221B Miscellaneous Notes on Contour Integrals

Contour integrals are very useful technique to compute integrals. For example, there are many functions whose indefinite integrals can't be written in terms of elementary functions, but their definite integrals (often from $-\infty$ to ∞) are known. Many of them were derived using contour integrals. Sometimes we are indeed interested in contour integrals for complex parameters; quantum mechanics brought complex numbers to physics in an intrinsic way. This note introduces the contour integrals.

1 Basics of Contour Integrals

Consider a two-dimensional plane (x, y), and regard it a "complex plane" parameterized by $z = x + iy$. On this plane, consider contour integrals

$$\int_C f(z) dz \tag{1}$$

where integration is performed along a contour C on this plane. The crucial point is that the function $f(z)$ is not an arbitrary function of x and y, but depends only on the combination $z = x + iy$. Such a function is said to be "analytic." Importance of this point will be clear immediately below.

What exactly is the contour integral? It is nothing but a line integral. This point becomes clear if you write $dz = dx + idy$,

$$\int_C f(z) dz = \int_C (f(x + iy)dx + if(x + iy)dy). \tag{2}$$

Therefore, it can be viewed as a line integral

$$\int_C \vec{A} \cdot d\vec{x}, \tag{3}$$

with

$$\vec{A} = (f(x + iy), if(x + iy)). \tag{4}$$

Now comes a crucial observation called Cauchy's theorem. *The contour can be continuously deformed without changing the result, as long as it doesn't hit a singularity and the end points are held fixed.* This is a very non-trivial and useful property. The proof is actually extremely simple. The "vector potential" does not have a "magnetic field," $B = \vec{\nabla} \times \vec{A} = 0$ (in two dimensions, there is only one component for the magnetic field "normal to the plane"), and it is analogous to Aharonov–Bohm effect! We can quickly check the curl

$$B = \vec{\nabla} \times \vec{A} = \partial_x A_y - \partial_y A_x = \partial_x i f(x+iy) - \partial_y f(x+iy) = i f' - i f' = 0. \tag{5}$$

The difference between integrals along two different contours with the same end points

$$\int_{C_1} f(z) dz - \int_{C_2} f(z) dz \tag{6}$$

is an integral over a closed loop $C_1 - C_2$

$$\oint_{C_1 - C_2} f(z) dz. \tag{7}$$

Using Stokes' theorem, this is given by the surface integral over the surface D, whose boundary is the closed loop $\partial D = C_1 - C_2$. But the integrand is the "magnetic field" which vanishes identically. Now you see that continuous deformation of the contour does not change the integral. Moreover, a contour integral along a closed contour is always zero!

But you have to be careful about singularities in the function $f(z)$. Suppose $f(z)$ has a pole at z_0,

$$f(z) = \frac{R}{z - z_0} + g(z), \tag{8}$$

where $g(z)$ is regular (no singularity). Consider a closed contour C that encircles z_0 anti-clockwise. Because the contour can be deformed, you can make the contour infinitesimally small to encircle z_0 with a radius ϵ. For the $g(z)$ piece, you can shrink the circle to zero ($\epsilon \to 0$) without encountering a singularity, and the piece vanishes. But you cannot do so with the singular piece. We define shifted coordiates $z - z_0 = x + iy = re^{i\theta}$. Then the integral along the small circle is nothing but an integral over the angle θ at the fixed radius $r = \epsilon$. Then

$$\oint_C \frac{R}{z - z_0} dz = \int_0^{2\pi} \frac{R}{\epsilon\, e^{i\theta}}\, \epsilon\, e^{i\theta} i d\theta. \tag{9}$$

Here I used $dz = d(\epsilon\, e^{i\theta}) = \epsilon\, e^{i\theta} i d\theta$. This integral can be done trivially because $e^{i\theta}$ cancels,

$$\oint_0^{2\pi} \frac{R}{\epsilon\, e^{i\theta}}\, \epsilon\, e^{i\theta} i d\theta = 2\pi i R. \tag{10}$$

The numerator R is called the "residue" at the pole.

It is remarkable that higher singularities, $1/(z-z_0)^n$ for $n>1$, actually give vanishing contribution to the contour integral. Following the same analysis,

$$\oint_C \frac{r}{(z-z_0)^n}dz = \int_0^{2\pi} \frac{r}{\epsilon^n e^{in\theta}}\epsilon\, e^{i\theta} i d\theta = \frac{r}{\epsilon^{n-1}} i \int_0^{2\pi} e^{-i(n-1)\theta} d\theta = 0. \tag{11}$$

Therefore, the only piece we need to pay attention to in closed-contour integrals is the single pole.

What was then wrong with the proof that contours can be continuously deformed, when the contour crosses a singularity? The function is still analytic, not depending on $\bar{z}$, but yet somehow we are not allowed to deform the contour across a singularity. Why?

It turns out that $1/z$ "secretly" depends on $\bar{z}$. It is a round-about story (that's why this is in small fonts), but it can be seen as follows.

We first define derivatives with respect to $z = x+iy$ and $\bar{z} = x-iy$ as $\partial = (\partial_x - i\partial_y)/2$ and $\bar{\partial} = (\partial_x + i\partial_y)/2$ such that $\partial z = \bar{\partial}\bar{z} = 1$, and $\partial \bar{z} = \bar{\partial} z = 0$. (Also note that ∂ and $\bar{\partial}$ commute, $[\partial, \bar{\partial}] = 0$.) This shows z and $\bar{z}$ are independent under differentiation. Then a useful identity is that the Laplacian on the plane is $\Delta = \partial_x^2 + \partial_y^2 = 4\bar{\partial}\partial$.

