COMPLEX ANALYSIS FOR QUANTUM PHYSICISTS

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These notes aim to introduce complex analysis to an audience of physicists and chemists. We will trade-off generality for simplicity, and several of our results are less powerful than they could be. The emphasis is on the applications of complex analysis to real analysis (rather than complex analysis for its own sake), based on the idea that "the shortest path between two truths of the real domain often passes through the complex one" (Painlevé). We only consider here complex *analysis*, defined as the study of functions of complex variables, as opposed to complex *algebra* (the use of complex numbers to compute expressions). Here is an example of questions purely about real numbers that can be settled very quickly using complex-analytic methods, but would be complicated (or impossible) without.

- What is the convergence radius of the Taylor series of $\frac{1}{1+x^2}$ around 0?
- Give an estimate of the number of points needed to approximate $\frac{1}{1+x^2}$ on $[-1, 1]$ using Chebyshev interpolation to machine precision.
- What is $\int_{-\infty}^{+\infty} \frac{1}{(1+x^2)^2} dx$?

0. Reminder in real analysis

We will use implicitly the dominated convergence theorem and its corollaries to take limits under the integral or sum sign. We recall that $\lim_{n\to\infty} \int f_n(x)dx = \int \lim_{n\to\infty} f_n(x)dx$ as long as there is a positive integrable function g such that $|f_n(x)| \le g(x)$. As a consequence, for instance, $\int \sum_{n=1}^{\infty} f_n(x)dx = \sum_{n=1}^{\infty} \int f_n(x)dx$ if $\int \sum_{n=1}^{\infty} |f_n|(x)dx < \infty$.

We recall that the power series of a function f around a point x_0 is

$$\sum_{n\ge 0} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

If this series converges for x close enough to x_0, f is said to be analytic at x_0. For any formal power series $\sum_{n\ge 0} a_n(x - x_0)^n$, there is a *radius of convergence* $0 \le r \le +\infty$ such that, if $x \in \mathbb{C}$ is such that $|x - x_0| < r$, the series converges absolutely, and if $|x - x_0| > r$, the series diverges. For instance, $\frac{1}{1-x} = \sum_{n\ge 0} x^n$ has radius of convergence 1 around $x = 0$.

The proof of the two preceding facts is the following. Assume without loss of generality that $x_0 = 0$, and let

$$r = \sup \left\{ |z| \in \mathbb{C}, \sum_{n\ge 0} a_n z^n \text{ converges.} \right\}$$

(this sup might be infinite). Let $|z| < r$. Then there is a z_0 with $|z| < |z_0| < r$ such that $\sum_{n\ge 0} a_n z_0^n$ converges; in particular, $a_n z_0^n$ is bounded by a constant C. Then

$$\sum_{n\ge 0} a_n z^n = \sum_{n\ge 0} \left(\frac{z}{z_0}\right)^n a_n z_0^n$$

whose general term is bounded by $C\left(\frac{|z|}{|z_0|}\right)^n$ and therefore converges absolutely.

1. Complex geometry

A complex number $z = x + iy \in \mathbb{C}$ can be seen as a point in $\mathbb{R}^2$. Any linear transform A of the complex plane can be seen as a 2×2 real matrix. A particular class is those transforms A_w that can be written as $A_w z = wz$ for some $w \in \mathbb{C}^*$. $wz = |w|\,|z|\, e^{i(\arg w + \arg z)}$ so these transformations are homotheties times rotations: they preserve shapes and angles. They are of the form

$$A_w = \begin{pmatrix} \operatorname{Re} w & -\operatorname{Im} w \\ \operatorname{Im} w & \operatorname{Re} w \end{pmatrix}$$

We have $A_{w_1 w_2} = A_{w_1} A_{w_2}$: A is a group homomorphism from $\mathbb{C}^*$ to GL(2). Reciprocally, all linear transformations that preserve angles are written in this form (they preserve $\cos\theta = \frac{\langle u,v\rangle}{|u|\,|v|}$, so they preserve inner products up to a constant, so they are homotheties times rotations). Not all linear transforms in $\mathbb{R}^2$ can be written as $z \mapsto wz$: examples are $z \mapsto \bar{z}$ (inverses angles), or $z \mapsto \operatorname{Re} z + 2\operatorname{Im} z$ (stretches axes, does not preserve shapes).

