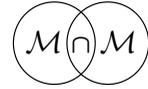# MATHEMATICS AND MECHANICS
of
Complex Systems

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QUANTUM MECHANICS:
SOME BASIC TECHNIQUES FOR SOME BASIC MODELS
II: THE TECHNIQUES

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This paper is a continuation of the previous one: "Quantum mechanics: some basic techniques for some basic models, I: The models". The main subject is the perturbation theory in quantum mechanics giving diverging perturbation series for the energy levels of the oscillators. Thus, a short historical introduction on the methods of the sum of diverging power series is given.

1. Introduction and some techniques

This is the second part of an article in honor of Professor Lucio Russo. In Section 2 there is a short history of the regular methods of the sum of divergent series. It starts with the formal series $\tilde{S}(a) = \sum_n a_n$, where $a = a_0, a_1, \ldots$ is considered a vector of components $a_n = (-1)^n$, with a possible sum $S(a) = \frac{1}{2}$ as suggested by Guido Grandi. The best proof of the value of this sum, if existent, is based on the assumption that $S(a)$ is a linear functional. The same linearity was used by Pietro Mengoli for the sum of some convergent series.

1a. *Quadratic estimates.* A family of analytic operators of type A should have constant domain [Kato 1966; Reed and Simon 1975; 1978]. For the control on the domain, the quadratic estimates can be used. We consider the simple closed PT operator $H := O_3(0) = p^2 + i x^3$, and we want to prove that $D(H) = D(p^2) \cap D(x^3)$, knowing that $D(p^2) \cap D(x^3) \subset D(H)$. We consider the quadratic norm as a quadratic form

$$\|H\psi\|^2 = \langle \psi, H^*H\psi \rangle \quad \text{for } \psi \in D(p^2) \cap D(x^3),$$

where

$$H^*H = p^4 + x^6 + 3[x^2, p]_+ = p^4 + x^6 + 3[(p+x^2)^2 - p^2 - x^4],$$

and we have the inequality

$$\|H\psi\|^2 \geq \|p^2\psi\|^2 - 3\|p\psi\|^2 + \|x^3\psi\|^2 - 3\|x^2\psi\|^2$$

$$> (1-\epsilon)(\|p^2\psi\|^2 + \|x^3\psi\|^2) - \frac{C}{\epsilon}\|\psi\|^2, \qquad \epsilon > 0, \ (1-\epsilon) > 0, \ C > 0,$$

so that $D(H)$ cannot be extended and $D(H) = D(p^2) \cap D(x^3)$.

1b. *The method of Loeffel and Martin for the confinement of the zeros.* We explain the Loeffel–Martin method [Loeffel et al. 1969] with a useful example. We consider a positive level $E = \hat{E}_m(0)$ with state $\psi(z) = \hat{\psi}_m(z)$, of the operator $O_3(0) = K(0)$ [Giachetti and Grecchi 2016a] transformed by the analytic translation $x \to x + iy$:

$$O_3(y, 0) = p^2 + i(x + iy)^3 = p^2 + i(x^2 - 3y^2)x + y^3 - 3yx^2 = p^2 + V_y(x).$$

Then

$$-\Im[\bar{\psi}(x+iy)\partial_x\psi(x+iy)] = \int_x^\infty \Im(V_y(s) - E)|\psi(s+iy)|^2\,ds$$

$$= \int_x^\infty (s^2 - 3y^2)s|\psi(s+iy)|^2\,ds = -\int_{-\infty}^x (s^2 - 3y^2)s|\psi(s+iy)|^2\,ds \neq 0 \quad (1\text{-}1)$$

for $|x| \geq \sqrt{3}|y|$, $y \in \mathbb{R}$. In this case we have a rigorous confinement of the nodes in the region

$$\mathbb{C}_\sigma = \{z = x + iy : y < 0, \ |x| < -\sqrt{3}y\} \subset \mathbb{C}_- = \{z \in \mathbb{C} : \Im z < 0\}.$$

Now we extend the Loeffel–Martin method to the case $\Im E \neq 0$, $x = 0$, obtaining the equation

$$\Im(\hbar^2\bar{\phi}(y)\partial_y\phi(y)) = -\Im E\int_y^\infty |\phi(s)|^2\,ds \quad \text{for all } y \in \mathbb{R}, \qquad (1\text{-}2)$$

where $\phi(y) = \psi(iy)$, if the integral in (1-2) exists and is bounded. Thus, the state of a nonreal level is free of imaginary zeros.

1c. *The exact quantization condition* [Giachetti and Grecchi 2016b]. We consider the semiclassical Hamiltonian

$$H_\hbar = \hbar^2 p^2 + V(x), \quad V(x) = i(x^3 - x), \ p^2 = -\frac{d^2}{dx^2}, \ \hbar > 0. \qquad (1\text{-}3)$$

Let us fix $\hbar > 0$ small, the level $E = E_n^+(\hbar) \in \mathbb{C}_-$ (the case $E_n^-(\hbar)$ is perfectly analogous) and the state $\psi_E(z) = \psi_n^+(\hbar, z)$ with n nodes in $\mathbb{C}^+ = \{z \in \mathbb{C} : \Re z > 0\}$. We have the exact quantization condition

$$J(E, \hbar) := \frac{\hbar}{2i\pi}\oint_\gamma \frac{\psi_E'(z)}{\psi_E(z)}\,dz + \frac{\hbar}{2} = \hbar(n + \tfrac{1}{2}), \qquad (1\text{-}4)$$

where $\gamma = \partial \Omega \subset \mathbb{C}^+$ and Ω is a connected domain large enough to contain all the nodes. The fixed number n and the isolation of the nodes allow us to bound the energy value.

In particular, for small $\hbar > 0$, and fixed $n \in \mathbb{N}$, the quantization rules (1-4) become the semiclassical quantization conditions for $E = E_n^+(\hbar)$

$$J(E, \hbar) = \frac{1}{2i\pi} \oint_\gamma p_0(E, z) \, dz + O(\hbar^2) = \hbar(n + \tfrac{1}{2}), \qquad (1\text{-}5)$$

where $p_0(E, z) = \sqrt{V(z) - E}$, and the path γ shrinks around the short Stokes line.

