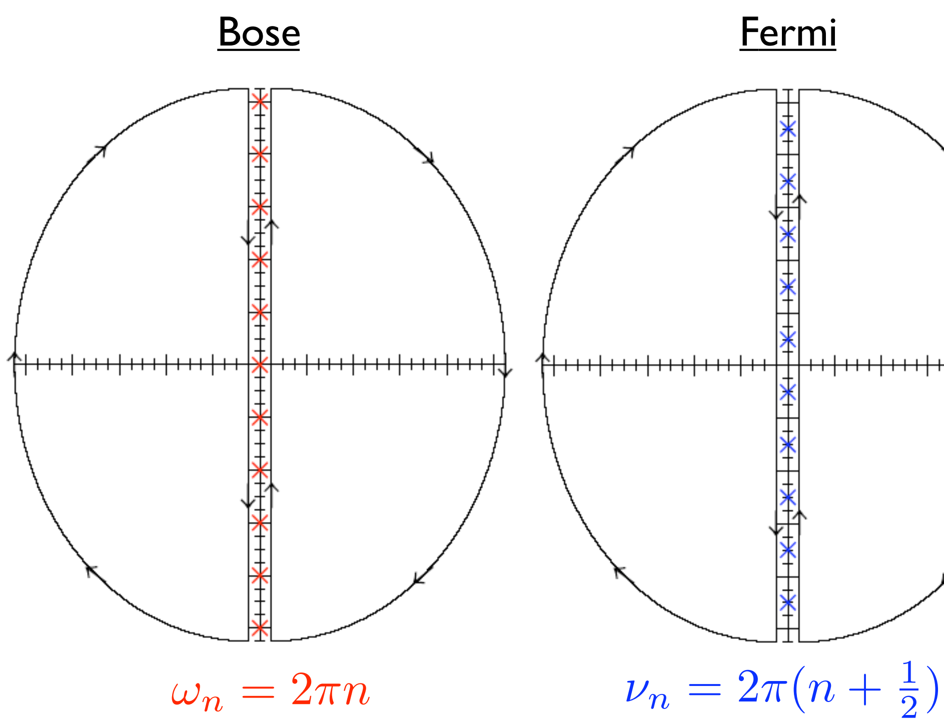

Figure 3.1: Integration contour for bosonic and fermionic Matsubara sums.

as shown in figure 3.1. We then have

$$H_{\rm B}(s) = \sum_{\omega_n} \hat{H}(i\omega_n)\, e^{i\omega_n s} \quad = \quad -\sum_{\widetilde{\omega}}{}' \,\text{Res}\left[n(\omega)\, H(\omega)\, e^{\omega s}\right]_{\omega=\widetilde{\omega}} \tag{3.18}$$

$$H_{\rm F}(s) = \sum_{\nu_n} \hat{H}(i\nu_n)\, e^{i\nu_n s} \quad = \quad +\sum_{\widetilde{\nu}}{}' \,\text{Res}\left[f(\nu)\, H(\nu)\, e^{\nu s}\right]_{\nu=\widetilde{\nu}}\ , \tag{3.19}$$

where $\widetilde{\omega}$ (or $\widetilde{\nu}$) denotes a pole of $\hat{H}$. The prime on the sum serves to remind us that we seek residues only in the left half plane (LHP) and right half plane (RHP) but not along the imaginary axis. Indeed, we have traded off the infinite sum over residues along the imaginary axis for a presumably simpler, finite sum of poles in the LHP and RHP. Note that the signs have changed on the right hand sides of 3.16 and 3.18 due to the fact that the integrations are clockwise around the contours.

One might worry that the exponential factors $e^{\omega s}$ and $e^{\nu s}$ will render the integrand unsuitable for closure at infinity, *i.e.* that Jordan's lemma is inapplicable. However, one can check that this is not the case. Suppose $s > 0$. The problem then comes at large positive values of ω (or ν), where these exponentials diverge. However, the Bose and Fermi functions are themselves decaying exponentially in this region, as $e^{-\omega}$. Since $0 \leq s < 1$, we have that the product $n(\omega)\exp(\omega s)$ does indeed satisfy Jordan's lemma, and the contours may be closed along semicircles of infinite radius in the left and right half planes.