2. Holomorphic functions

There are at least three notions of derivatives of complex maps, that should not be confused

(1) The derivative of a $\mathbb{R} \to \mathbb{C}$ map: $f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$
(2) The gradient of a $\mathbb{C} \to \mathbb{R}$ map: $\nabla f(z) = \frac{\partial f}{\partial \operatorname{Re} z} + \frac{\partial f}{\partial \operatorname{Im} z} i$, so that $f(z+h) = f(z) + \operatorname{Re}(\overline{\nabla f(z)} h) + O(|h|^2)$ (used in optimisation, e.g. $\min \langle x, Ax\rangle / \langle x, x\rangle$)
(3) The derivative of a holomorphic $\mathbb{C} \to \mathbb{C}$ map, simply called "the complex derivative"

The first two do not explicitly take into account the structure of complex numbers, and treat them simply as vectors in $\mathbb{R}^2$. We are interested in the last one. Let $f : \mathbb{C} \to \mathbb{C}$, and $z \in \mathbb{C}$. We will note $z = x + iy$ and $f(z) = u(z) + iv(z)$. We assume that f is C^2 (differentiable with twice continuous derivatives) as a function $\mathbb{R}^2 \to \mathbb{R}^2$. As a function $\mathbb{R}^2 \to \mathbb{R}^2$, it has a Jacobian

$$J_f(z) = \begin{pmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{pmatrix}.$$

We will say that f is *holomorphic* on some open set $\Omega \subset \mathbb{C}$ if it preserves shapes locally, i.e. if its Jacobian preserves shapes: if U is an infinitesimally small arbitrary shape around $z \in \Omega$, then $f(U) = \{f(w), w \in U\}$ is a translated, scaled and rotated version of U around $f(z)$. As we have seen before, this implies a particular form for $J_f(z)$: we must have

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y},$$
$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}.$$

These are the *Cauchy-Riemann equations.*

An equivalent definition is that f is *complex-differentiable*: for every $z \in \Omega$, there is $w \in \mathbb{C}$ such that

$$f(z+h) = f(z) + wz + O(|z|^2)$$

This (unique) w is called the *derivative* of f at z, noted $f'(z)$. Note in particular that this implies that $f'(z) = \lim_{h\to 0} \frac{f(z+h)-f(z)}{h}$ and that this limit is independent on the particular way h goes to zero. Complex differentiability is a much stronger condition than simply real differentiability of $(x,y) \to \Big(\operatorname{Re} f(x+iy), \operatorname{Im} f(x+iy)\Big)$ as a $\mathbb{R}^2 \to \mathbb{R}^2$ map: as we will see, it implies very strong constraints on the function (*rigidity*).

Holomorphic functions are also called *analytic* (we will see why). Holomorphic functions defined on $\Omega = \mathbb{C}$ are called *entire*. Holomorphic functions defined everywhere on Ω except on a discrete set of isolated points are called *meromorphic* on Ω.

- Find examples of simple holomorphic and non-holomorphic functions
- Prove that the addition, multiplication, composition and division of non-zero holomorphic functions produces holomorphic functions
- Where is $\frac{1}{z}$ holomorphic? $\frac{1}{1+z^2}$? $\frac{1}{1+|z|^2}$? $\frac{1}{1+e^x}$? $\frac{\sin x}{x}$?
- Prove that there are no non-constant real-valued holomorphic function
- Propose a Newton method to find a zero of a function $f : \mathbb{C} \to \mathbb{C}$. What is its relationship to the Newton method for a function $f : \mathbb{R}^2 \to \mathbb{R}^2$, in the case where f is holomorphic? In the case where it is not?
- If $f : \mathbb{R} \to \mathbb{R}$ extends to a holomorphic function around $x \in \mathbb{R}$, prove that $\frac{\operatorname{Im} f(x+\varepsilon i)}{\varepsilon} \to f'(x)$. Why is this more accurate than a regular finite difference approximation in the presence of roundoff error?
- Prove that a real function defined by a power series at x with radius of convergence r can be extended to a function that is holomorphic inside in a disk centered at x of radius r. Prove that exp, cos, sin are entire.