1d. *The generalized changes of representation* [Aguilar and Combes 1971]. A change of representation is given by a unitary transform $U_\delta \neq U_0 = I$, where δ is any nonzero real number and I is the identity operator, giving a new Hamiltonian $H_\delta = U_\delta H U_\delta^*$ unitarily equivalent to the original one. In this case, a level of the Hamiltonian is the same as that of the original one, $E_n(\delta) = E_n(0)$, and the state is transformed into $\psi_n(\delta) = U_\delta \psi_n$. Let H_δ be an *analytic* family of operators of type A in the parameter $\delta \in \Omega \subset \mathbb{C}$, with $\mathbb{R} \subset \Omega$, and let H have discrete spectrum $\{E_n\}_n$. Then the operator H_δ, $\delta \in \Omega \subset \mathbb{C}$, is *isospectral* to $H := H_0$ so that

$$E_n(\delta) = E_n, \qquad (1\text{-}6)$$

and the vector $\psi_n(\delta) = U_\delta \psi_n$, $\delta \in \Omega$ and $\delta = i\theta$, $\theta \in \mathbb{R}$, is the state ψ_n in a generalized representation.

Actually, there are more general changes of representation with definite transformations of the eigenvalues

$$E_n(\delta) = f_\delta(E_n).$$

1e. *The Stokes sectors, the asymptotic behavior, the Riccati equation* [1761] ***and the semiclassical series expansion.*** We recall the asymptotic behavior of the states at infinity, the Stokes sectors and the Carlini semiclassical series expansion [Plana 1832; Fröman and Fröman 1965].

Let us fix a direction in the complex plane of the variable $\arg(z) = \alpha$. The asymptotic behavior of a fundamental solution of $H_\hbar$ (see (1-3)) at infinity in this direction is given by [Sibuya 1975]

$$\hbar \lim_{\substack{|z| \to \infty \\ \arg z = \alpha}} \frac{\ln \psi_n(z)}{\int^z \sqrt{V(w)} \, dw} = \pm 1.$$

The Stokes directions α_j are defined by the oscillatory condition of the fundamental solutions at infinity:

$$\lim_{|z| \to \infty} \arg(\ln \psi_n(z)) = \pi/2 + j\pi, \quad j = -2, -1, 0, 1, 2.$$

A Stokes sector of the complex plane is a minimal sector between two Stokes directions. In the case of the cubic oscillator $H_\hbar$, the Stokes directions $\arg(z) = \alpha_j$ are

$$\lim_{|z|\to\infty} \arg(\ln \psi_n(z)) = 5\arg(iz)/2 = \pi/2 + j\pi, \quad j = -2, -1, 0, 1, 2,$$

and the Stokes sectors

$$S_j = \{z \in \mathbb{C} : |\arg(iz) - 2j\pi/5| < \pi/5\}, \quad j = -2, -1, 0, 1, 2. \tag{1-7}$$

A state $\psi_n(\hbar)$ of the Hamiltonian $H_\hbar$ is exponentially decreasing at infinity in the sectors $S_{\pm 1}$ and exponentially increasing in the sectors S_0 and $S_{\pm 2}$.

This state has large zeros only in the imaginary asymptotic direction. If we label the zeros Z_j such that $|Z_j| \to \infty$ for $j \to \infty$,

$$\arg(Z_j) \to \alpha_{\pm 2} = \pi/2 \quad \text{as } j \to \infty. \tag{1-8}$$

Remark. In the case of a double-well cubic oscillator, this result is not sufficient for our purposes. We have proven that in the case of positive levels E_m the large zeros of ψ_m are exactly imaginary. Moreover, we have $\mp \Im E_n^\pm > 0$ and the large zeros of $\psi_n^\pm$ are in $\mathbb{C}^\mp$.

We express two fundamental solutions, in a given sector S_j, of the Schrödinger equation

$$(\hbar^2 p^2 + p_0^2(z))\psi(z) = 0, \quad p^2 = -\frac{d^2}{dz^2}, \quad p_0^2(z) = V(z) - E,$$

in the form

$$\psi_\pm(z) = \exp\left(\pm\frac{1}{\hbar}\int_0^z p_\hbar(w)\,dw\right),$$

where $p_\hbar(z)$ satisfies the Riccati equation

$$p_\hbar^2(z) + \hbar p_\hbar'(z) = p_0^2(z), \quad p_0^2(z) = V(z) - E. \tag{1-9}$$

We formally solve by the Carlini series

$$p_\hbar(z) \sim \sum_n p_n(z)\hbar^n,$$

where the coefficients are computed recursively starting from the *positive* definition of the classical momentum: $p_0(z) = \sqrt{V(z) - E}$ and

$$p_1(z) = \frac{ip_0'(z)}{2p_0(z)},$$

$$p_n(z) = -\frac{1}{2p_0(z)}\left(\sum_{j=1}^{n-1} p_{n-j}(z)p_j(z) + ip_{n-1}'(z)\right), \quad n = 2, 3, \ldots. \tag{1-10}$$

Defining

$$p_\hbar(z) = P_\chi(z) + \hbar Q_\chi(z), \quad \chi = \hbar^2,$$

we get the equation for $P_\chi(z)$

$$P_\chi^2(z) - p_0^2(z) = -\chi(Q_\chi^2(z) + Q_\chi'(z)), \tag{1-11}$$

where

$$Q_\chi(z) = -\frac{P_\chi'(z)}{2P_\chi(z)}.$$

We thus have the equivalent expression of the solutions

$$\psi_\pm(z) = \frac{1}{\sqrt{P_\chi(z)}} \exp\left(\pm\frac{1}{\hbar}\int_0^z P_\chi(w)\,dw\right), \tag{1-12}$$

where the Riccati solution $P_\chi(z)$ has the even part of the Carlini expansion:

$$P_\chi(z) \sim \sum_{j\in\mathbb{N}} \chi^j p_{2j}(z) \quad \text{with truncations } P_\chi^N(z) \sim \sum_j^N \chi^j p_{2j}(z). \tag{1-13}$$

Thus, the semiclassical momentum $P_\chi(z)$ is an asymptotic notion, and the coefficients of the Carlini series are singular near the turning points. In certain cases, the exact momentum $P_\chi(z)$ is the Borel sum of the series in (1-13) [Voros 1994; Delabaere et al. 1997]. Notice that the behaviors of the fundamental solutions, for large $|z|$ in a Stokes sector, are given by (1-12) at a zeroth order of approximation with $p_0(z)$ in place of $P_\chi(z)$ [Sibuya 1975].

