Appendix A

Literature

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  (also available in English)

- *R. Shankar*
  Principles of Quantum Mechanics
  2nd edition, Kluwer Academic / Plenum Publishers (1994), ISBN 0306447908
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  Relativistic Quantum Mechanics / Relativistische Quantenmechanik
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All prices from amazon.de, 01/2005

Appendix B

Theory of complex functions (essentials)

1. **Definition**

Let $z = x + iy \in \mathbb{C}$ and

$$f: \quad z \longmapsto f(z) = u(x,y) + i\,v(x,y) \quad \in \mathbb{C} \tag{B.1}$$

a complex function of z, with real part $u(x,y)$ and imaginary part $v(x,y)$.
The function f is called *analytic* in a region $A \subset \mathbb{C}$, if the partial derivatives $\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial v}{\partial x}, \frac{\partial v}{\partial y}$ exist, *and*

$$\boxed{\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} &= -\frac{\partial v}{\partial x} \end{aligned}} \tag{B.2}$$

for $z = x + iy \in A \subset \mathbb{C}$.

QM.pdf **Examples:**

(a) $f(z) = z^n, n = 0, 1, 2, \ldots$ is analytic in $\mathbb{C}$.

Proof: Complete induction

1. $n = 1:$

$$f(z) = x + iy = u + iv \tag{B.3}$$

$$\frac{\partial u}{\partial x} = 1 = \frac{\partial v}{\partial y} \tag{B.4}$$

$$\frac{\partial u}{\partial y} = 0 = -\frac{\partial v}{\partial x} \tag{B.5}$$

2. $f_n(z) = z^n$ is analytic

3.
$$f_{n+1}(z) = z^{n+1} = f_n(z) \cdot z \tag{B.6}$$
$$= \underbrace{(u_n x - v_n y)}_{u_{n+1}} + i \underbrace{(v_n x + u_n y)}_{v_{n+1}} \tag{B.7}$$
$$\frac{\partial u_{n+1}}{\partial x} = \frac{\partial v_n}{\partial y} x + u_n + \frac{\partial u_n}{\partial y} y \tag{B.8}$$
$$= \frac{\partial v_{n+1}}{\partial y} \tag{B.9}$$
$$\frac{u_{n+1}}{\partial y} = -\frac{\partial v_n}{\partial x} x - \frac{\partial u}{\partial x} y - v_n \tag{B.10}$$
$$= -\frac{\partial v_{n+1}}{\partial x} \tag{B.11}$$

(b) Any complex function $f(z)$ which has a Taylor expansion around $z_0 \in \mathbb{C}$ with a finite radius of convergence in the complex plane is analytic in z_0.

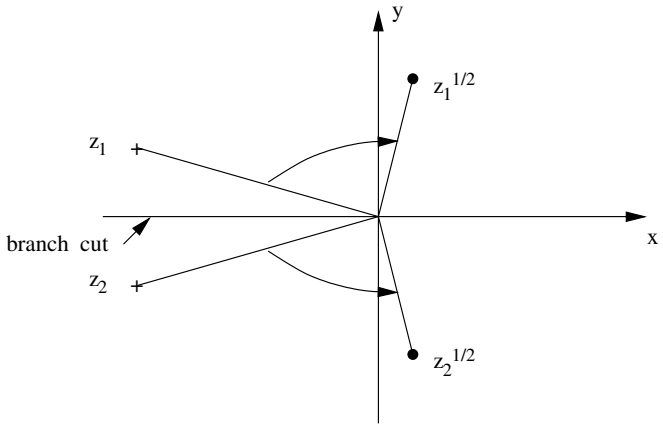
$$f(z) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(z_0)(z - z_0)^n \tag{B.12}$$

Counter examples:

(c) $f(z) = z^* = x - iy$ is not analytic for $z \neq 0$.

(d) Functions with discontinuities:

– $f(z) = z^{1/2}$ is not analytic for $y = 0, x \leq 0$.



Remark:
A continuous line of analytic points z_0 of a function f is called *branch cut*) of f.

– $f(z) = |z| = \sqrt{x^2 + y^2}$ is not analytic in $z = 0$.

– $f(z) = \mathrm{Re}\, t$ is not analytic for any $z \in \mathbb{C}$.

– $f(z) = \widetilde{f}(z)\theta(y)$ is not analytic for $\mathrm{Im}\, z = 0$.