3.2.1 Example #1

Consider the case

$$H_{\rm F}(s) = \sum_{\nu_n} \frac{e^{i\nu_n s}}{i\nu_n + E} \ . \tag{3.20}$$

Then $\hat{H}(\nu) = 1/(\nu + E)$ has one simple pole, located at $\nu = -E$. According to 3.19, then,

$$H_{\rm F}(s) = {\rm Res}\left[\frac{1}{e^\nu + 1}\,\frac{e^{\nu s}}{\nu + E}\right]_{\nu=-E} = \frac{e^{(1-s)E}}{e^E + 1} \ . \tag{3.21}$$

A peculiarity with this example is that

$$H_{\rm F}(0) = \frac{e^E}{e^E + 1} \qquad , \qquad H_{\rm F}(1) = \frac{1}{e^E + 1} = 1 - H_{\rm F}(0) \ , \tag{3.22}$$

which seems to contradict the general result that $H_{\rm F}(s)$ is antiperiodic with period 1. The resolution to this conundrum is that $H_{\rm F}(s)$ is indeed antiperiodic, but that in this case it also has a *discontinuity* at all integer values of s. When s is an integer, the exponential factor is always unity, and the summand, $(i\nu_n + E)^{-1}$ decays sufficiently slowly that the sum is only conditionally convergent. See figure 3.2 for a sketch of $H_{\rm F}(s)$ in this case.

For the bosonic case, following 3.18,

$$H_{\rm B}(s) = \sum_{\omega_n} \frac{e^{i\omega_n s}}{i\omega_n + E} = -{\rm Res}\left[\frac{1}{e^\omega - 1}\,\frac{e^{\omega s}}{\omega + E}\right]_{\omega=-E} = \frac{e^{(1-s)E}}{e^E - 1} \ . \tag{3.23}$$

This diverges as $E \to 0$ due to the $\omega_n = 0$ term in the Matsubara sum.

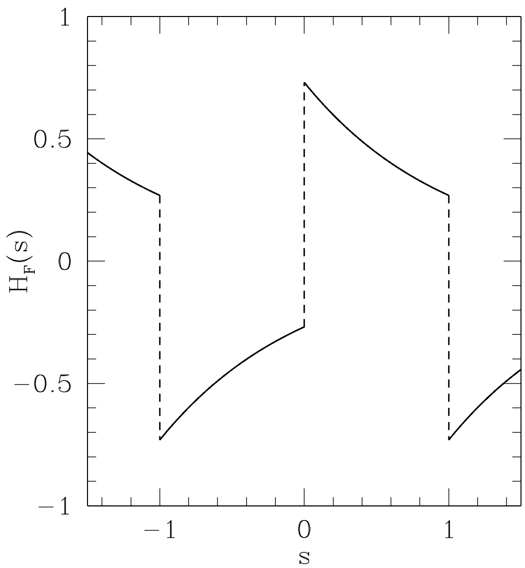

Figure 3.2: The function $H_{\rm F}(s)$ from example #1, with $E = 1$. Note the discontinuities at integer values of s.

3.2.2 Example #2

Consider next the sum

$$H_{\rm F}(s) = \sum_{\nu_n} \frac{e^{i\nu_n s}}{(i\nu_n + E)(i\nu_n + E + \Delta)} \ . \tag{3.24}$$

Now the summand decays as n^{-2} for large $|n|$ and we should have no discontinuities in $H_{\rm F}(s)$. Evaluating the sum according to 3.19,

$$\begin{aligned} H_{\rm F}(s) &= \sum_{\widetilde{\nu}} {\rm Res}\bigg[\frac{1}{e^\nu + 1}\,\frac{e^{\nu s}}{(\nu + E)(\nu + E + \Delta)}\bigg]_{\nu=\widetilde{\nu}} \\ &= \frac{1}{\Delta}\bigg\{ e^{(1-s)E}\, f(E) - e^{(1-s)(E+\Delta)}\, f(E+\Delta)\bigg\} \ , \end{aligned} \tag{3.25}$$

where the poles are at $\widetilde{\nu} = -E$ and $\widetilde{\nu} = -(E + \Delta)$. Note that in this case

$$H_{\rm F}(1) = -H_{\rm F}(0) = \frac{1}{\Delta}\Big\{ f(E) - f(E+\Delta)\Big\} \ , \tag{3.26}$$

and the function $H_{\rm F}(s)$ is continuous and antiperiodic.