The example above show that we can sometimes define *analytic continuations* to the complex plane of functions that are only a priori defined on the real line, by exploiting the fact that power series converge in disks. This gives a definition of e.g. $\exp(1+2i)$ by expanding exp as a power series around 0. But the choice of 0 was arbitrary: what is to say that the expansion around 1 does not converge to another value? We will prove later on the following

Theorem (Isolated zeroes)**.** *If f and g are holomorphic on a connected domain D and agree on a segment included in D, they are equal everywhere on D.*

This justifies that we can speak of *the* analytic continuation of a real analytic function. In practice this is rarely done so explicitly; given a real-analytic function $f(x)$, it is often more convenient to give directly a value to $f(z)$ for z in some subset of the complex plane, and then check that this agree with $f(x)$ on the real line. For instance, here we could have used $\exp(x+iy) = \exp(x)\exp(iy) = \exp(x)(\cos y + i \sin y)$.

Can we find an analytic continuation of log? We want $\exp \log z = z$ to hold, and so if $z = re^{i\theta}$, we want $\log z = \log r + i(\theta + 2\pi k)$ for some $k \in \mathbb{Z}$. The problem is how to choose k, which implies a phase determination. The best we can do is to choose a *branch cut*: require $\theta \in (-\pi, \pi]$, for instance. log is then holomorphic on $\mathbb{C} \setminus \mathbb{R}^-$. The same is true for functions defined using logs, like the square root. Alternatively, we can define log as a *multi-valued function*: $\log z = \log r + i\theta + 2\pi i\mathbb{Z}$. This can be visualized by plotting the imaginary part(s) of $\log z$ as a function of z, giving a staircase (called a Riemann surface). Note that the multiple definitions of log do not violate the previous theorem, as the places where they would match ($\mathbb{R}^-$) is excluded from the domain of definition.

- Note that a power series around x with radius of convergence r can be re-expanded in a power series around y when $|x-y| < r$. What happens if you play this game with $\log x$ starting at $x = 1$? With $\sqrt{x}$?
- Prove that $\sum_{n \geq 0} z^n$ defined on $(-1, 1)$ can be analytically continued on $\mathbb{C} \setminus \{1\}$. What "is" $1 + 2 + 4 + \ldots$?
- Prove that the Riemann zeta function

$$\zeta(z) = \sum_{n=1}^{\infty} n^{-z}$$

defines a holomorphic function on the set $\operatorname{Re} z > 1$. It can actually be analytically extended to $\mathbb{C} \setminus \{1\}$; since analytic continuations are unique, it is a well-defined mathematical question (the \$1M-worth Riemann hypothesis) to inquire about the location of the zeros of *the* Riemann zeta function in $\mathbb{C} \setminus \{1\}$.
- Prove that

$$\sum_{m,n,o \in \mathbb{Z}^3} \frac{(-1)^{m+n+o}}{(m^2+n^2+o^2)^{s/2}}$$

is convergent for $\operatorname{Re} s > 1$, but not absolutely convergent at $s = 1$. This function can be analytically extended to $s = 1$, giving the Madelung constant of salt. This quantity can also be obtained by expanding cubes (but not balls) or by the Ewald method.

3. Harmonic functions

Recall that a function $u : \mathbb{R}^2 \to \mathbb{R}$ is *harmonic* if it is a solution of the Laplace equation $\Delta u = 0$. Such functions model an electrostatic/gravitation potential in vacuum, the potential of a 2D irrotational incompressible flow, or the steady-state distribution of heat. If $f = u + iv$ is holomorphic and u and v are C^2, then $\Delta u = \Delta v = 0$: holomorphic functions are harmonic. Like harmonic functions, holomorphic functions are smooth and determined by their boundary values.

Holomorphic functions can be used as Lego bricks to build harmonic functions: we just have to find the holomorphic function that satisfies the correct boundary conditions. For instance, the Joukowsky transform $z \mapsto z + \frac{1}{z}$ happens to map the circle to something resembling an airfoil. Since we know how to solve the potential flows around a disk and the composition of holomorphic functions is holomorphic, we know how to compute flow around an airfoil, which was important historically. Similarly, many problems in electrostatics can be solved in this way (although this is limited to 2D problems).

4. Contour integrals

We now turn to the notion of contour integral, which defines a version of integration that is adapted to the complex derivative, in the sense that, if $F'(z) = f(z)$, then "$\int_a^b f(z)dz = F(b) - F(a)$". However, in the complex case, there are multiple paths from a to b, so that $\int_a^b$ is not well-defined. In fact, it turns out that the dependence of this integral on paths is more interesting that the integral itself, and we will therefore be concerned with contour integrals on closed paths.