1f. *The Stokes lines and the classical trajectories.* Here we also examine the critical energies at the semiclassical limit $\hbar = 0$.

Let us consider the real cubic oscillator

$$H_r(\hbar) := \hbar^2 p^2 + V^r(x), \quad V^r(x) = x^3 - x, \ \hbar > 0,$$

and the energy range $R_0 = [-E_0, E_0]$, where $E_0 = 2/3\sqrt{3}$. The *union of the trajectories of the classical motion $M(E)$* consists of the *oscillation range $\sigma(E) := [I_-, I_+]$* and the *escape route $B(E) := (-\infty, I_0]$, $I_0 < -1/\sqrt{3} < I_- < I_+$*. We recall the definition of the Stokes lines at energy E. A Stokes line is tangent at each one of its points z to the direction $dz^2(z)$, where $p(z)^2\,dz^2(z) < 0$, $p(z)^2 = V^r(z) - E$, and starts from a turning point I. From the complex semiclassical point of view, $\sigma(E)$ is the internal Stokes line and $B(E)$ is the exceptional Stokes line [Giller 2011].

The fundamental state $\psi_E^0(\hbar, x)$, $E \in R_0$, subdominant in the positive semiaxis,

$$\psi_E^0(\hbar, x) \sim \frac{1}{\sqrt{p(x)}} \exp\left(-\frac{1}{\hbar}\int_{I_+}^x p(w)\,dw\right),$$

for large $x > 0$, can be continued onto the complex plane cut along $\sigma(E)$ and $B(E)$. We extend the approximate fundamental state by setting $\psi_E^0(\hbar, x) = (\psi_E^0(\hbar, x+i0) + \psi_E^0(\hbar, x-i0))/2$ for all $x \in M(E)$. This approximation oscillates in $M(E)$ as the exact fundamental state. In the limit $\hbar \to 0$ all the zeros of the exact fundamental state $\psi_E(\hbar)$ tend to $M(E)$ as $\hbar \to 0$ [Giller 2011]. The union of the trajectories of the classical motion $M(E)$ is singular at $E = E_0 = 2/3\sqrt{3}$, where the escape route $B(E)$ touches the oscillation range $\sigma(E)$.

Now we consider the PT-symmetric double well with Hamiltonian $H_\hbar = \hbar^2 p^2 + i(x^3 - x)$, for $\hbar > 0$. For $E > 0$ large, the escape route is part of the imaginary axis, while the oscillation range should be computed numerically.

The union of the trajectories of the classical motion $M(E)$ has the singular point $E^c = 0.352268\ldots$ where the escape route touches the oscillation range at its middle point. For larger $E > E^c$ the escape route and the oscillation range are separated. The energy levels $E_n(\hbar)$ are positive for large $\hbar > 0$ and are imaginary at the limit $\hbar \to 0$. This means the existence of (at least) a singularity and a crossing at $\hbar_n > 0$ for each pair of functions $E_n^\pm(\hbar)$, $0 < \hbar < \hbar_n$. The crossing parameters $\hbar_n > 0$ and the energy crossings $E_n^c > 0$ have the limits $\hbar_n \to 0$ and $E_n^c = E_n^\pm(\hbar_n) \to E^c$ as $n \to \infty$. The approximate actions around the oscillation range defined at the crossing, $J_n := n\hbar_n$, have limit $J(E^c, 0)$ as $n \to \infty$ (see (1-5)), the action integral around the oscillation range $\sigma(E)$.

We now consider the two cases denoted by the signs $\pm$ together. At energies $E_n^\mp(0) = \pm i E_0$, the oscillation range $\sigma(E)$ reduces to the points $I_- = I_+ = \mp 1/\sqrt{3}$, respectively. It is possible to prove that the escape route $B(E)$ starts at $I_0 = \pm 2/\sqrt{3}$ and goes toward $+i\infty$ staying in the half-plane $\mathbb{C}^\pm$. Moreover, the levels $E_n^\pm(\hbar)$ are nonreal for $\hbar < \hbar_n$ and the zeros of $\psi_n^\pm(\hbar)$ cannot be on the imaginary axis. Thus, the n nodes of $\psi_n^\pm(\hbar)$ are stable in $\mathbb{C}^\mp$ for $0 < \hbar < \hbar_n$.

1g. *The theory of the regular perturbations.* Let H_0 be a self-adjoint operator on the Hilbert space $\mathcal{H}$ with compact resolvent, so that the spectral theorem takes the expression

$$H_0 = \sum_n E_n P_n, \quad \mathbf{1} = \sum_n P_n, \quad P_n P_k = \delta_n^k P_n, \quad P_n^* = P_n,$$

where the set of real eigenvalues $\{E_n\}_n$ (the spectrum of H_0: $\sigma(H_0)$) have no accumulation points in $\mathbb{R}$ and the orthogonal projectors P_n have a finite-dimensional image: $m_n = \dim(P_n \mathcal{H}) \in \mathbb{N}$.

Resolvent. For $z \in \mathbb{C} - \sigma(H_0)$ the resolvent of H_0 with parameter z,

$$R_0(z) = (H_0 - z)^{-1} = \sum_n (E_n - z)^{-1} P_n, \tag{1-14}$$

is a compact operator, with norm

$$\|R_0(z)u\|^2 \leq \max_n |E_n - z|^{-2} \sum_n \|P_n u\|^2 = \|u\|^2 / \rho(z, \sigma(H_0))^2,$$

where $\rho(z, \sigma(H_0))$ is the distance of z from the spectrum of H_0. In particular, if $u = P_j u$, we have

$$\|R_0(z)u\| = 1/\rho(z, E_j).$$

Operator V relatively bounded with respect to H_0 (Kato). Let V be another operator on $\mathcal{H}$ such that $D(H_0) \subset D(V)$ and

$$\|Vu\| \leq a\|H_0 u\| + b\|u\| \quad \text{for all } u \in D(H_0)$$

for positive constants a and b. We use the notation $V < H_0$.