The point is that two-dimensional Coulomb potential is a logarithm,

$$\Delta\left(\frac{1}{4\pi}\log r^2\right) = \delta^2(\vec{r}). \tag{12}$$

Now we rewrite this Green's equation in terms of complex coordinate z and $\bar{z}$. Because $r^2 = z\bar{z}$, we find

$$4\bar{\partial}\partial\frac{1}{4\pi}\log(z\bar{z}) = \delta^2(\vec{r}). \tag{13}$$

Because $\log(z\bar{z}) = \log z + \log\bar{z}$, doing the derivative ∂ with respect to z gives

$$\frac{1}{2\pi}\bar{\partial}\frac{1}{z} = \delta^2(\vec{r}). \tag{14}$$

Now we see that $1/z$ actually "depends" on $\bar{z}$ and its $\bar{z}$-derivative gives a delta function! This is precisely the contribution that gives the extra piece from the pole when the contour crosses a singularity.

The "magnetic flux" of the pole $1/z$ is

$$B = \vec{\nabla}\times\vec{A} = \partial_x A_y - \partial_y A_x = \partial_x i\frac{1}{z} - \partial_y\frac{1}{z} = 2i\bar{\partial}\frac{1}{z} = 2\pi i\delta^2(\vec{r}). \tag{15}$$

Now it is easy to see that the contour integral around the pole gives the "magnetic flux" of $2\pi i$.

When a function of z has poles, it is said to be meromorphic, while an analytic function without a pole is said to be holomorphic.

The general formula we then keep in our mind is

$$\oint_C \frac{f(z)}{z - z_0} dz = 2\pi i f(z_0) \tag{16}$$

for any function $f(z)$ regular at z_0, if the contour C encircles the pole z_0 counter-closewise.

If there is a multiple pole together with a regular function, the contribution comes from Taylor-expanding the integrand up to the order that gives a single pole.

$$\begin{aligned}
&\oint_C \frac{f(z)}{(z - z_0)^n} dz \\
&= \oint_C \frac{f(z_0) + (z - z_0) f'(z_0) + \cdots + \frac{1}{(n-1)!}(z - z_0)^{n-1} f^{(n-1)}(z_0) + \cdots}{(z - z_0)^n} dz \\
&= \oint_C \frac{\frac{1}{(n-1)!} f^{(n-1)}(z_0)}{z - z_0} dz \\
&= 2\pi i \frac{1}{(n-1)!} f^{(n-1)}(z_0).
\end{aligned} \tag{17}$$

2 A Few Checks

Let us do a few checks to see the contour integrals gives the same result as what you do in normal integrals.

Consider

$$\int_{-\infty}^{\infty} \frac{dx}{x^2 + a^2}. \tag{18}$$

The standard way to do it is first do the indefinite integral

$$\int \frac{dx}{x^2 + a^2} = \frac{1}{a} \arctan \frac{x}{a}. \tag{19}$$

Then evaluate the definite integral

$$\int_{-\infty}^{\infty} \frac{dx}{x^2 + a^2} = \lim_{\substack{A \to \infty \\ B \to -\infty}} \int_B^A \frac{dx}{x^2 + a^2}$$

$$
\begin{aligned}
&= \lim_{\substack{A\to\infty \\ B\to-\infty}} \frac{1}{a}\left(\arctan\frac{A}{a} - \arctan\frac{B}{a}\right) \\
&= \frac{1}{a}\left(\frac{\pi}{2} - \left(-\frac{\pi}{2}\right)\right) = \frac{\pi}{a}. \qquad (20)
\end{aligned}
$$

On the other hand, this is what we would do with contour integrals. First of all, we regard this integral as a contour integral along the real axis on the complex plane. (We now view x as a complex parameter.) At the inifinity $|x| \to \infty$, no matter at what angle, the integrand damps as $1/|x|^2$. Therefore, even if we add a contour from $+\infty$ going up in circle and come down at $-\infty$, the additional piece can give correction suppressed by $1/|x|$ and hence vanishes. What it means is that we can regard the integral as a closed-contour integral along the real axis, going up at the infinity on the upper half plane, coming back to the real axis at $-\infty$. On the other hand, the integrand can be rewritten as

$$
\frac{1}{x^2+a^2} = \frac{1}{(x+ia)(x-ia)}. \qquad (21)
$$

Therefore in the closed contour described above, the pole at $x = +ia$ is encircled. The factor $1/(x+ia)$ corresponds to $f(z)$ in Eq. (16). Then the result can be obtained immediately as

$$
\oint_C \frac{dx}{x^2+a^2} = \oint_C \frac{1/(x+ia)}{x-ia} dx = 2\pi i \frac{1}{ia+ia} = \frac{\pi}{a}. \qquad (22)
$$

This result indeed agrees with the standard method.

When we extended the contour at the infinity, we could have actually go down on the lower half plane. This defines another contour C' that encircles the other pole at $x = -ia$. Do we obtain the same result this way, too? Let's do it:

$$
\oint_{C'} \frac{dx}{x^2+a^2} = \oint_{C'} \frac{1/(x-ia)}{x+ia} dx = -2\pi i \frac{1}{-ia-ia} = \frac{\pi}{a}. \qquad (23)
$$

Here, we had to be careful about the fact that the contour C' encircles the pole clockwise, that made the overall contribution of the residue come with the coefficient $-2\pi i$ instead of $2\pi i$. Now we see that contour integrals indeed work!