Let C be a *contour* (a directed closed piecewise smooth curve in $\mathbb{C}$), and let f be holomorphic on an open set containing C. We proceed by approximation and approximate C by a sequence $\widetilde{C}$ of directed segments $\widetilde{C}_i = [z_i, z_{i+1}]$ with $|z_{i+1} - z_i| < h$. We define

$$\oint_C f(z)dz = \lim_{h \to 0} \sum_i f(z_i)(z_{i+1} - z_i)$$

where the convergence of the limit is guaranteed by the smoothness of f and C. Assume C is parametrized by a curve $\gamma(t)$, with $\gamma(a) = \gamma(b)$. Then

$$\oint_C f(z)dz = \int_a^b f(\gamma(t))\gamma'(t)dt,$$

(which is independent of the parametrization γ).

Contour integrals do not have a real analogue, because of the complex multiplication in their definition. They are not related to an average value of f (that would be $f(\gamma(t))|\gamma'(t)|$), nor are they doing a circulation of f seen as a 2D vector field (this would be $\operatorname{Re} \overline{f(\gamma(t))}\gamma'(t)$). For instance, in the simple case $f(z) = z$, and C being the circle of radius 1 centered around 0, we can use the parametrization $\gamma(t) = e^{2\pi i t}$ to compute

Interpretation	Formula	$f(z) = 1$	$f(z) = z$	$f(z) = iz$	$f(z) = \overline{z} = 1/z$
Line integral	$\int_a^b f(\gamma(t))\|\gamma'(t)\|dt$	2π	0	0	0
Circulation	$\int_a^b \operatorname{Re}(\overline{f(\gamma(t))}\gamma'(t))dt$	0	0	2π	0
Contour integral	$\oint_C f(z)dz$	0	0	0	$2\pi i$

Contour integrals are particularly simple for functions that have a complex antiderivative: if there is $F(z)$ holomorphic on a neighborhood of C such that $F'(z) = f(z)$, then

$$\oint_C f(z)dz = \int_a^b F'(\gamma(t))\gamma'(t) = \int_a^b \frac{d}{dt}F(\gamma(t))dt = 0.$$

Therefore, for instance, $\oint_C (w_1 + w_2 z)dz = 0$ (it has antiderivative $w_1 z + \frac{w_2}{2}z^2$). It is not always true that a function admits an antiderivative: for instance, $1/z$ would have a natural antiderivative log, but this is not holomorphic on the unit circle. In fact, when going around the circle, log picks up an extra $2\pi i$. This can be checked explicitly: if C is the unit circle oriented trigonometrically, with $\gamma(t) = e^{it}$ we get

$$\oint_C \frac{1}{z}dz = i\int_0^{2\pi} e^{-it}e^{it}dt = 2\pi i.$$

More generally $\oint_C z^n = 2\pi i \delta_{n,-1}$ (because there is an antiderivative when $n \neq -1$)

Let Ω be a disk centered around z_0, C be its (oriented) boundary, and f be holomorphic inside Ω. Define $F(z) = \int_{[z_0,z]} f(w)dw = (z - z_0)\int_0^1 f(z_0 + t(z - z_0))dt$. F is C^2 and

$$F(z+h) = F(z) + h\int_0^1 f(z_0 + t(z - z_0))dt + h(z - z_0)\int_0^1 tf'(z_0 + t(z - z_0))dt + O(h^2) = F(z) + f(z)h + O(h^2)$$

so $F'(z) = f(z)$ and $\oint_C f(z)dz = 0$. More generally,

Theorem (Cauchy integral theorem, 1825)**.** *Let C be the piecewise smooth oriented boundary of a simply connected open set Ω, and f be holomorphic on a neighborhood of $\overline{\Omega}$. Then*

$$\oint_C f(z)dz = 0$$

Proof. Approximate Ω from the interior by a union Ω_h of squares S_i of size h. The contour integral is approximated by that on the boundary of Ω_h. This is equal to a sum of contour integrals over the boundary of each square (because the inner segments cancel out). On each square S_i, we have the expansion $f(z) = w_1 + w_2 z + O(|h|^2)$, and so $\oint_{S_i} f(z)dz = O(|h|^3)$, and $\oint_C f(z)dz = O(|h|) \to 0$.