(e) Functions with point singularities:

$$f(z) = (z - z_0)^{-n}, n = 1, 2, 3, \ldots \tag{B.13}$$

has pole of order n in $z = z_0 \in \mathbb{C}$.

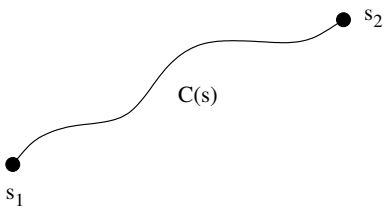
(f) $f(z) = \sum_{n=n_0}^{\infty} a_n (z - z_0)^n, n_0 \in \mathbb{Z}$

- has poles of order $n_0, n_0 - 1, \ldots, -1$, if $n_0 < 0$.
- has essential singularity, if $n_0 \to -\infty$.

2. Contour integrals

A contour in the complex plane is a continuous mapping

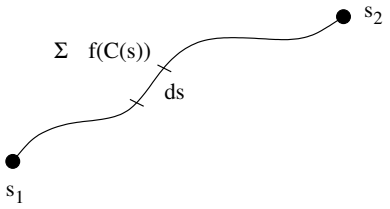
$$\begin{aligned} C: \quad \mathbb{R} &\longrightarrow \mathbb{C} \\ s &\longmapsto C(s), \quad s \in [s_1, s_2] \end{aligned} \tag{B.14}$$



s parametrizes the line $C(s)$ in the complex plane. The integral along the contour C

$$\int_C dz\, f(z) = \int_{s_1}^{s_2} ds\, f(C(s)) \tag{B.15}$$

is called *contour integral*.



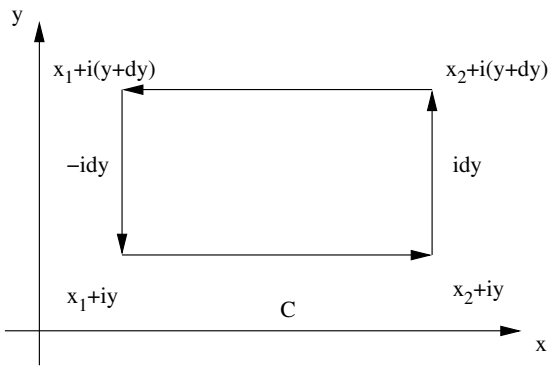
3. Theorem:

The *closed contour integral* of a function $f(z)$ enclosing a region A in $\mathbb{C}$, where $f(z)$ is analytic, is zero.

$$\boxed{\oint dz\, f(z) = 0, \quad f \text{ analytic in } A} \tag{B.16}$$

Proof: $f(z)$ analytic in a region A

(a) Consider closed, rectangular contour in A with infinitesimal extension in y-coordinate:



$$\oint dz\, f(z) = \int_{x_1}^{x_2} dx[f(x,y) - \underbrace{f(x,y+dy)}_{(*)}] \tag{B.17}$$
$$+idy[f(x_2,y) - f(x_1,y)]$$
$$= \int_{x_1}^{x_2} dx\left[\frac{\partial v(x,y)}{\partial x}dy - i\frac{\partial u(x,y)}{\partial x}dy\right] \tag{B.18}$$
$$+dy(-v(x_2,y) + v(x_1,y))$$
$$+idy(u(x_2,y) - u(x_1,y))$$
$$= 0 \tag{B.19}$$
$$(*) \qquad f(x,y+dy) = f(x,y) + \frac{\partial f(x,y)}{\partial y}dy \tag{B.20}$$
$$= f(x,y) + \left[\frac{\partial u}{\partial y} + i\frac{\partial v}{\partial y}\right]dy \tag{B.21}$$

(b) Since f is analytic in A, any contour A can be composed of infinitesimal contours considered in (a).

4. **Cauchy theorem:**

$$f(z) = \frac{a_{-1}}{z - z_0} + \sum_{n=0}^{\infty} a_n (z - z_0)^n \tag{B.22}$$