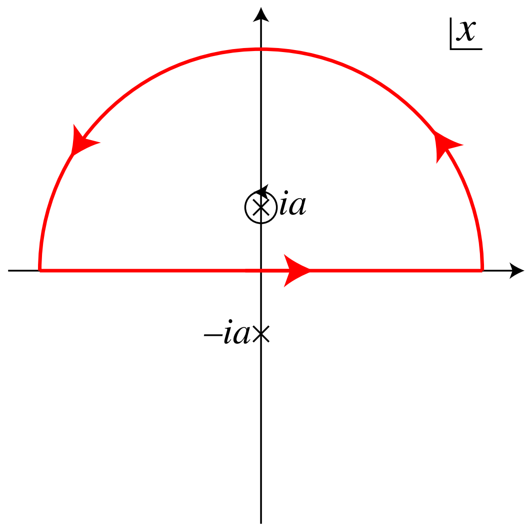

Figure 1: Contour for the integrand $1/(x^2+a^2)$.

3 More non-trivial cross-checks

Now consider the following example[1]

$$\int_{-\infty}^{\infty} \frac{dx}{\cosh x}. \tag{24}$$

The standard method is to find the indefinite integral, which is known to be

$$\int \frac{dx}{\cosh x} = 2 \arctan \tanh \frac{x}{2}, \tag{25}$$

which is easy to verify by differentiating it. Given this indefinite integral, the definite integral is simply

$$\int_{-\infty}^{\infty} \frac{dx}{\cosh x} = \left[2 \arctan \tanh \frac{x}{2} \right]_{-\infty}^{\infty} = \frac{\pi}{2} - \left(-\frac{\pi}{2} \right) = \pi. \tag{26}$$

We calculate this integral using a contour integral. The orignal integral is done along the real axis C_1 on complex x plane. Now we add another section in the opposite direction parallel to the real axis but with the imaginary part π: C_2. Note that

$$\cosh(x+i\pi) = \frac{e^{x+i\pi}+e^{-(x+i\pi)}}{2} = \frac{-e^{x}-e^{-x}}{2} = -\cosh x. \tag{27}$$

[1] I thank Roni Harnik for this example.

Therefore, the integral along C_2 must be the same as that along C_1. Finally, we can close the contour at $-\infty$ and ∞ because $\cosh x$ grows exponentially and hence $1/\cosh x$ is exponentially damped there. Then the closed contour integral, first along the real axis C_1, up to the imaginary part $i\pi$ at ∞, then back parallel to the real axis C_2, and down to the real axis at $-\infty$, must give twice of the original integral we wanted.

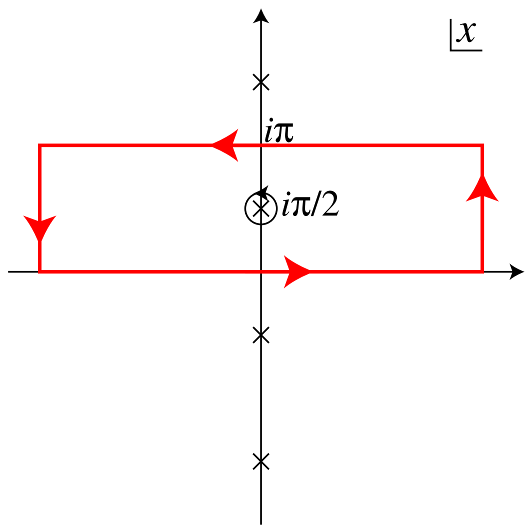

Figure 2: The integration countour for the integral $1/\cosh x$. It can be smoothly deformed to that around the pole at $x = i\pi/2$.

The poles of $1/\cosh x$ are all along the imaginary axis at $x = i(n + \frac{1}{2})\pi$. In the closed contour integral, only the pole at $x = i\pi/2$ is encircled counter-clockwise. To identify the residue, we expand $\cosh x$ at $x = i\pi/2$ as

$$\cosh\left(i\frac{\pi}{2} + x'\right) = \cosh i\frac{\pi}{2} + x' \sinh i\frac{\pi}{2} + O(x')^2 = 0 + ix' + O(x')^2. \quad (28)$$

Therefore, the contour integral reduces to that around the pole

$$\oint \frac{dx}{\cosh x} = \oint_0 \frac{dx'}{ix'} = 2\pi i \frac{1}{i} = 2\pi. \quad (29)$$

Because this is supposed to be twice as large as the original integral along the real axis, the wanted result is π. It agrees indeed with the conventional method.