Theorem. *With V as above, the operator*

$$A := A(z) := V R_0(z) \tag{1-15}$$

for $z \notin \sigma(H_0)$ is a bounded *operator.*

Proof. Let us consider any $v \in \mathcal{H}$; then $Av = Vu$, where $u = R_0(z)v$, with norm $\|u\| \leq \|R_0(z)\|\|v\| \equiv c\|v\|$. For the *relative boundedness* we have $\|Vu\| \leq a\|H_0 u\| + b\|u\|$, where $\|H_0 u\| = \|H_0 R_0(z)v\| = \|v + zu\| \leq \|v\| + |z|\|u\|$; hence, $\|Av\| \leq (a(1 + |z|c) + bc)\|v\|$, whence A is a bounded operator with norm

$$\|A\| \leq a(1 + |z|c) + bc. \qquad \square$$

Analytic family of operators. Let us consider the analytic family of operators $H_\epsilon = H_0 + \epsilon V$ for $\epsilon \in \mathbb{C}$.

Theorem. *The resolvent of H_ϵ, $R_\epsilon(z) = B_\epsilon$ for a fixed $z \notin \sigma(H_\epsilon)$, is an analytic family of bounded operators on the domain $|\beta| < b_0$.*

Proof. We have

$$B_\epsilon = R_\epsilon(z) = ((H_0 - z) + \epsilon V)^{-1} = R_0(z)(1 + \epsilon A)^{-1} = R_0(z)\sum_n (-\epsilon A)^n,$$

where A is defined in (1-15) and the series of powers of operators converges in norm for $|\epsilon| < b_0 = 1/\|A\|$. $\qquad \square$

Norm convergence of the resolvents. We have that

$$\|B_\epsilon - B_0\| \leq \|R_0(z)\| \sum_{n=1}^{\infty} (|\epsilon|\|A\|)^n$$

vanishes as $\epsilon \to 0$. Analogously, for $b_1 > 0$ small and $|\epsilon_1| < b_1$, $\|B_\epsilon - B_{\epsilon_1}\| \to 0$ as $\epsilon \to \epsilon_1$.

Perturbation not relatively bounded.

Quadratic estimate 1. For any $u \in D(H_0) \cap D(V)$, there exist $a, b > 0$ such that

$$\|H_0 u\|^2 + |\epsilon|^2 \|V u\|^2 \le a \|H_\epsilon u\|^2 + b \|u\|^2.$$

Let $V = V_0 V'$ such that $V' < H$ and $V_0 = V_0^* < H_0$.

Quadratic estimate 2. For any $u \in D(H_0) \cap D(V)$, there exist positive constants a and b such that

$$\|V' u\|^2 \le a \|H_\epsilon u\|^2 + b \|u\|^2.$$

We have

$$R_\epsilon - R_0 = \epsilon R_0 V R_\epsilon = \epsilon A_0 A',$$

where the $z \notin \sigma(H_0)$ dependence is omitted. Both the operators $A_0 = R_0 V_0$ and $A' = V' R_\epsilon$ are uniformly bounded as $\epsilon \to 0$. Thus, we have the *norm resolvent convergence*

$$\|R_\epsilon - R_0\| \le |\epsilon| \|A\| \|A'\| \to 0$$

as $\epsilon \to 0$.

In our case, we have $H_0 = p^2 + \alpha x^2$, $|\alpha| = 1$, $V_0 = x$, $V' = i x^2$ and $\epsilon = \sqrt{b} \ge 0$.

Projector on an isolated part of the spectrum. Let $\gamma = \partial \Gamma$ be a regular closed positively oriented curve in $\mathbb{C}$ encompassing a simple isolated eigenvalue of H_0 once:

$$\sigma_\Gamma := E_j = \Gamma \cap \sigma(H_0), \qquad \gamma \cap \sigma(H_0) = \varnothing.$$

For instance, let γ be the *circle* $|z - E_j| = d/2$, where $d > 0$ is the isolation distance of E_j. We have

$$P_j = -(1/2\pi i) \int_\gamma R_0(z) \, dz,$$

because of (1-14) and the residue theorem. Because of the norm convergence of the resolvents and γ being a compact set, we have the norm convergence of the projectors $P_j(\epsilon) := P_\epsilon$,

$$\|P_\epsilon - P_j\| \to 0$$

for $|\epsilon| \to 0$, and there exists $b_0 > 0$ such that

$$P_j \epsilon = -(1/2\pi i) \int_\gamma R_\epsilon(z) \, dz,$$

for $0 < \epsilon < b_0$.

Perturbation expansion of P_ϵ. The set of projectors P_ϵ is an *analytic family* of projectors, and its power series expansion is

$$P_\epsilon = \sum_n \epsilon^n Q_n,$$

where

$$Q_n = -(2\pi i)^{-1} \int_\gamma R_0(z)(-V R_0(z))^n \, dz.$$

Continuity and stability of the spectrum. Let $m_\epsilon = \dim(P_\epsilon \mathcal{H}) \in \mathbb{N}$ be the total multiplicity of the eigenvalues of H_ϵ contained in Γ. This is a *continued* function for $0 < \epsilon \le \epsilon_0$ and, being *discrete-valued*, is *constant*. This means that in Γ we always have the only eigenvalue $E_j(\epsilon)$ near E_j, for ϵ small, and we can compute this analytic eigenvalue by the perturbation method.