This theorem can also be proven in a more algebraic fashion:

$$\oint_C f(z)dz = \oint_C (u+iv)(\vec{dl}\cdot(\vec{e_x}+i\vec{e_y})) = \oint (u\vec{e_x}-v\vec{e_y})\cdot\vec{dl} + i\oint_C (u\vec{e_y}+v\vec{e_x})\cdot\vec{dl}$$

Now we use the Stokes formula on the two parts separately. The curl vanishes from the Cauchy-Riemann equations, and we get the result. Note that this proof is equivalent to the one above (which essentially reproved the Stokes formula). □

Therefore, contour integrals can be *deformed* without changing their value, as long as the function is holomorphic inside.

This formula only applies if f is holomorphic inside Ω. If f has poles inside Ω, additional terms appear: as we have seen, poles like $1/z$ have a prescribed contour integral around 0, which can be amplified to

Theorem (Cauchy integral formula)**.** *Let C be the piecewise smooth boundary of a simply connected open set Ω, oriented trigonometrically. Let $w \in \Omega$, and f be holomorphic on a neighborhood of $\overline{\Omega}$. Then*

$$f(w) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{z-w}dz$$

Proof. Shrink C to a circle C_ε of radius ε around z_0. This does not change the value of the integral. Then

$$\frac{1}{2\pi i}\oint_{C_\varepsilon} \frac{f(z)}{z-w}dz = \frac{1}{2\pi i}\oint_{C_\varepsilon} \frac{f(w)}{z-w}dz + O(\varepsilon) \to f(w).$$

□

This formula expresses f inside Ω as a function of the values of $f(z)$ on the boundary $\partial\Omega$. This is not surprising: the real and imaginary parts of f are solutions of Laplace's equation inside Ω, and can be determined from their boundary values using Green's function techniques.

More generally, a *meromorphic function* (a function that is holomorphic on Ω except at some isolated points) will have a contour interal determined by the local behavior near its singularities (the *residues*). As the previous theorem shows, a function behaving like $\frac{a}{z-z_0}$ will give a term $2\pi i a$. One might think that a function behaving like $\frac{a}{(z-z_0)^2}$ gives a zero contribution, but this forgets the higher order terms: $\frac{a+b(z-z_0)}{(z-z_0)^2}$ will give a term $2\pi i b$. It is useful to think of meromorphic functions with singularities as analogous to electric potentials: they are determined by their values on the boundary of the domain, and by the presence of singularities (charges, dipoles, etc., corresponding to poles of order 1, 2, etc.) The analogy is however imperfect because electrostatics is not 2D.

This representation of f has a very simple dependence on w, and we have the central result

Theorem (Holomorphic functions are analytic)**.** *Under the same conditions as before, f is analytic at any point $z_0 \in \Omega$. Its radius of convergence is at least the distance of z_0 to the boundary of Ω, and*

$$f^{(n)}(z_0) = \frac{n!}{2\pi i}\oint_C \frac{f(z)}{(z-z_0)^{n+1}}dz$$

Proof. If $z \neq z_0$, then for $|w-z_0| < |z-z_0|$ we have the convergent power series expansion near z_0

$$\frac{1}{z-w} = \sum_{n\geq 0} \frac{1}{(z-z_0)^{n+1}}(w-z_0)^n.$$

The result then follows from

$$f(w) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{z-w}dz$$

□

We can now prove the isolated zeroes theorem above: if f and g are holomorphic on a connected domain, and agree on a segment, then they agree everywhere on the domain. This is because we can expand $f-g$ in a power series at a point on the segment, and from there continue in circles to reach every point in the domain.

If the radius of convergence of f goes beyond the boundary of Ω, then f can be continued beyond Ω. The radius of convergence of a power series is therefore determined by the point up to which the function cannot be continued holomorphically. This happens when the holomorphic function encounters a singularity, like a pole, a log or a square root.