4 New Integrals

There are many integrals I cannot imagine doing without using contour integrals. Here is one simple example,

$$\int_{-\infty}^{\infty} \frac{e^{iqx}}{q^2+a^2} dq. \tag{30}$$

We assume $a > 0$ without loss of generality. When $x > 0$, we can add an additional arc at the infinity on the upper half plane because that section gives an exponentially damped contribution. This makes the contour closed and it encirles the pole at $q = ia$. Hence the result is

$$\int_{-\infty}^{\infty} \frac{e^{iqx}}{q^2+a^2} dq = \oint_{ia} \frac{e^{iqx}}{(q+ia)(q-ia)} dq = 2\pi i \frac{e^{-ax}}{2ia} = \pi \frac{e^{-ax}}{a}. \tag{31}$$

On the other hand, when $x < 0$, the same added section is exponentially enhanced instead of damped, and we cannot add it. Instead, we add a section at the infinity on the lower half plane. Then the contour encircles the pole at $q = -ia$ clockwise, and hence

$$\int_{-\infty}^{\infty} \frac{e^{iqx}}{q^2+a^2} dq = -\oint_{-ia} \frac{e^{iqx}}{(q+ia)(q-ia)} dq = -2\pi i \frac{e^{ax}}{-2ia} = \pi \frac{e^{ax}}{a}. \tag{32}$$

Either way, the result can be summarized as $\pi e^{-a|x|}/a$.

This is actually the Yukawa-potential in one-dimension, or Green's function for the equation

$$(\partial_x^2 - a^2) G(x) = -2\pi\delta(x). \tag{33}$$

This is easy to see from the integral expression,

$$\begin{aligned} (\partial_x^2 - a^2) \int_{-\infty}^{\infty} \frac{e^{iqx}}{q^2+a^2} dq &= \int_{-\infty}^{\infty} \frac{(-q^2-a^2)e^{iqx}}{q^2+a^2} dq \\ &= -\int_{-\infty}^{\infty} e^{iqx} dq \\ &= -2\pi\delta(x). \end{aligned} \tag{34}$$

The result of the contour integral can be verified to satisfy this equation,

$$\begin{aligned} (\partial_x^2 - a^2)\frac{\pi}{a} e^{-a|x|} &= \partial_x(-\pi(\text{sign } x) e^{-a|x|}) - \pi a e^{-a|x|} \\ &= \pi a (\text{sign } x)^2 e^{-a|x|} - 2\pi\delta(x) e^{-a|x|} - \pi a e^{-a|x|} \\ &= -2\pi\delta(x). \end{aligned} \tag{35}$$

Here we used

$$\partial_x |x| = \text{sign } x = \begin{cases} +1 & x > 0 \\ -1 & x < 0 \end{cases}, \tag{36}$$

$(\text{sign } x)^2 = 1$, and $\partial_x \text{sign } x = 2\delta(x)$.

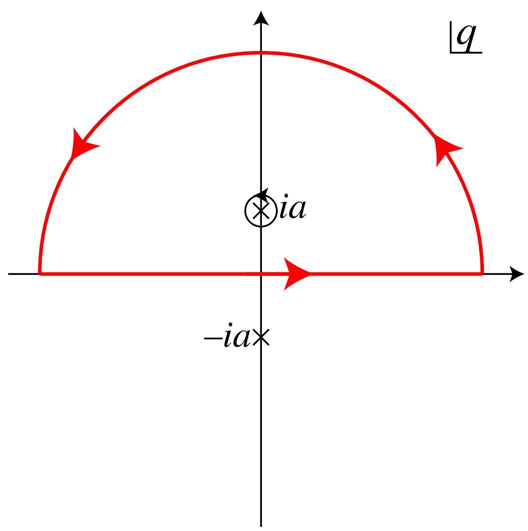

Figure 3: The contour for the integrand $e^{iqx}/(q^2+a^2)$ when $x > 0$. The added arc section on the upper half plane is exponentially damped and vanishes in the limit of taking the arc to infinity. When $x < 0$, an arc on the lower half plane is added instead.

If we have only one pole instead of one, *e.g.*,

$$G(x) = \int_{-\infty}^{\infty} \frac{e^{iqx}}{q - ia} dq, \tag{37}$$

the result is more interesting: it vanishes when $k < 0$ because the contour on the lower half plane does not encirle a pole. The result is therefore

$$G(x) = 2\pi i \theta(x) e^{-ax}, \tag{38}$$

where $\theta(x)$ is the step function

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0. \end{cases} \tag{39}$$

As a limit, $a \to 0$ gives just the step function with an exponential factor.

This $G(x)$ can also be viewed as a Green's function for a differential equation. From the definition,

$$(\partial_x + a)G(x) = \int_{-\infty}^{\infty} \frac{(iq+a)e^{iqx}}{q - ia} dq = \int_{-\infty}^{\infty} ie^{iqx} dq = 2\pi i \delta(x). \tag{40}$$

It is straightforward to check that our result $G(x) = \theta(x)e^{-ax}$ satisifes the differential equation, noting $\partial_x \theta(x) = \delta(x)$.

5 Real-Life Examples

Here are some real-life examples.

5.1 Three-dimensional Coulomb potential

This is an example well-known to you. The scalar potential in electromagnetism satisfies the Poisson equation

$$\Delta\phi = -4\pi\rho, \tag{41}$$

where ρ is the charged density. (In MKSA system, the r.h.s. is $-\rho/\epsilon_0$.) The standard way to solve this equation is to first solve the Green's equation

$$\Delta G(\vec{x} - \vec{x}') = \delta(\vec{x} - \vec{x}'). \tag{42}$$

Once you have a solution "Green's function," the solution to the original equation is given simply by

$$\phi(\vec{x}) = -4\pi \int d\vec{x}' G(\vec{x} - \vec{x}')\rho(\vec{x}'). \tag{43}$$

The way to solve the Green's equation is to use a Fourier transform,

$$G(\vec{x}) = \int \frac{d\vec{q}}{(2\pi)^3} \tilde{G}(\vec{q}) e^{i\vec{q}\cdot\vec{x}}. \tag{44}$$