1h. *Perturbation expansion of a simple isolated eigenvalue.* Let $E(0)$ be a simple isolated eigenvalue of H_0, with normalized eigenvector u_0 and projector P_0, so that $H_0 u_0 = E(0) u_0$ and $P_0 u_0 = u_0$. We have $\|P_\epsilon - P_0\| \to 0$ as $\epsilon \to 0$ so that $u_\epsilon = P_\epsilon u_0 \to u_0$ as $\epsilon \to 0$ is an eigenvector: $H_\epsilon u_\epsilon = E(\epsilon) u_\epsilon$, $\|u_\epsilon\| > 0$. Thus, $\langle u_0, P_\epsilon u_0 \rangle = \langle P_\epsilon u_0, P_\epsilon u_0 \rangle \to 1$ as $\epsilon \to 0$. We can compute $E(\epsilon)$ by the expression

$$
\begin{aligned}
E(\epsilon) &= \langle u_0, H_\epsilon P_\epsilon u_0 \rangle / \langle u_0, P_\epsilon u_0 \rangle \\
&= E(0) + \epsilon \langle u_0, V P_\epsilon u_0 \rangle / \langle u_0, P_\epsilon u_0 \rangle \\
&= E(0) + \epsilon \frac{\sum_n \epsilon^n \langle u_0, V Q_n u_0 \rangle}{\sum_n \epsilon^n \langle u_0, Q_n u_0 \rangle} \\
&= E(0) + \epsilon \langle u_0, V u_0 \rangle + O(\epsilon^2) = \sum_n \epsilon^n c_n,
\end{aligned}
$$

where the $\{c_n\}_n$ are the coefficients of the power series expansion given by the perturbation theory as a ratio of two power series. Since the two series are geometric, it is possible to evaluate the *remainder*, and it turns out to be of the same order as the next perturbation coefficient.

1i. *Divergent perturbation series.* If V is not bounded with respect to H_0, but any vector $V Q_n u_0$ or $Q_n u_0$, $n \in \mathbb{N}$, is bounded, we have bounded coefficients of a divergent perturbation series. We do not use the estimates of the growing of the coefficients and the remainders made with the perturbation theory because we have the exact behavior from the Stieltjes property and the behavior of the imaginary part of the "resonances".

Now it is useful to recall the method of summing the divergent perturbation series.

2. Divergent power series regular sum: a short story

The formal series [Akhiezer 1965] as a vector function with specified terms

$$\tilde{S}(a) := \sum_{k=0}^{\infty} a_k := \sum a_k, \quad a = \{a_k\}_{k \in \mathbb{N}}, \ a_k \in \mathbb{C}, \tag{2-1}$$

is convergent (Cauchy) with *sum* $S(a)$, if there exists

$$S(a) = \lim_{n \to \infty} S_n(a) \in \mathbb{C}, \quad S_n(a) = \sum_{k=0}^{n} a_k.$$

Actually Pietro Mengoli's [1650] idea of a convergent series was not so different.

For the simple *formal series* $\tilde{S}(a)$ as a function of the sequence of its terms

$$a = \{a_k = (-1)^k\}_{k \in \mathbb{N}}, \tag{2-2}$$

Guido Grandi [1703], obviously unaware of the Cauchy condition, suggested that the only possible sum of the series $S(a)$ is $\frac{1}{2}$.

Let us recall a possible *proof*.

We assume that the sum $S(a)$ is a linear functional of the vector a. Now we recall some obvious facts.

The sum of a series with only one nonzero term must exist:

$$\text{if } b = b_0, 0, 0, 0, \ldots, \quad S(b) = b_0. \tag{2-3}$$

The invariance of the series by translation of the indexes is obvious:

$$\tilde{S}(Ta) = \tilde{S}(a), \quad a = a_0, a_1, \ldots, \ Ta = 0, a_0, a_1, \ldots.$$

So we must admit the same invariance for the sum

$$S(Ta) = S(a). \tag{2-4}$$

The proof that $S(a)$, for a as in (2-2), if it exists, must be equal to $\frac{1}{2}$, is based on the extension of the linearity of the sum used by Pietro Mengoli for convergent series.

Hypothesis 1. *The sum of a series $S(a)$ is a linear function of the vector of its elements a:*

$$S(a) = S(b) + \lambda S(c), \quad a = b + \lambda c, \tag{2-5}$$

if all the sums exist.

Proposition. *Assuming the existence of the sum $S(a)$ of the formal series* (2-2),

$$S(a) = \tfrac{1}{2}. \tag{2-6}$$

Proof. We decompose the vector a as $a = b + a_0'$, where $b = a_0, 0, 0, \ldots$ and $a_0' = 0, a_1, a_2, \ldots = -Ta$. Thus, since $a = b + \lambda Ta$ where $\lambda = -1$, by Hypothesis 1,

$$S(c) = S(b) + \lambda S(Ta) = b_0 + \lambda S(a), \tag{2-7}$$

if $\lambda \in \mathbb{C}$, $c = b + \lambda Ta$ and b is as above in (2-3). The sum of the series satisfies a linear equation

$$S(a) = S(b) - S(Ta) = a_0 - S(a) = 1 - S(a),$$

with the unique solution $S(a) = \frac{1}{2}$. $\qquad\square$

Notice that Mangione [1971] says that the statement of the existence of the sum of the series $\tilde{S}(a)$ is a mistake (obviously it is, assuming the Cauchy definition of the sum).

Later Cesaro proposed his method of the sum (1894–1897). The partial sums of $\tilde{S}(a)$ are

$$S_n(a) = \frac{1}{2} + \frac{1}{2}(-1)^n, \quad n = 0, 1, 2, \ldots,$$

so that the mean values of the first sums are

$$S_N^c(a) = \sum_{n=0}^{N-1} \frac{S_n(a)}{N} = \frac{1}{2} + \frac{1}{2N}(-1)^{N-1}, \quad N = 1, 2, \ldots.$$

The Cesaro sum of the series, $\lim_{N\to\infty} S_N^c(a)$, exists and coincides with Grandi's.

2a. *The Taylor expansion of a function.* An analytic function is the sum of its power series expansion on a disk:

$$f(z) = \sum_{k=0}^{\infty} c_k z^k, \quad c_k = \frac{f^{(k)}(0)}{k!}, \ |c_k| = \frac{1}{r_k^k}, \ |z| < r, \tag{2-8}$$

where $r = \underline{\lim} \, r_k > 0$.

Example 1. We have the expansion

$$f(z) = \frac{1}{1+z} = \sum_{k=0}^{\infty} c_k z^k = \sum_{k=0}^{\infty} c_k z^{-k-1}, \quad c_k = (-1)^k, \tag{2-9}$$

on the open disk $|z| < 1$. Extending the sum by *continuity* to the point $z = 1$, we get the Grandi proof of the Grandi sum of the Grandi series.