- What is the radius of convergence of the power series expansion of $\frac{1}{1+x^2}$ at 0? Of $\sqrt{1+x^2}$?
- Compute $\int_{-\infty}^{+\infty} \frac{1}{1+x^2} dx$ and $\int_{-\infty}^{+\infty} \frac{1}{(1+x^2)^2} dx$ by contour integration. Compute the Fourier transform of $\frac{1}{1+x^2}$.
- Prove that if f is bounded and entire, then it is constant (Liouville theorem). Use this to prove that every non-constant polynomial vanishes somewhere in $\mathbb{C}$, and therefore that any polynomial can be factored in $\mathbb{C}$.
- Prove that if f is non-constant and holomorphic in an open set Ω, $|f|$ does not admit a local maximum (or minimum) inside Ω.
- Prove that if f is meromorphic inside a contour C, then
$$\oint \frac{f'(z)}{f(z)} dz = 2\pi i(N - P)$$
where N is the number of zeroes and P the number of poles, counting multiple zeroes and poles with their order (ie z^{-2} contributes -2 to P)

5. Functional calculus and perturbation theory

Let H be a Hermitian matrix of size N, with eigenvalues λ_n and eigenvectors $|n\rangle$. Recall that matrix functions $f(H)$ are defined as $\sum_{n=1}^N f(\lambda_n)|n\rangle\langle n|$. Letting C be a trigonometrically oriented contour that encloses all the spectrum of H, and assuming f is holomorphic inside C, we have

$$f(\lambda_n) = \frac{1}{2\pi i}\oint_C f(z)\frac{1}{z-\lambda_n}dz$$

and so

$$f(H) = \sum_{n=1}^N \frac{1}{2\pi i}\oint_C f(z)\frac{1}{z-\lambda_n}|n\rangle\langle n|dz = \frac{1}{2\pi i}\oint_C f(z)\frac{1}{z-H}dz$$

- Let P be the spectral projector on the eigenspace associated with an isolated simple eigenvalue λ. Prove that $P = \frac{1}{2\pi i}\oint_C \frac{1}{z-H}dz$, where C is a small circle around λ, oriented trigonometrically. Generalize this to the case of the spectral projector on the eigenspace associated with several eigenvalues, isolated from the rest of the spectrum.

This form of functional calculus (functions of matrices) is convenient for a number of applications, notably perturbation theory. Let $H(\varepsilon) = H_0 + \varepsilon H_1$ where H_0 and H_1 are Hermitian matrices. We want to expand various quantities in powers of ε, using the formulas above. This is based on the following expansion of the resolvent (also known as Green's function) $(z - H_\varepsilon)^{-1}$, for $z \notin \sigma(H_0)$. We let $G = (z - H_\varepsilon)^{-1}$ and $G_0 = (z - H_0)^{-1}$, and obtain

$$\begin{aligned} G &= \Big((z-H_0)(1-\varepsilon G_0 H_1)\Big)^{-1} \\ &= (1-\varepsilon G_0H_1)^{-1}G_0 \\ &= G_0 + \varepsilon G_0H_1G_0 + \varepsilon^2 G_0H_1G_0H_1G_0 + \dots \end{aligned}$$

(note that this computation is also sometimes written as the Dyson equation $G = G_0 + G_0H_1G$.) The n-th term in this expansion is bounded by $\|G_0\|^{n+1}\|H_1\|^n \leq \frac{\|H_1\|^n}{d(z,\sigma(H_0))^{n+1}}$, and therefore converges if $\varepsilon < \frac{d(z,\sigma(H_0))}{\|H_1\|}$.

- Prove that the following quantities are analytic at $\varepsilon = 0$, estimate the radius of convergence in terms of the problem parameters (H_1, gap, β, t), and write down explicitly the first order using an eigenbasis of H_0.
  1. The projector $P(\varepsilon)$ on the eigenspace corresponding to the ground state of $H(\varepsilon)$, assuming it is non-degenerate at $\varepsilon = 0$
  2. The ground state energy, under the same hypothesis
  3. The propagator $e^{-itH(\varepsilon)}$, at t fixed.
  4. The Fermi-Dirac weighted density matrix $\frac{1}{1+e^{\beta H}}$
- Compute the kernel of the free particle Green's function $G = (z + \Delta)^{-1}$, a priori defined on $\mathbb{C} \setminus [0, +\infty)$. Prove that $G(z)$ can be continued through the branch cut $(0, +\infty)$, either from above or from below.