Of course the delta function is a Fourier-transform of unity,

$$\delta(\vec{x}) = \int \frac{d\vec{q}}{(2\pi)^3} e^{i\vec{q}\cdot\vec{x}}. \tag{45}$$

By substituting these expressions into the Green's equation, we find

$$-\vec{q}^2\tilde{G}(\vec{q}) = 1. \tag{46}$$

Therefore, $\tilde{G}(\vec{q}) = 1/\vec{q}^2$ and hence

$$G(\vec{x}) = \int \frac{d\vec{q}}{(2\pi)^3}\frac{-1}{\vec{q}^2}e^{i\vec{q}\cdot\vec{x}}. \tag{47}$$

Now we go to spherical coordinates,

$$G(\vec{x}) = -\int \frac{q^2 dq d\cos\theta d\phi}{(2\pi)^3}\frac{1}{q^2}e^{iqr\cos\theta}. \tag{48}$$

The integral over the azimuth is trivial: just a factor of 2π. Then the integral over $\cos\theta$ can be done and we find

$$G(\vec{x}) = -\int_0^\infty \frac{dq}{(2\pi)^2}\frac{1}{iqr}\left(e^{iqr} - e^{-iqr}\right). \tag{49}$$

Of course I can write the integrand in terms of $\sin qr$, but let me keep it that way. The integration over q is from 0 to ∞, but the integrand is an even function of q, and we can extend it to the entire real axis with a factor of a half,

$$G(\vec{x}) = -\frac{1}{8\pi^2 i}\frac{1}{r}\int_{-\infty}^\infty dq\frac{e^{iqr} - e^{-iqr}}{q}. \tag{50}$$

The integrand is regular at $q = 0$ because of the numerator. Therefore, we can safely regard it as a limit of the integral

$$\int_{-\infty}^\infty dq\frac{e^{iqr} - e^{-iqr}}{q + i\epsilon}. \tag{51}$$

There is now a pole at $q = -i\epsilon$. Let us assume $\epsilon > 0$ for the moment. Note that $r > 0$. Therefore, for the piece e^{iqr}, we can extend the contour on the upper half plane. This contour does not encirle the pole. On the other hand, for the piece e^{-iqr}, we can extend the contour on the lower half plane, and pick up the pole. Therefore,

$$\int_{-\infty}^\infty dq\frac{e^{iqr} - e^{-iqr}}{q + i\epsilon} = -2\pi i(-e^{-\epsilon r}). \tag{52}$$

Suppose now that $\epsilon < 0$. In this case the opposite happens. We now get the contribution from the pole for the piece e^{iqr}, and we find

$$\int_{-\infty}^{\infty} dq \frac{e^{iqr} - e^{-iqr}}{q + i\epsilon} = 2\pi i(e^{\epsilon r}). \tag{53}$$

Either way, we find the same result $2\pi i$ in the limit $\epsilon \to 0$. Therefore,

$$G(\vec{x}) = -\frac{1}{8\pi^2 i}\frac{1}{r}2\pi i = -\frac{1}{4\pi}\frac{1}{r}. \tag{54}$$

This is nothing but the Coulomb potential.

A by-product of this calculation is the formula

$$\int_{-\infty}^{\infty} dq \frac{\sin qr}{q} = \pi, \tag{55}$$

independent of r. The indefinite integral is called Sine-Integral function Si (x),

$$\text{Si } (x) = \int_0^x \frac{\sin t}{t} dt, \tag{56}$$

which cannot be expressed in terms of elementary functions. What we learned from the contour integral is Si $(\infty) = \pi/2$.

5.2 Lippmann–Schwinger Kernel

In the Lippmann–Schwinger equation, we need the operator $1/(E - H_0 + i\epsilon)$. In the position representation, it defines a Green's function

$$G(\vec{x} - \vec{x}') = \lim_{\epsilon \to +0} \langle \vec{x}| \frac{1}{E - H_0 + i\epsilon} |\vec{x}'\rangle \tag{57}$$

which satisfies the equation

$$\begin{aligned}
\left(E + \frac{\hbar^2 \Delta}{2m}\right) G(\vec{x} - \vec{x}') &= \left(E + \frac{\hbar^2 \Delta}{2m}\right) \langle \vec{x}| \frac{1}{E - H_0 + i\epsilon} |\vec{x}'\rangle \\
&= \langle \vec{x}| \left(E - \frac{\vec{p}^2}{2m}\right) \frac{1}{E - H_0 + i\epsilon} |\vec{x}'\rangle \\
&= \langle \vec{x}|\vec{x}'\rangle \\
&= \delta(\vec{x} - \vec{x}'). \qquad (58)
\end{aligned}$$

Here, the one-sided limit $\epsilon \to +0$ is understood but not written explicitly.