As a bonus, let's set $E = \Delta = 0$ and compute

$$H_{\rm F}(0) = \sum_{\nu_n} \frac{1}{(i\nu_n)^2} = -\frac{2}{\pi^2} \sum_{k \text{ odd}} \frac{1}{k^2} \ , \tag{3.27}$$

where the sum on k is over all positive odd integers. For general E and $\Delta \to 0$,

$$H_{\rm F}(0) = \frac{df}{dE} = -\frac{e^E}{(e^E + 1)^2} \ , \tag{3.28}$$

hence setting $E = 0$ gives $H_{\rm F}(0) = -\frac{1}{4}$. We therefore conclude

$$\sum_{k \text{ odd}} \frac{1}{k^2} = \frac{\pi^2}{8} \ . \tag{3.29}$$

In the bosonic case, one finds

$$H_{\rm B}(s) = \frac{1}{\Delta} \bigg\{ e^{(1-s)E}\, n(E) - e^{(1-s)(E+\Delta)}\, n(E+\Delta) \bigg\} \ . \tag{3.30}$$

3.3 Response Functions

3.3.1 Forced Damped Harmonic Oscillator

Consider a forced, damped harmonic oscillator which obeys the equation

$$\ddot{x} + 2\beta\dot{x} + \omega_0^2 x = f(t) \ , \tag{3.31}$$

where $\beta > 0$ is a damping constant, ω_0 is the natural freqency, and where we have expressed the force in units of the mass m. Fourier transforming this equation, using

$$x(t) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \hat{x}(\omega)\, e^{-i\omega t} \qquad \Longleftrightarrow \qquad \hat{x}(\omega) = \int\limits_{-\infty}^{\infty} dt\, x(t)\, e^{+i\omega t} \ , \tag{3.32}$$

we have $d/dt \longleftrightarrow (-i\omega)$, and

$$\big(-\omega^2 - 2i\beta\omega + \omega_0^2 \big)\, \hat{x}(\omega) = \hat{f}(\omega) \ . \tag{3.33}$$

We define the frequency-dependent *susceptibility* $\hat{\chi}(\omega)$ as

$$\hat{\chi}(\omega) = \frac{1}{\omega_0^2 - 2i\beta\omega - \omega^2} \ , \tag{3.34}$$

in which case

$$\hat{x}(\omega) = \hat{\chi}(\omega)\,\hat{f}(\omega) \tag{3.35}$$

Fourier transforming back to the time domain, we obtain the general solution

$$x(t) = x_{\rm h}(t) + \int\limits_{-\infty}^{\infty} dt'\,\chi(t-t')\,f(t')\ , \tag{3.36}$$

where $x_{\rm h}(t)$ is the solution to the homogeneous equation, *i.e.* with zero forcing.

What equation 3.36 says is that the response at time t depends on the forcing at all other times t'. We can thereby write the susceptibility kernel as a functional derivative

$$\chi(t-t') = \frac{\delta x(t)}{\delta f(t')}\ , \tag{3.37}$$

which tells us how sensitive the response at time t is to the forcing at time t'. That is, a system subjected to a Δ-function forcing $f(t) = A\,\Delta(t-t_0)$ will result in a response $x(t) = A\,\chi(t-t_0)$.

Now, if our system is *causal*, then we must have $\chi(t-t') = 0$ for $t < t'$. That is, the system only responds to external forces it was subjected to *in the past*. It is easy to see that this requires that $\hat{\chi}(\omega)$ be analytic in the upper half plane. We can see this by writing $\chi(s)$ as

$$\chi(s) = \int\limits_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\hat{\chi}(\omega)\,e^{-i\omega s}\ . \tag{3.38}$$

If $s > 0$, we close in the LHP, where $\text{Im}(\omega) < 0$. The result is that we pick up contributions from residues at all the poles of $\hat{\chi}(\omega)$. When $s < 0$, we close in the UHP and pick up contributions from residues at poles therein. Any pole structure is inconsistent with $\chi(s) = 0\ \forall\ s < 0$.