6. Fourier transforms

6.1. **Fourier transforms of causal functions: the $i0^+$ trick.** Let f be a causal function, ie $f(t) = 0$ for $t < 0$. This is the case for the response function of a linear causal time-invariant system, which relates an input I to an output O by $O(t) = (I * f)(t)$. Assume for the moment that f is continuous and decays quickly enough at infinity (the system returns to its equilibrium state). Then the Fourier transform

$$\hat{f}(\omega) = \int_{-\infty}^{+\infty} f(t) e^{i\omega t} dt$$

is well defined for real ω (note inverse convention from the usual in mathematics: this is natural because solutions to $i\partial_t \psi = \omega\psi$ are $e^{-i\omega t}$). It is also well-defined for complex ω, as long as $\operatorname{Im}\omega \geq 0$, so that the exponential decays; it is even holomorphic there.

Assume now that f does not decay, but rather oscillates. This is an important case because this is what response functions of quantum mechanical systems are: a superposition of oscillations whose frequencies are the excitation energies. What sense should the Fourier transform of f have? Clearly it cannot be defined as an integral because this does not converge. The mathematical definition that makes sense is that of distribution theory, in which $\hat{f}$ is defined by its action on nicely-behaved (Schwartz) test functions: $\langle \hat{f}, \phi\rangle = \langle f, \hat{\phi}\rangle$. For instance, $\langle \hat{1}, \phi\rangle = \langle 1, \hat{\phi}\rangle = \int_{-\infty}^{\infty} \hat{\phi} = 2\pi\check{\hat{\phi}}(0) = 2\pi\phi(0)$ and so $\hat{1} = 2\pi\delta_0$. How can we compute this in practice? The trick is to *regularize*: find a sequence of functions f_η such that $f_\eta \to f$ (in a distributional sense, which is usually very easy to check), compute the Fourier transform (in the usual sense) of f_η, and pass to the limit. This is the same trick used to make sense of the 3D Fourier transform of $1/r$ (which is not integrable at infinity, and not even square-integrable): compute the Fourier transform of $\frac{e^{-\eta r}}{r}$, and pass to the limit.

It should now be clear what to do to compute the (distributional) Fourier transform of a causal but non-decaying function. Regularize the integral by a factor $e^{-\eta r}$, and then pass to the (distributional) limit. This is physically equivalent to artificially stabilizing the system (e.g. because of a small interaction with a bath). This is equivalent to computing $\hat{f}(\omega + i\eta)$, and then passing to the limit $\eta \to 0$. This is the "$i0^+$ trick": the (distributional) Fourier transform of a causal function f (defined above) is obtained by the limit $\hat{f}(\omega + i0^+)$.

6.2. **Kramers-Kronig relations.** Assume now that f is causal, smooth and decays quickly (for simplicity; generalizations are possible). Fix $\eta > 0$ and $\omega \in \mathbb{R}$. Integrate $\frac{\hat{f}(\omega')}{\omega'-\omega}$ around a semicircle of radius L in the upper plane, with base starting at $i\eta$. Since $\hat{f}$ decays at complex infinity, in the $L \to \infty$ limit the contribution of the semicircle vanishes and we are left with

$$0 = \int_{\mathbb{R}} \frac{\hat{f}(\omega' + i\eta)}{\omega' - \omega + i\eta} d\omega' = \int_{\mathbb{R}} \frac{\hat{f}(\omega' + i\eta)((\omega' - \omega) - i\eta)}{(\omega' - \omega)^2 + \eta^2} d\omega' \to \mathcal{P}\int_{-\infty}^{+\infty} \frac{\hat{f}(\omega')}{\omega' - \omega} d\omega' - i\pi\hat{f}(\omega).$$

and so

$$\hat{f}(\omega) = \frac{1}{i\pi}\mathcal{P}\int_{-\infty}^{+\infty} \frac{\hat{f}(\omega')}{\omega' - \omega} d\omega'$$

where $\mathcal{P}$ denotes the Cauchy principal value, defined as

$$\mathcal{P}\int_{-\infty}^{+\infty} \frac{\phi(\omega)}{\omega} d\omega = \lim_{\eta\to 0} \int_{[-\infty,\infty]\setminus[-\eta,\eta]} \frac{\phi(t)}{t} dt = \lim_{\eta\to 0} \int_{-\infty}^{+\infty} \frac{\phi(t)}{t + \eta^2} dt.$$

These are known as the Kramers-Kronig relations. The significance of this is that single i at the denominator, which gives the real part of $\hat{f}$ as a function of the imaginary part. This means for instance that if you know how a medium absorbs light, you know its diffraction index.