By inserting the complete set of states in the momentum representation, and using the fact that H_0 is diagonal in the momentum space, we find

$$\begin{aligned} G(\vec{x}, \vec{x'}) &= \int d\vec{p} \langle \vec{x} | \vec{p} \rangle \frac{1}{E - \vec{p}^2/2m + i\epsilon} \langle \vec{p} | \vec{x'} \rangle \\ &= \int d\vec{p} \frac{e^{i\vec{x}\cdot\vec{p}/\hbar}}{(2\pi\hbar)^{3/2}} \frac{1}{E - \vec{p}^2/2m + i\epsilon} \frac{e^{-i\vec{x'}\cdot\vec{p}/\hbar}}{(2\pi\hbar)^{3/2}} \\ &= \int d\vec{p} \frac{e^{i(\vec{x}-\vec{x'})\cdot\vec{p}/\hbar}}{(2\pi\hbar)^3} \frac{1}{E - \vec{p}^2/2m + i\epsilon}. \end{aligned} \tag{59}$$

There are many ways to do this integration. One way is to use polar coordinates for $\vec{p}$ defining the polar angle relative to the direction of $\vec{r} = \vec{x} - \vec{x'}$ such that

$$\begin{aligned} G(\vec{r}) &= \int_0^\infty p^2 dp \int_{-1}^1 d\cos\theta \int_0^{2\pi} d\phi \frac{e^{ipr\cos\theta/\hbar}}{(2\pi\hbar)^3} \frac{1}{E - p^2/2m + i\epsilon} \\ &= \frac{2\pi}{(2\pi\hbar)^3} \int_0^\infty p^2 dp \frac{e^{ipr/\hbar} - e^{-ipr/\hbar}}{ipr/\hbar} \frac{1}{E - p^2/2m + i\epsilon} \\ &= \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^\infty p dp \frac{e^{ipr/\hbar}}{ir} \frac{-2m}{p^2 - 2mE - i\epsilon} \\ &= \frac{1}{(2\pi\hbar)^2} \frac{2mi}{r} \int_{-\infty}^\infty dp \frac{p e^{ipr/\hbar}}{(p - \sqrt{2mE} - i\epsilon)(p + \sqrt{2mE} + i\epsilon)}. \end{aligned} \tag{60}$$

Because of the numerator $e^{ipr/\hbar}$, we can extend the integration contour to go along the real axis and come back at the infinity on the upper half plane. Then the contour integral picks up only the pole at $p = \sqrt{2mE} + i\epsilon = \hbar k + i\epsilon$, and we find

$$\begin{aligned} G(\vec{r}) &= \frac{1}{(2\pi\hbar)^2} \frac{2mi}{r} 2\pi i \frac{\hbar k e^{ikr}}{2\hbar k} \\ &= -\frac{2m}{\hbar^2} \frac{e^{ikr}}{4\pi r}. \end{aligned} \tag{61}$$

This Green's function describes the wave propagating outwards from a point source.

If we had approached the pole from the opposite side, we had gotten a different result. The contour on the upper half plane would pick the pole at

$p = -\sqrt{2mE} = -\hbar k$ instead, and we find

$$
\begin{aligned}
G(\vec{r}) &= \frac{1}{(2\pi\hbar)^2}\frac{2mi}{r}2\pi i\frac{-\hbar k e^{-ikr}}{-2\hbar k} \\
&= -\frac{2m}{\hbar^2}\frac{e^{-ikr}}{4\pi r}.
\end{aligned} \tag{62}
$$

This Green's function describes the wave propagating towards a point sink. It is hard to imagine setting up an initial condition so that the wave would converge exactly to a point. Because of this reason, this Green's function is not used in the scattering problem.

6 Principal Value Integral

Here, we introduce the following identity

$$
\frac{1}{x \pm i\epsilon} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x). \tag{63}
$$

When one encounters an integral of the type

$$
\int_{-a}^{b} \frac{f(x)}{x} dx \tag{64}
$$

along the real axis, it is ill-defined at $x = 0$ unless $f(x) = 0$. It is a mild logarithmic singularity, but it is a singularity nonetheless. One way to define such an integral is as a limit of

$$
\lim_{\epsilon \to +0} \int \frac{f(x)}{x \pm i\epsilon} dx. \tag{65}
$$

It turns out that the result depends on which way you avoid the singularity (choice of the sign of $i\epsilon$ in the denominator). It is always assumed that $\epsilon > 0$ and hence the one-sided limit $\epsilon \to +0$.

Let us first study the limit

$$
\lim_{\epsilon \to +0} \int \frac{f(x)}{x - i\epsilon} dx. \tag{66}
$$

In this case, the pole is at $x = +i\epsilon$ and above the real axis. Therefore, the limit $\epsilon \to 0$ defines the integral along the contour shown in the figure Fig. 4.

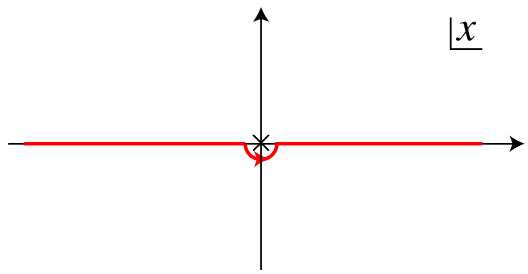

Figure 4: The integral $1/(x - i\epsilon)$ defined by the limit $\epsilon \to +0$.