In the case of the damped harmonic oscillator, we have

$$\hat{\chi}(\omega) = -\frac{1}{(\omega-\omega_+)(\omega-\omega_-)} \tag{3.39}$$

$$\omega_\pm = -i\beta \pm \sqrt{\omega_0^2 - \beta^2}\ . \tag{3.40}$$

Hence, with $\beta > 0$, both poles are in the LHP, as required for causality. The susceptibility $\chi(s)$ is then given by a sum over the two poles:

$$\chi(s) = -i \sum_{\omega=\omega_\pm} \text{Res}\left[\hat{\chi}(\omega)\, e^{-i\omega s}\right] \Theta(s) \tag{3.41}$$

$$= \frac{1}{\sqrt{\omega_0^2 - \beta^2}} \exp(-\beta s) \sin\left(\sqrt{\omega_0^2 - \beta^2}\, s\right) \Theta(s) \ , \tag{3.42}$$

where $\Theta(s)$ is the step function. Note that $\chi(s)$ starts from zero at $s = 0$. The reason is that the particle has inertia, so even a Δ-function impulse, which results in an instantaneous change in velocity, will not instantaneously change the position. As s increases from $s = 0$, $\chi(s)$ increases linearly, and eventually reaches a maximum and then turns around. $\chi(s)$ is negative over certain time intervals, corresponding to delays such that the particle rebounds from its initial push. At large times, the susceptibility decays to zero exponentially, with time scale β^{-1}. This is the time scale on which the system 'loses its memory' of its initial conditions.

Finally, the homogeneous solution is

$$x_{\mathrm{h}}(t) = A_+\, e^{-i\omega_+ t} + A_-\, e^{-i\omega_- t} \ , \tag{3.43}$$

where $A_\pm$ are two constants of integration, as required for a second order ODE. For real $x(t)$, we must have $A_- = A_+^*$.

3.3.2 General Linear Autonomous Inhomogeneous ODEs

This method immediately generalizes to the case of general autonomous linear inhomogeneous ODEs of the form

$$\frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \cdots + a_1 \frac{dx}{dt} + a_0\, x = f(t) \ . \tag{3.44}$$

In Fourier space, this equation becomes

$$\hat{Q}(\omega)\, \hat{x}(\omega) = \hat{f}(\omega) \ , \tag{3.45}$$

where

$$Q(\omega) = \sum_{k=0}^{n} a_k\, (-i\omega)^k \tag{3.46}$$

and $a_n \equiv 1$. According to the Fundamental Theorem of Algebra, the $n^{\rm th}$ degree polynomial $\hat{Q}(\omega)$ may be uniquely factored over the complex ω plane into a product over n roots:

$$\hat{Q}(\omega) = (-i)^n \, (\omega - \omega_1)(\omega - \omega_2) \cdots (\omega - \omega_n) \ . \tag{3.47}$$

If the $\{a_k\}$ are all real, then $\big[\hat{Q}(\omega)\big]^* = \hat{Q}(-\omega^*)$, hence if $\varOmega$ is a root then so is $-\varOmega^*$. Thus, the roots appear in pairs which are symmetric about the imaginary axis. *I.e.* if $\varOmega = a + ib$ is a root, then so is $-\varOmega^* = -a + ib$. The general solution to the homogeneous equation is

$$x_{\rm h}(t) = \sum_{i=1}^n A_i \, e^{-i\omega_i t} \ , \tag{3.48}$$

which involves n arbitrary complex constants. The susceptibility $\hat{\chi}(\omega)$ is simply

$$\hat{\chi}(\omega) = \frac{1}{\hat{Q}(\omega)} = \frac{i^n}{(\omega - \omega_1)(\omega - \omega_2) \cdots (\omega - \omega_n)} \ , \tag{3.49}$$

and the general solution to the inhomogeneous equation is again given by equations 3.36 and 3.38.