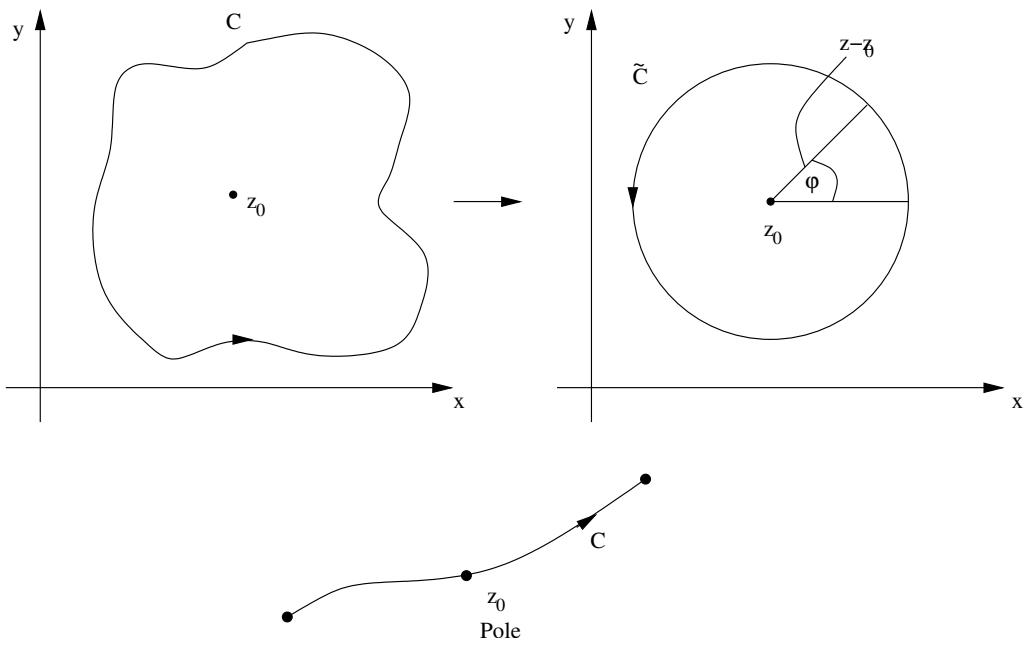
f is a complex function with a pole of first order in z, and analytic everywhere else. C is an arbitrary contour encircling z_0 *counter clockwise*.

Then:

$$\boxed{\oint_C dz\, f(z) = 2\pi i a_{-1}} \quad \text{Cauchy theorem (Residue theorem)} \tag{B.23}$$

The coefficient a_{-1} of the first order pole is called *residue* of f in z_0.

Proof:



According to 4., the contour C can be deformed to a *circle* $\widetilde{C}$, without changing the $\oint dz\, f(z)$, such that $z \in \widetilde{C}$ differs from z_0 only by an infinitesimal number ε.

$$|z - z_0| = \varepsilon \quad \text{on contour } \widetilde{C} \tag{B.24}$$

$$\oint_C dz\, f(z) = \oint_{\widetilde{C}} dz \frac{\sum_{n=-1}^{\infty} a_n (z - z_0)^{n+1}}{z - z_0} \tag{B.25}$$

$$\overset{(*)}{=} i \int_0^{2\pi} d\varphi \left(\sum_{n=-1}^{\infty} a_n \underbrace{(z - z_0)^{n+1}}_{re^{i\varphi} = r(\cos\varphi + i \sin\varphi)} \right) \tag{B.26}$$

$$= 2\pi i a_n \tag{B.27}$$

$$(*) \quad \text{parametrization of the circular contour } \widetilde{C}, \tag{B.28}$$

$$dz = i(z - z_0) d\varphi$$

$$z = z_0 + |z - z_0| e^{i\varphi} \tag{B.29}$$

$$|z - z_0| = \varepsilon = \text{const. on } \widetilde{C} \tag{B.30}$$

Remark:
For $f(z) = \frac{a}{z - z_0}$ the contour integral along a circle centered around z_0 is independent of the radius of the circle.

Corollary:

$$\oint_C dz \frac{b}{(z - z_0)^k} = 0 \quad \text{for} \quad k = 2, 3, 4, \ldots, \quad b \in \mathbb{C}\,\text{const.} \tag{B.31}$$

Proof:
Parametrization:

$$z - z_0 = re^{i\varphi} \tag{B.32}$$

$$dz = ire^{i\varphi}d\varphi \tag{B.33}$$

$$= i(z - z_0)d\varphi \tag{B.34}$$

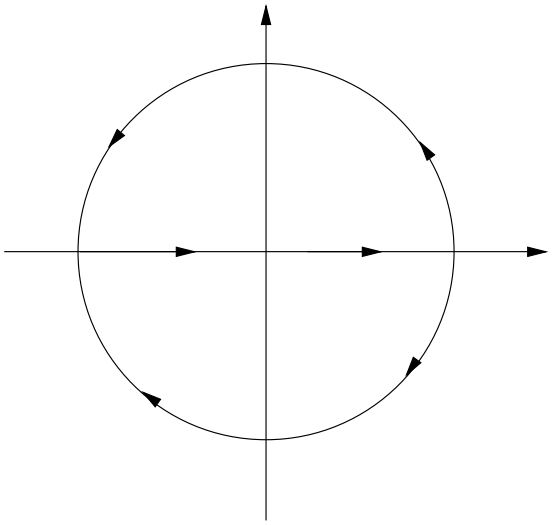
$$\oint_C dz \frac{b}{(z - z_0)^k} = \int_0^{2\pi} d\varphi \frac{ib}{re^{i\varphi}} \tag{B.35}$$

$$= \frac{ib}{r}\int_0^{2\pi} d\varphi \underbrace{e^{-i\varphi}}_{\cos\varphi(-i)\sin\varphi} \tag{B.36}$$

$$= 0 \tag{B.37}$$

Independent of $r > 0$!

5. **Treatment of poles on the integration contour**



The integral along a contour containing a pole is a priory not well-defined. Such an integral must be treated as the limit of a well-defined contour integral, where the pole is "shifted" away from the contour by an infinitesimal amount. The manner, in which the pole is shifted, is usually imposed by the physical boundary conditions.

Example: Pole on the real axis

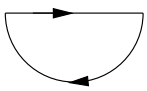
$$G_k(z) = \frac{1}{z - \varepsilon_k} = f(z) \tag{B.38}$$

The integral

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\frac{1}{\omega - \varepsilon_k} \tag{B.39}$$

is interpreted as the $t \to 0$ limit of a Fourier transform of $G_k(z)$:

$$G_k(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{\omega - \varepsilon_k} \tag{B.40}$$



We want to use contour integration so we need a closed contour.

Evaluation of $G_k(t)$ using contour integration:

1. $\underline{t > 0:}$

$$\int_C \frac{dz}{2\pi} \frac{e^{-izt}}{z - \varepsilon_k} = \int_0^{-\pi} \frac{d\varphi}{2\pi} \left. \frac{iz \exp\left(-ir(\cos\varphi + i\sin\varphi)t\right)}{z - \varepsilon_k} \right|_{r\to\infty} = 0, \tag{B.41}$$

where C is the contour of the lower complex half plane and

$$z = re^{i\varphi}, \quad r \to \infty, \quad -\pi < \varphi < 0 \quad (\varphi \neq 0, \pi), \tag{B.42}$$

since the real part of the exponent, $rt\sin\varphi$, is $-\infty$ for any $\varphi \in]-\pi, 0[, r \to \infty, t > 0$. [Order of limits $\varphi \to -\pi, 0, r \to \infty$ is essential: $r \to \infty$ first.]

2. $\underline{t < 0:}$

$$\int_{r\to\infty} \frac{dz}{2\pi} \frac{e^{-izt}}{z - \varepsilon_k} = \int_0^{\pi} \frac{d\varphi}{2\pi} \left. \frac{iz \exp\left(-ir(\cos\varphi + i\sin\varphi)t\right)}{z - \varepsilon_k} \right|_{r\to\infty} = 0, \tag{B.43}$$

since $\mathrm{Re}\,(rt\sin\varphi) \to -\infty$ for any $\varphi \in]0, \pi[, t < 0, r \to \infty$.

$$\Rightarrow \quad \underline{t > 0:} \tag{B.44}$$

$$G_k(t) = \oint_{C_{\text{lower half plane}}} \frac{dz}{2\pi} \frac{e^{-izt}}{z - \varepsilon_k} \tag{B.45}$$

$$\underline{t < 0:} \tag{B.46}$$

$$G_k(t) = \int_{C_{\text{upper half plane}}} \frac{dz}{2\pi} \frac{e^{-izt}}{z - \varepsilon_k} \tag{B.47}$$

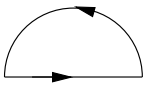
From Cauchy's theorem, these integrals are given by the residues of the pole(s) inside the contour. In particular, $\oint dz \ldots = 0$, if there is no pole inside.
To obtain a t-dependent $G_k(t)$ with $G_k(t < 0) = 0$ (retarded G-function), shift pole at $z = \varepsilon_k$ outside of the upper complex half plane, i.e. *define*:

$$G_k^R(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega - \varepsilon_k + i\eta} \tag{B.48}$$

$$= \begin{cases} -i\exp\left(-i\varepsilon_k t\right), & t > 0 \\ 0, & t < 0 \end{cases} \tag{B.49}$$

$$G_k^A(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega - \varepsilon_k - i\eta} \tag{B.50}$$

$$= \begin{cases} 0, & t > 0 \\ -i\exp\left(-i\varepsilon_k t\right), & t < 0 \end{cases} \tag{B.51}$$