The integral consists of three pieces. First, the integral along the real axis, except that the singularity is avoided symmetrically around the origin. In other words, there is an integral

$$\left[\int_{-a}^{-\varepsilon} + \int_{\varepsilon}^{b}\right] dx \frac{f(x)}{x}. \tag{67}$$

By taking ε infinitesimally small, the singularity cancels between the contributions from the left and right of the pole. This way, the integral is made well-defined. This contribution is called the *principal value integral*, and denoted by

$$\mathcal{P}\int_{-a}^{b} \frac{f(x)}{x} dx = \left[\int_{-a}^{-\varepsilon} + \int_{\varepsilon}^{b}\right] dx \frac{f(x)}{x}. \tag{68}$$

Second, there is an arc below the pole. By taking the radius of the circle infinitesimally small, we can take $f(x)$ to be constant $f(0)$, and the integral along the semi-circle is a half of that from a closed contour integral. Therefore, the additional piece is

$$i\pi f(0) = \int_{-\varepsilon}^{\varepsilon} i\pi\delta(x) f(x) dx. \tag{69}$$

The whole integral then is given by the sum of two pieces,

$$\lim_{\epsilon\to 0} \int_{-a}^{b} \frac{f(x)}{x - i\epsilon} dx = \mathcal{P}\int_{-a}^{b} \frac{f(x)}{x} dx + \int_{-a}^{b} i\pi\delta(x) f(x) dx. \tag{70}$$

To express this identity, we can write

$$\frac{1}{x - i\epsilon} = \mathcal{P}\frac{1}{x} + i\pi\delta(x), \tag{71}$$

as long as it is understood that $\mathcal{P}$ is the principal value integral and the entire right-hand side is inside an integral.

The case with the opposite way to avoid the pole $1/(x+i\epsilon)$ is done very similarly, and we find

$$\frac{1}{x+i\epsilon} = \mathcal{P}\frac{1}{x} - i\pi\delta(x). \tag{72}$$

The source of the minus sign in front of the second term is because the semi-circle around the pole goes clockwise in this case.

We can test these formulae with a simple example,

$$\int_{-\infty}^{\infty} dx \frac{\cos x}{x - i\epsilon}. \tag{73}$$

Writing $\cos x = (e^{ix} + e^{-ix})/2$, the first term allows us to add a semi-circle on the upper half plane, while the second term on the lower half plane. Because the pole is at $x = +i\epsilon$, only the semi-circle on the upper half plane encirles the pole. Therefore,

$$\int_{-\infty}^{\infty} dx \frac{\cos x}{x - i\epsilon} = 2\pi i \frac{1}{2} = i\pi. \tag{74}$$

On the other hand, the principal value intergral is

$$\mathcal{P}\int_{-\infty}^{\infty} dx \frac{\cos x}{x} = 0. \tag{75}$$

This follows from the definition

$$\mathcal{P}\int_{-\infty}^{\infty} dx \frac{\cos x}{x} = \lim_{\epsilon\to 0}\left[\int_{-\infty}^{-\epsilon} dx \frac{\cos x}{x} + \int_{\epsilon}^{\infty} dx \frac{\cos x}{x}\right] \tag{76}$$

together with the change of the variable $x \to -x$ in the first term,

$$= \lim_{\epsilon\to 0}\left[-\int_{\epsilon}^{\infty} dx \frac{\cos x}{x} + \int_{\epsilon}^{\infty} dx \frac{\cos x}{x}\right] = 0. \tag{77}$$

It is crucial that the principal value prescription is symmetric around the pole. Finally,

$$\int_{-\infty}^{\infty} dx \cos x i\pi\delta(x) = i\pi. \tag{78}$$

Putting Eqs. (74,77,78) together, the formula Eq. (71) indeed holds.

Another way to look at the principal value integral is by combining Eqs. (71,72),

$$\mathcal{P}\frac{1}{x} = \frac{1}{2}\left(\frac{1}{x - i\epsilon} + \frac{1}{x + i\epsilon}\right). \tag{79}$$

The two terms in the r.h.s. avoid the pole from above and below. Therefore, you can also express it as

$$\mathcal{P}\int_a^b dx \frac{f(x)}{x} = \frac{1}{2}\lim_{\epsilon\to 0}\left(\int_{a-i\epsilon}^{b-i\epsilon} dx \frac{f(x)}{x} + \int_{a+i\epsilon}^{b+i\epsilon} dx \frac{f(x)}{x}\right), \tag{80}$$

as shown graphically in Fig. 5.

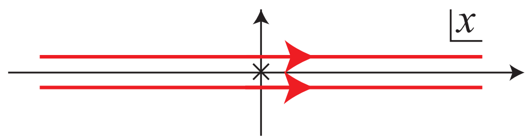

Figure 5: The principal value integral is the same as the average of integrals just above and just below the pole.

7 Crazy Examples

Now equipped with contour integrals and principal value integrals, we can prove some crazy examples I found in math books. For example,

$$\int_0^\infty dx \frac{\sin ax}{\sin bx}\frac{1}{1+x^2} = \frac{\pi}{2}\frac{\sinh a}{\sinh b} \qquad \text{if } |a| < |b|. \tag{81}$$

This looks really crazy; how come is the integral of an oscillating function given in terms of hyperbolic functions?