3.3.3 Kramers-Krönig Relations

Suppose $\hat{\chi}(\omega)$ is analytic in the UHP. Then for all ν, we must have

$$\int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi} \, \frac{\hat{\chi}(\nu)}{\nu - \omega + i\epsilon} = 0 \ , \tag{3.50}$$

where ϵ is a positive infinitesimal. The reason is simple: just close the contour in the UHP, assuming $\hat{\chi}(\omega)$ vanishes sufficiently rapidly that Jordan's lemma can be applied. Clearly this is an extremely weak restriction on $\hat{\chi}(\omega)$, given the fact that the denominator already causes the integrand to vanish as $|\omega|^{-1}$.

Let us examine the function

$$\frac{1}{\nu - \omega + i\epsilon} = \frac{\nu - \omega}{(\nu - \omega)^2 + \epsilon^2} - \frac{i\epsilon}{(\nu - \omega)^2 + \epsilon^2} \ . \tag{3.51}$$

which we have separated into real and imaginary parts. Under an integral sign, the first term, in the limit $\epsilon \to 0$, is equivalent to taking a *principal part* of the integral. That is, for any function $F(\nu)$ which is regular at $\nu = \omega$,

$$\lim_{\epsilon\to 0} \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi} \, \frac{\nu - \omega}{(\nu-\omega)^2 + \epsilon^2} \, F(\nu) \equiv \mathcal{P} \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi} \, \frac{F(\nu)}{\nu - \omega} \ . \tag{3.52}$$

The principal part symbol $\mathcal{P}$ means that the singularity at $\nu = \omega$ is elided, either by smoothing out the function $1/(\nu - \epsilon)$ as above, or by simply cutting out a region of integration of width ϵ on either side of $\nu = \omega$.

The imaginary part is more interesting. Let us write

$$h(u) \equiv \frac{\epsilon}{u^2 + \epsilon^2} \ . \tag{3.53}$$

For $|u| \gg \epsilon$, $h(u) \simeq \epsilon/u^2$, which vanishes as $\epsilon \to 0$. For $u = 0$, $h(0) = 1/\epsilon$ which diverges as $\epsilon \to 0$. Thus, $h(u)$ has a huge peak at $u = 0$ and rapidly decays to 0 as one moves off the peak in either direction a distance greater that ϵ. Finally, note that

$$\int\limits_{-\infty}^{\infty} du \, h(u) = \pi \ , \tag{3.54}$$

a result which itself is easy to show using contour integration. Putting it all together, this tells us that

$$\lim_{\epsilon\to 0} \frac{\epsilon}{u^2 + \epsilon^2} = \pi \Delta(u) \ . \tag{3.55}$$

Thus, for positive infinitesimal ϵ,

$$\frac{1}{u \pm i\epsilon} = \mathcal{P} \, \frac{1}{u} \mp i\pi\Delta(u) \ , \tag{3.56}$$

a most useful result.

We now return to our initial result 3.50, and we separate $\hat{\chi}(\omega)$ into real and imaginary parts:

$$\hat{\chi}(\omega) = \hat{\chi}'(\omega) + i\hat{\chi}''(\omega) \ . \tag{3.57}$$

We therefore have, for every real value of ω,

$$0 = \int\limits_{-\infty}^{\infty} \frac{d\nu}{2\pi} \Big[\chi'(\nu) + i\chi''(\nu) \Big] \Big[\mathcal{P} \, \frac{1}{\nu - \omega} - i\pi\Delta(\nu - \omega) \Big] \ . \tag{3.58}$$

Taking the real and imaginary parts of this equation, we derive the *Kramers-Krönig relations*:

$$\chi'(\omega) = +\mathcal{P}\int_{-\infty}^{\infty} \frac{d\nu}{\pi}\,\frac{\hat{\chi}''(\nu)}{\nu-\omega} \tag{3.59}$$

$$\chi''(\omega) = -\mathcal{P}\int_{-\infty}^{\infty} \frac{d\nu}{\pi}\,\frac{\hat{\chi}'(\nu)}{\nu-\omega}\ . \tag{3.60}$$