Conversely, the Fourier transform of the retarded and advanced Green's functions from t to ω space are defined such that the t-integral converges for $t > 0$ or $t < 0$, respectively:

$$G_k^R(\omega) = \int_0^\infty dt\,(-i)e^{-i\varepsilon_k t} \underbrace{e^{i(\omega+i\eta)t}}_{\text{convergence factor}} = \frac{1}{\omega - \varepsilon_k + i\eta} \tag{B.52}$$

$$G_k^A(\omega) = \int_{-\infty}^0 dt\, ie^{-i\varepsilon_k t}e^{i(\omega-i\eta)t} = \frac{1}{\omega - \varepsilon_k - i\eta} \tag{B.53}$$

6. **Kramers-Kroenig relation**
Let $G^R(z)$ be an analytic function in the upper complex half plane (e.g. $G^R(z)$ is retarded Green's function: no pole in upper half plane $\Rightarrow G^R(t) = 0$ for $t < 0$.).
$G^R(z)$ has the integral representation:

$$\boxed{G^R(z) = -\int_{-\infty}^{+\infty} \frac{d\varepsilon}{\pi} \frac{A(\varepsilon)}{z - \varepsilon + i\eta}} \tag{B.54}$$

where $A(\varepsilon) = \operatorname{Im} G^R(\varepsilon) \in \mathbb{R}$.

Proof:

1. $G^R(z)$ defined by (A.54) is analytic for $z > 0$, since, by construction, it has no pole in the upper half plane ($A(\varepsilon)$ is real function).

2. From (A.54) we have for $\omega \in \mathbb{R}$:

$$\operatorname{Im} G^R(\omega) = -\int_{-\infty}^{+\infty} \frac{d\varepsilon}{\pi} \underbrace{\left.\frac{-\eta}{(\omega-\varepsilon)^2 + \eta^2}\right|_{\eta\to 0}}_{=-\pi\delta(\omega-\varepsilon)} A(\varepsilon) = A(\omega) \tag{B.55}$$

   The function $A(\varepsilon) \in \mathbb{R}, \varepsilon \in \mathbb{R}$ determines the imaginary part of G^R on the real axis as $\operatorname{Im} G^R(\omega) = u(x, y = 0) = A(\omega)$.

3. Since $\operatorname{Im} G^R(\omega)$ uniquely determines $G^R(z)$ in the complete domain of analyticity via the differential equations, and since (A.54) is analytic in upper half plane, (A.54) determines the complete $G^R(z)$, and in particular, the real part on the real axis:

$$\operatorname{Re} G^R(\omega) = -\operatorname{Re} \int_\infty^{+\infty} \frac{d\varepsilon}{\pi} \frac{\operatorname{Im} G^R(\varepsilon)}{\omega - \varepsilon + i\eta} \tag{B.56}$$

$$\boxed{\operatorname{Re} G^R(\omega) = -\mathcal{P} \int \frac{d\varepsilon}{\pi} \frac{\operatorname{Im} G^R(\varepsilon)}{\omega - \varepsilon}} \tag{B.57}$$

This is the *Kramers-Kroenig relation.* (A.54) is called *analytic continuation.*

$$\mathcal{P}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{\pi}\frac{A(\varepsilon)}{\omega-\varepsilon} = \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{\pi}\mathrm{Re}\left(\frac{1}{\omega-\varepsilon+i\eta}\right)A(\varepsilon) \tag{B.58}$$

$$= \lim_{\eta\to 0^+}\int_{-\infty}^{+\infty}\frac{d\varepsilon}{\pi}\frac{\omega-\varepsilon}{(\omega-\varepsilon)^2+\eta^2}A(\varepsilon) \tag{B.59}$$

$$= \lim_{\eta\to 0^+}\left[\int_{-\infty}^{\omega-\eta}\frac{d\varepsilon}{\pi}+\int_{\omega+\eta}^{+\infty}\frac{d\varepsilon}{\pi}\right]\frac{A(\varepsilon)}{\omega-\varepsilon} \tag{B.60}$$