First of all, the integrand has many poles along the real axis, $x = n\pi/b$. The prescription employed in math books is often the principal value prescription. Using the idea in Fig. 5, we first rewrite the integral as

$$= \frac{1}{2}\lim_{\epsilon\to 0}\left[\int_\epsilon^{\infty+i\epsilon} dx \frac{\sin ax}{\sin bx}\frac{1}{1+x^2} + \int_{-\epsilon}^{\infty-i\epsilon} dx \frac{\sin ax}{\sin bx}\frac{1}{1+x^2}\right]. \tag{82}$$

Then we change the variable from x to $-x$ in the second term,

$$\begin{aligned} &= \frac{1}{2}\lim_{\epsilon\to 0}\left[\int_\epsilon^{\infty+i\epsilon} dx \frac{\sin ax}{\sin bx}\frac{1}{1+x^2} + \int_{-\infty+i\epsilon}^{\epsilon} dx \frac{\sin ax}{\sin bx}\frac{1}{1+x^2}\right] \\ &= \frac{1}{2}\lim_{\epsilon\to 0}\int_{-\infty+i\epsilon}^{\infty+i\epsilon} dx \frac{\sin ax}{\sin bx}\frac{1}{1+x^2}. \end{aligned} \tag{83}$$

The integration is above the real axis. Now the trick is to use the pole at $x = +i$. Because of the assumption $|a| < |b|$, the behavior of $\sin ax/\sin bx$ on the infinite semi-circle on the upper half plane is (for example when both a, b are positive),

$$\frac{\sin ax}{\sin bx} = \frac{e^{iax} - e^{-iax}}{e^{ibx} - e^{-ibx}} \sim \frac{e^{-iax}}{e^{-ibx}} = e^{-i(a-b)x} \to 0. \tag{84}$$

Cases with other signs of a, b can also be seen easily and $\sin ax/\sin bx \to 0$. Therefore, we can add the inifinite semi-circle on the upper half plane to the integration contour, which closes the contour. The only pole inside the contour is at $x = +i$, and the by-now-standard steps lead to the result

$$= \frac{1}{2}\lim_{\epsilon\to 0} 2\pi i \frac{\sin ia}{\sin ib}\frac{1}{2i} = \frac{\pi}{2}\frac{\sinh a}{\sinh b}. \tag{85}$$

Exactly the same method proves another formula

$$\int_0^\infty dx \frac{\sin ax}{\cos bx}\frac{x}{1+x^2} = -\frac{\pi}{2}\frac{\sinh a}{\cosh b} \qquad \text{if } |a| < |b|. \tag{86}$$

The next one can be done with an indefinite integral, but is much easier with a contour integral:

$$\int_0^{2\pi} \frac{dx}{1 - 2a\cos x + a^2} = \frac{2\pi}{|1-a^2|} \qquad (a \neq \pm 1). \tag{87}$$

We assume $a > 0$ for the discussions below, but the case $a < 0$ can be done the same way.

Along the real axis, $1 - 2a\cos x + a^2 = (1-a)^2 + 2a(1-\cos x) = (1-a)^2 + 4a\sin^2\frac{x}{2} > 0$. However, along the imaginary axis $x = i\chi$, $1 - 2a\cos x + a^2 = 1 - 2a\cosh\chi + a^2 = 0$ at $\chi = \cosh^{-1}\frac{1+a^2}{2a}$. Therefore there is a pole along the imaginary axis.

Let us first shift the integration region to $[-\pi, \pi]$ using the periodicity of $\cos x$. Then further consider a rectangle as shown in Fig. 6. We will send the top side all the way to infinite in the end. The main point is that left and right sides cancel due to the periodicity in $\cos x$. Moreover, the integral along the top side goes to zero in the limit because $\cos x = \cosh\chi \to \infty$. Therefore, the integration along the real axis (the bottom side) is the same as the contour integral along the rectangle. Then the contour integral encircles the pole at $x_0 = i\chi_0 = i\cosh^{-1}\frac{1+a^2}{2a}$, where

$$1 - 2a\cos x + a^2 = 0 + (x - x_0)2ai\sinh\chi_0 + O(x-x_0)^2. \tag{88}$$

The integral is easily done as

$$\int_0^{2\pi} \frac{dx}{1-2a\cos x+a^2} = 2\pi i \frac{1}{2a\sin x_0}. \tag{89}$$

The rest is to rewrite $\sin x_0$. Because $\cosh\chi_0 = \frac{1+a^2}{2a}$, $\sinh^2\chi_0 = \cosh^2\chi_0 - 1 = \frac{(1-a^2)^2}{4a^2}$, and hence $\sinh\chi_0 = \frac{|1-a^2|}{2a}$. Therefore, we find

$$\int_0^{2\pi} \frac{dx}{1-2a\cos x+a^2} = 2\pi i \frac{1}{2ai\sinh\chi_0} = \frac{2\pi}{|1-a^2|}. \tag{90}$$

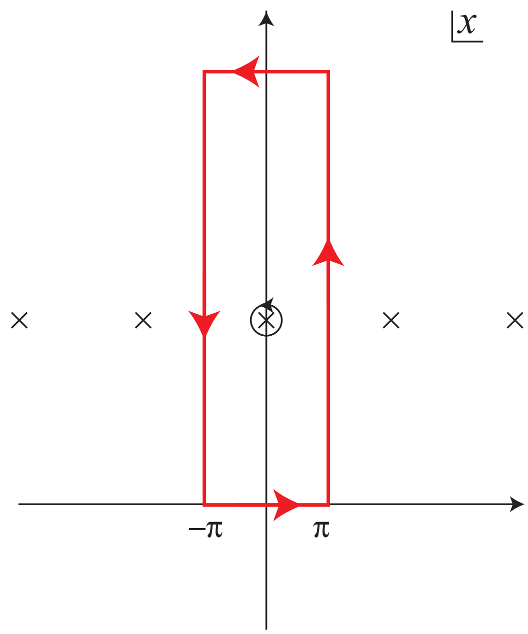

Figure 6: The integration contour to study Eq. (87).