We now state some definitions and results.

2b. *A divergent power series asymptotic to a function* (*Poincaré*). A divergent power series is asymptotic to a function f when

$$\left| f(x) - \sum_{n=0}^{N-1} c_n x^n \right| \le C_N x^N, \quad 0 < x < X. \tag{2-10}$$

The astronomer approximants. Let $C_N = a^N N!$, where $a > 0$. For any x as above, we fix $N(x) = [1/ax]$ and we take the approximant

$$\sum_{n=0}^{N(x)-1} c_n x^n,$$

with an *error exponentially small* as $x \to 0$.

Remark. The asymptotic function $f(x)$ in (2-10) is *not unique*; there is also the family of functions $f_\epsilon(x) = f(x) + \epsilon \exp(-1/ax)$ for $\epsilon \ne 0$ with $|\epsilon|$ small enough.

2c. *Strong asymptotics and uniqueness of the function* (*Carleman*). Consider the formal power series $\sum_n^\infty c_n z^n$ and the function $f(z)$. If there exist $X, C_N > 0$ such that

$$\sum_N \frac{1}{\sqrt[N]{C_N}} = \infty$$

and $f(z)$ is analytic on

$$D_X = \{z : |z| \le X, \ |\arg(z)| \le \pi/2\}$$

with

$$\left| f(z) - \sum_n^{N-1} c_n z^n \right| \le C_N |z|^N$$

uniformly for $N \in \mathbb{N}$ and $z \in D_X$, then the function $f(z)$ is uniquely defined on D_X by the formal series and is called the sum of the series.

2d. *Direct methods of sum.* We define more general approximants of the series (2-8), not only the polynomials $S_n(z) = \sum_{k=0}^n c_k z^k$ but also the rational functions called diagonal *Padé approximants*:

$$\frac{Q_j(z)}{P_j(z)} = S_{2j}(z) + O(z^{2j+1})$$

where $P_j(z)$ and $Q_j(z)$ are polynomials of degree j, with $P_j(0) = 1$. If they converge, we say that the series is summable, and the limit is called the Padé sum. Let us notice that in the case (2-9) the approximants are *exact*:

$$\frac{Q_j(z)}{P_j(z)} = f(z), \quad z \ne -1,$$

for all $j \ge 1$.

Another *regular method of sum is the Borel* one.

For the series of Example 1, we call the *Borel* transform the entire function defined by the convergent series

$$f^B(z) = \sum_{k=0}^{\infty} \frac{c_k}{k!} z^k = \sum_{k=0}^{\infty} \frac{1}{k!} (-z)^k = \exp(-z),$$

and we get the *sum* of the original series by the integral

$$f(z) = \int_0^{\infty} f^B(tz) \exp(-t) \, dt = \int_0^{\infty} \exp(-t(1+z)) \, dt$$

on the *half-plane* $\Re z > -1$.

Example 2 (Euler function (1770)). We may take

$$f(z) = \int_0^{\infty} \frac{1}{1+zt} \exp(-t) \, dt = \sum_{k=0}^{\infty} c_k z^k, \quad c_k = (-1)^k k!.$$

In this case, the power series converges nowhere, but we understand by inspection that it is the *Borel sum* of the Borel transform, $f^B(z) = (1+z)^{-1}$, on the *half-plane* $\Re z > 0$.

Remark. In this case, the Borel transform is not entire, and the analytic continuation of the Borel transform on the half-axis is not automatic. In any case, the Borel summability *does not directly give convergent approximants*, but it is not difficult to find them by mapping the region of analyticity of the Borel transform on a disk containing the origin.

Criterion of Borel summability of a series to a function (*Nevanlinna*) [Caliceti et al. 1986]. Let us consider the formal power series $\sum_n^{\infty} c_n z^n$ and the function $f(z)$. If there exist $X, C_N > 0$ such that

$$C_N = O(A^N N!)$$

and the function is analytic and

$$\left| f(z) - \sum_n^{N-1} c_n z^n \right| \le C_N |z|^N, \qquad D_X = \{z : |z - X| < X\}$$

uniformly for N and z, then the function is uniquely defined as the Borel sum of the formal series.

Returning to the problem, is it possible for the *Padé approximants* to do better? Yes! Stieltjes (1894) proved the convergence of the Padé approximants on all of *the cut plane* $\mathbb{C}_c = \{z \in \mathbb{C} : z \neq 0, \ |\arg(z)| < \pi\}$. Our function can be written

$$f(z) = yg(y) = y \int_0^{\infty} \frac{1}{y+t} \exp(-t) \, dt = \int_0^{\infty} \frac{1}{1+tz} \exp(-t) \, dt = \sum_j (-1)^j c_j z^j,$$

where $y = 1/z$ and $g(y)$ is a Stieltjes function with the associated *continued fraction* (Laguerre) [Wall 1948]

$$g(y) = 1/(y + 1/(1 + 1/(y + 2/(1 + 2/(y + 3/(\cdots)))))).$$

The approximants of the continued fraction are the *Padé approximants* of the series.

Definition. A *Stieltjes function* is a bounded analytic function on the cut plane, real for $z > 0$, with $\overline{g(z)} = g(\bar{z})$, which satisfies the *Herglotz* property [Shohat and Tamarkin 1943, Lemma 2.2],

$$\frac{\Im g(z)}{\Im z} < 0, \quad \Im z \neq 0,$$

vanishing at ∞. In this case, by the Stieltjes–Stone inversion formula, the nondecreasing measure $\mu(t)$ with $\mu(-\infty) = \mu(0) = 0$ and $\mu(t) = (\mu(t-0) + \mu(t+0))/2$ is defined by

$$\mu(b) - \mu(a) = \lim_{\epsilon \to 0} -\frac{1}{2i\pi} \int_a^b (g(t + i\epsilon) - g(t - i\epsilon))\, dt,$$

for any a and b with $0 \leq a < b$, such that

$$g(z) = \int_0^\infty \frac{1}{z+t}\, d\mu(t) := S\left(\frac{1}{z+t}\right).$$

Definition of the series of Hamburger (*more general than the Stieltjes one*) *and the Hamburger moment problem.* Let us consider the real sequence $c := \{c_n\}_{n \in \mathbb{N}}$. There exists a nondecreasing function μ, taking on infinitely many values in the interval $[-\infty, \infty)$, such that the sequence c is the sequence of the *moments* of the *measure $d\mu$*:

$$c_n = \int_{-\infty}^\infty t^n d\mu(t) := S(t^n) \in \mathbb{R} \quad \text{for all } n \in \mathbb{N}.$$

The existence of a measure is proved if and only if we have the *positivity* of the sequence of $n \times n$ matrices

$$(A_n)_{j,k} = c_{j+k}$$

so that the determinants

$$D_n = \det A_n > 0 \quad \text{for all } n \in \mathbb{N}.$$

We can set $c_0 = D_0 = D_{-1} = 1$.