- Compute the Fourier transform of $\theta(t)e^{-i\omega_0 t}$, where $\theta(t)$ is the Heaviside function.
- Derive the response function of a harmonic oscillator $\ddot{O}(t) + \omega^2 O(t) = I(t)$, $O(-\infty) = \dot{O}(-\infty) = 0$, and its Fourier transform. Check that the Kramers-Kronig relations are satisfied.
- Derive the response to first order of an observable $\langle \psi(t), \mathcal{O}\psi(t)\rangle$ where ψ starts in the ground state a finite-dimensional Hamiltonian H_0 and evolves according to the perturbed Hamiltonian $H_0 + I(t)H_1$. Write it in the form $O(t) = (f * I)(t)$, identifying f. Compute its Fourier transform $\hat{f}$.
- Derive the Kramers-Kronig relations from $f(t) = \theta(t)f(t)$ and the convolution theorem.

7. Paley-Wiener theory

We know that the Fourier transform of a C^k functions decays like $1/|x|^k$, and vice versa. What should we impose on a function to have an exponentially decaying Fourier transform? The following transform gives us a hint:

$$\widehat{e^{-\alpha|t|}} = \frac{2\alpha}{\alpha^2 + \omega^2}$$

Exponential decay at rate α corresponds to analyticity up to $\pm i\alpha$.

Theorem (Paley-Wiener)**.** *Let f be holomorphic on $\mathbb{R} + i[-\alpha, \alpha]$, and assume that there is $C > 0$ such that $|f(t)| \le C|t|^{-2}$ on that domain, so that $\hat{f}$ is bounded and continuous. Then there is $C' > 0$ such that $|\hat{f}(\omega)| \le C'e^{-\alpha|\omega|}$. Conversely, if $\hat{f}$ is continuous and satisfies $|\hat{f}(\omega)| \le C'e^{-\alpha|\omega|}$, its inverse Fourier transform is holomorphic on $\mathbb{R} + i(-\alpha, \alpha)$.*

Proof.

$$\hat{f}(\omega) = \int_{-\infty}^{+\infty} f(t)e^{i\omega t}dt = \int_{-\infty}^{+\infty} f(t + i\alpha)e^{i\omega(t+i\alpha)}dt$$

$$|\hat{f}(\omega)| \le e^{-\alpha\omega} \int_{-\infty}^{+\infty} |f(t + i\alpha)|dt$$

where we have shifted the contour from $\mathbb{R}$ to $\mathbb{R} + i\alpha$, picking up a vanishing term (because f decays at infinity). Similarly, $|f(t)| \le e^{\alpha t} \int_{-\infty}^{+\infty} |\hat{f}(t - i\alpha)|dt$.

The converse follows by noting that the formula defining f in terms of $\hat{f}$ makes sense on $\mathbb{R} + i(-\alpha, \alpha)$, and is holomorphic there. □

This is a new step in the "hierarchy of smoothness": continuous, differentiable, C^1, C^k, C^∞, real-analytic, analytic on a complex strip, entire, entire with exponential growth. These correspond to increasing decay of the Fourier transform.

- Prove that no function can be compactly supported both in real and in Fourier space
- State and prove a Paley-Wiener theorem for the Fourier coefficients of a periodic function.
- Estimate the error on the Fourier interpolation of $\frac{1}{1+\cos\theta^2}$. Recalling that the Chebyshev interpolation of a function f on the interval $[-1, 1]$ is the Fourier interpolation of $f(\cos\theta)$ on $[0, 2\pi]$, estimate the error on the Chebyshev interpolation of $\frac{1}{1+x^2}$ on $[-1, 1]$.
- The free electron gas has density matrix $P = f(-\Delta)$, with f the Fermi-Dirac function. This acts on functions as $\widehat{P\psi}(q) = f(|q|^2)\widehat{\psi}(q)$, and so has kernel $P(x, y) = (\mathcal{F}^{-1}f(|q|^2))(x - y)$. What is the off-diagonal decay rate of P? What happens with the Boltzmann distribution instead?
- If you know Bloch theory, use the Paley-Wiener theorem for periodic functions to prove that, for an insulator, the error on the energy per unit volume in the supercell method decays exponentially with the supercell size.

8. References

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