2e. *The Stieltjes series and the Stieltjes moment problem.* Let us consider the real sequence $c := \{c_n\}_{n\in\mathbb{N}}$. There exists a nondecreasing function μ, taking on infinitely many values in the interval $[0, \infty)$, such that the sequence c is the sequence of the *moments* of the *measure $d\mu$*:

$$c_n = \int_0^\infty t^n \, d\mu(t) := S(t^n) \in \mathbb{R} \quad \text{for all } n \in \mathbb{N}.$$

The existence is proved if and only if we have the *positivity* of the two sequences of $n \times n$ matrices

$$(A_n)_{j,k} = c_{j+k}, \qquad (B_n)_{j,k} = c_{j+k+1}$$

so that we have

$$D_n = \det A_n > 0 \quad \text{for all } n \in \mathbb{N}.$$

We can set $c_0 = D_0 = D_{-1} = 1$.

2f. *Definition of orthonormal polynomials.* The orthonormal polynomials $P_n(t)$ for the measure $d\mu$ and the mean S,

$$S(P_n P_m) = \delta_m^n,$$

have an explicit expression:

$$P_n(t) = \frac{1}{\sqrt{D_{n-1}D_n}} \det \begin{pmatrix} c_0 & c_1 & \cdots & c_n \\ c_1 & c_2 & \cdots & c_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n-1} & c_n & \cdots & c_{2n-1} \\ 1 & t & \cdots & t^n \end{pmatrix} = \frac{\sqrt{D_{n-1}}}{\sqrt{D_n}} t^n + R_{n-1}(t).$$

It is easy to prove that

$$S(P_n(t)t^m) = \sqrt{(D_n/D_{n-1})}\,\delta_n^m$$

if $m \le n$. Let us expand

$$t\,P_n(t) = a_{n,n+1} P_{n+1}(t) + a_{n,n} P_n(t) + a_{n,n-1} P_{n-1}(t) + \cdots.$$

Comparing the leading coefficients, we get

$$a_{n,n+1} = \frac{\sqrt{D_{n-1}D_{n+1}}}{D_n}.$$

Multiplying by $P_m(t)$ and taking the mean, we get

$$a_{n,n-j} = S(t\,P_n(t)P_{n-j}(t)) = 0 \quad \text{for all } j > 1, \qquad a_{n,n-1} = a_{n-1,n}.$$

Setting $b_n = a_{n,n+1}$ and $a_n = a_{n,n}$, we get the difference equation

$$t P_n(t) = b_n P_{n+1}(t) + a_n P_n(t) + b_{n-1} P_{n-1}(t), \quad n \in \mathbb{N},$$

with the boundary conditions given by $b_{-1} = 0$ and $P_0(t) \equiv 1$.

2g. *The determination of the moment problem and the essential self-adjointness of an operator!* The determination of the Stieltjes moment problem can be seen as the *essential self-adjointness* of a *positive* operator B in $\mathcal{H}$. Let us consider a generating vector e_0 on the domain of all the operators $D = \bigcap_n B^n$ and the linear space $L = L(B, e_0)$ generated by the vectors $\{e'_n := B^n e_0\}_n$ and the Hilbert subspace $\mathcal{H}(B, e_0)$, the closure of $L(B, e_0)$ in $\mathcal{H}$. $\dot{A}$ is B restricted to L. If $\dot{A}$ is essentially self-adjoint, we call A its positive self-adjoint closure in $\mathcal{H}(A, e_0)$ with spectral function $E(x)$, $x \geq 0$. In this case, the unique measure $\mu(x)$ is the mean value of the spectral function on the generating vector e_0, $\langle e_0, E(x) e_0 \rangle$, and the Stieltjes function given by the mean value of the *resolvent* for $-z \in \mathbb{C}_c$,

$$g(z) = -\left\langle e_0, \frac{1}{A-z} e_0 \right\rangle = \int_0^\infty \frac{1}{z-x} \, d\mu(x)$$
$$= \frac{c_0}{z} + \frac{c_1}{z^2} + \cdots + \frac{c_{2n-1}}{z^{2n}} + O(1/z^{2n+1}), \tag{2-11}$$

for $|z|$ large, is the Stieltjes sum of its asymptotic series. Let us consider the infinite real *Jacobian matrix* as the representation of the linear operator $\dot{A}$ on the canonical basis $\{e_n = P_n(\dot{A}) e_0\}_n$ so that

$$\dot{A} e_k = b_{k-1} e_{k-1} + a_k e_k + b_k e_{k+1}, \quad b_k > 0, \ k \in \mathbb{N}, \ b_{-1} = 0.$$

The operator $\dot{A}$ is defined as a *symmetric* operator on the *dense* set of *finite* vectors, $g_N = \sum^N x_k e_k$. We define the adjoint operator $\dot{A}^*$ by the condition $g = \sum x_k e_k \in D(\dot{A}^*)$ if there exists $g^* = \sum y_k e_k$ such that

$$\langle \dot{A} e_k, g \rangle = \langle e_k, g^* \rangle \quad \text{for all } k \in \mathbb{N} \text{ with } g^* := \dot{A}^* g$$

or

$$b_{k-1} x_{k-1} + a_k x_k + b_k x_{k+1} = y_k \quad \text{for all } k \in \mathbb{N}.$$

Thus, the vector $g \in D(\dot{A}^*)$ if g^* is in the space l^2:

$$\sum_k |b_{k-1} x_{k-1} + a_k x_k + b_k x_{k+1}|^2 < \infty.$$

The *deficiency index* of the operator $\dot{A}$ is $(0, 0)$ or $(1, 1)$.
We look for complex eigenvalues of $\dot{A}^*$:

$$\dot{A}^* g = \sum (b_{k-1} x_{k-1} + a_k x_k + b_k x_{k+1}) e_k$$
$$= \sum x_k (b_{k-1} e_{k-1} + a_k e_k + b_k e_{k+1}) = \lambda \sum x_k e_k := \lambda g$$

so that

$$\lambda x_k = b_{k-1} x_{k-1} + a_k x_k + b_k x_{k+1}, \quad k \in \mathbb{Z}_+, \qquad (2\text{-}12)$$

with boundary conditions $\lambda x_0 = a_0 x_0 + b_0 x_1$ or $x_1 = (\lambda - a_0) x_0 / b_0$, $x_0 = c \neq 0$, so that $x_k = c P_k(\lambda)$. The same recurrence relation (2-12), with initial conditions $Q_0(\lambda) = 0$ and $Q_1(\lambda) = 1/b_0$, defines the polynomials $Q_k(\lambda)$.

It is equivalent to consider the relation

$$z Y_{k+1}(z) = (z - a_k) Y_k(z) - b_{k-1}^2 Y_{k-1}(z), \quad k \in \mathbb{Z}_+, \qquad (2\text{-}13)$$

with solutions N_k and M_k for boundary conditions $N_0 = Q_0 = 0$, $N_1 = 1$, $M_0 = P_0 = 1$ and $M_1 = z - a_0$:

$$M_k(z) = b_0 b_1 \cdots b_{k-1} P_k(z), \quad N_k(z) = b_0 b_1 \cdots b_{k-1} Q_k(z), \quad k > 0,$$

$$g(z) = 1/(z - a_0 - b_0^2/(z - a_1 - b_1^2/(z - a_2 - b_2^2/(z - a_3 - \cdots))))$$

$$= \frac{Q_k(z)}{P_k(z)} + O(1/z^{2k+1}).$$

In the determined case the sequence of diagonal Padé approximants converge for $z \in \mathbb{C}_c$ to the function

$$g(z) = \lim_{k \to \infty} \left(\frac{N_k(z)}{M_k(z)} \equiv \frac{Q_k(z)}{P_k(z)} \right).$$

Thus, we have deficiency index $(0, 0)$ if and only if

$$\sum_k |P_k(\lambda)|^2 = \infty. \qquad (2\text{-}14)$$

We have the analogue of the Liouville–Ostrogradskii formula for $k \in \mathbb{Z}_+$:

$$b_{k-1} P_{k-1} Q_k - P_k b_{k-1} Q_{k-1} = -b_k P_{k+1} Q_k + P_k b_k Q_{k+1} = b_0 P_0 Q_1 - P_1 b_0 Q_0 = 1$$

or

$$P_{k-1} Q_k - P_k Q_{k-1} = P_{k-1} Q'_{k-1} - P'_{k-1} Q_{k-1} = \frac{1}{b_{k-1}}, \qquad (2\text{-}15)$$

where

$$Q'_{k-1} = Q_k - Q_{k-1}, \qquad P'_{k-1} = P_k - P_{k-1}.$$

Theorem (Hellinger). *Let us fix z, $n \in \mathbb{Z}_+$ and*

$$w_n(t) := w_n(z, t) = -\frac{Q_n(z) - t Q_{n-1}(z)}{P_n(z) - t P_{n-1}(z)}, \quad \Im(z) \neq 0,$$

where $w_n(z, \infty) = w_{n-1}(z, 0)$. The images of $w_n : \mathbb{R} \to \mathbb{C}$ are nested circles of n-decreasing radii

$$r = r(n, z) = \frac{1}{|\Im z|} \frac{1}{\sum_{k=0}^{n-1} |P_k(z)|^2}.$$

In the case of zero deficiency index, we have the limit point *case:* $r(n, z) \to 0$, *as* $n \to \infty$, *and* $w_n(z, t)$ *have a t-independent limit as* $n \to \infty$.

Theorem (criterion). *Let*

$$\sum_n \frac{1}{b_n} = \infty.$$

The J-matrix is determinate: *we have a unique solution of the moment problem and convergence of the continued fraction.*

Proof. Use the formula (2-15):

$$\sum_{k=1}^{n} \frac{1}{b_{k-1}} = \left| \sum_{k=1}^{n} (P_{k-1} Q_k - P_k Q_{k-1})(\lambda) \right|$$

$$\leq 2 \sqrt{\sum_{k=0}^{n} |Q_k^2(\lambda)| \sum_{k=0}^{n} |P_k^2(\lambda)|}. \qquad \square$$

Theorem (Carleman criterion). *If*

$$\sum_n \frac{1}{\sqrt[2n]{c_{2n}}} = \infty,$$

then the Hamburger moment problem

$$c_k = \int_{-\infty}^{\infty} x^k \, d\mu(x),$$

is determinate.

Proof. From (2-12) we have

$$b_0 b_1 \cdots b_{n-1} P_n(\lambda) = \lambda^n + O(\lambda^{n-1})$$

for λ large. Hence,

$$b_0 \cdots b_{n-1} S(P_n^2) = \int_{-\infty}^{\infty} x^n P_n(x) \, d\mu(x) \leq \sqrt{c_{2n}} \sqrt{S(P_n^2)},$$

or since $S(P_n^2) = 1$,

$$b_0 \cdots b_{n-1} \leq \sqrt{c_{2n}},$$

and

$$\infty = \sum_n \frac{1}{\sqrt[2n]{c_{2n}}} \leq \sum_n \frac{1}{\sqrt[n]{b_0 \cdots b_{n-1}}} < e \sum_n \frac{1}{b_n}$$

for a general inequality of Carleman.

The determined Hamburger moment problem corresponds to *a determined Stieltjes* one:

$$c_n' = \int_0^\infty y^n \, d\mu'(y)$$

where $c_n' = c_{2n}$, $y = x^2$ and

$$d\mu'(y) := d\mu(\sqrt{y}) + d\mu(-\sqrt{y})$$

is the unique solution.   □

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