Appendix J

Infinite dimensional operators

(A. Wirzba)

This appendix taken from ref. [J.1] summarizes the definitions and properties for trace-class and Hilbert-Schmidt matrices, the determinants over infinite dimensional matrices and possible regularization schemes for matrices or operators which are not of trace-class.

J.1 Matrix-valued functions

(P. Cvitanović)

As a preliminary we summarize some of the properties of functions of finite-dimensional matrices.

The derivative of a matrix is a matrix with elements

$$A'(x) = \frac{dA(x)}{dx}\,, \qquad A'_{ij}(x) = \frac{d}{dx}A_{ij}(x)\,. \tag{J.1}$$

Derivatives of products of matrices are evaluated by the chain rule

$$\frac{d}{dx}(A\mathbf{B}) = \frac{dA}{dx}\mathbf{B} + A\frac{d\mathbf{B}}{dx}\,. \tag{J.2}$$

A matrix and its derivative matrix in general do not commute

$$\frac{d}{dx}A^2 = \frac{dA}{dx}A + A\frac{dA}{dx}\,. \tag{J.3}$$

The derivative of the inverse of a matrix, follows from $\frac{d}{dx}(AA^{-1}) = 0$:

$$\frac{d}{dx}A^{-1} = -\frac{1}{A}\frac{dA}{dx}\frac{1}{A}\,. \tag{J.4}$$

A function of a single variable that can be expressed in terms of additions and multiplications generalizes to a matrix-valued function by replacing the variable by the matrix.

In particular, the exponential of a constant matrix can be defined either by its series expansion, or as a limit of an infinite product:

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k \,, \qquad A^0 = \mathbf{1} \tag{J.5}$$

$$= \lim_{N\to\infty} \left(\mathbf{1} + \frac{1}{N} A\right)^N \tag{J.6}$$

The first equation follows from the second one by the binomial theorem, so these indeed are equivalent definitions. That the terms of order $O(N^{-2})$ or smaller do not matter follows from the bound

$$\left(1 + \frac{x-\epsilon}{N}\right)^N < \left(1 + \frac{x+\delta x_N}{N}\right)^N < \left(1 + \frac{x+\epsilon}{N}\right)^N \,,$$

where $|\delta x_N| < \epsilon$. If $\lim \delta x_N \to 0$ as $N \to \infty$, the extra terms do not contribute.

Consider now the determinant

$$\det\left(e^A\right) = \lim_{N\to\infty} \left(\det\,(\mathbf{1} + A/N)\right)^N \,.$$

To the leading order in $1/N$

$$\det\,(\mathbf{1} + A/N) = 1 + \frac{1}{N}\mathrm{tr}\,A + O(N^{-2})\,.$$

hence

$$\det e^A = \lim_{N\to\infty} \left(1 + \frac{1}{N}\mathrm{tr}\,A + O(N^{-2})\right)^N = e^{\mathrm{tr}\,A} \tag{J.7}$$

Due to non-commutativity of matrices, generalization of a function of several variables to a function is not as straightforward. Expression involving several matrices depend on their commutation relations. For example, the commutator expansion

$$e^{t\mathbf{A}}\mathbf{B}e^{-t\mathbf{A}} = \mathbf{B} + t[\mathbf{A},\mathbf{B}] + \frac{t^2}{2}[\mathbf{A},[\mathbf{A},\mathbf{B}]] + \frac{t^3}{3!}[\mathbf{A},[\mathbf{A},[\mathbf{A},\mathbf{B}]]] + \cdots \tag{J.8}$$

sometimes used to establish the equivalence of the Heisenberg and Schrödinger pictures of quantum mechanics follows by recursive evaluation of t derivaties

$$\frac{d}{dt}\left(e^{t\mathbf{A}}\mathbf{B}e^{-t\mathbf{A}}\right) = e^{t\mathbf{A}}[\mathbf{A},\mathbf{B}]e^{-t\mathbf{A}}\,.$$

Manipulations of such ilk yield

$$e^{(\mathbf{A}+\mathbf{B})/N} = e^{\mathbf{A}/N}e^{\mathbf{B}/N} - \frac{1}{2N^2}[\mathbf{A},\mathbf{B}] + O(N^{-3})\,,$$

and the Trotter product formula: if $\mathbf{B}$, $\mathbf{C}$ and $\mathbf{A} = \mathbf{B}+\mathbf{C}$ are matrices, then

$$e^{\mathbf{A}} = \lim_{N\to\infty}\left(e^{\mathbf{B}/N}e^{\mathbf{C}/N}\right)^N \tag{J.9}$$

J.2 Operator norms

(R. Mainieri and P. Cvitanović)

The limit used in the above definition involves matrices - operators in vector spaces - rather than numbers, and its convergence can be checked using tools familiar from calculus. We briefly review those tools here, as throughout the text we will have to consider many different operators and how they converge.

The $n \to \infty$ convergence of partial products

$$\mathbf{E}_n = \prod_{0\le m<n}\left(\mathbf{1} + \frac{t}{m}A\right)$$

can be verified using the Cauchy criterion, which states that the sequence $\{\mathbf{E}_n\}$ converges if the differences $\|\mathbf{E}_k - \mathbf{E}_j\| \to 0$ as $k, j \to \infty$. To make sense of this we need to define a sensible norm $\|\cdots\|$. Norm of a matrix is based on the Euclidean norm for a vector: the idea is to assign to a matrix $\mathbf{M}$ a norm that is the largest possible change it can cause to the length of a unit vector $\hat{n}$:

$$\|\mathbf{M}\| \;=\; \sup_{\hat{n}}\|\mathbf{M}\hat{n}\|\,, \qquad \|\hat{n}\| = 1\,. \tag{J.10}$$

We say that $\|\cdot\|$ is the operator norm induced by the vector norm $\|\cdot\|$. Constructing a norm for a finite-dimensional matrix is easy, but had $\mathbf{M}$

been an operator in an infinite-dimensional space, we would also have to specify the space $\hat{n}$ belongs to. In the finite-dimensional case, the sum of the absolute values of the components of a vector is also a norm; the induced operator norm for a matrix $\mathbf{M}$ with components M_{ij} in that case can be defined by

$$\|\mathbf{M}\| = \max_i \sum_j |M_{ij}| \,. \tag{J.11}$$

The operator norm (J.11) and the vector norm (J.10) are only rarely distinguished by different notation, a bit of notational laziness that we shall uphold.

Now that we have learned how to make sense out of norms of operators, we can check that

$$\|e^{tA}\| \leq e^{t\|A\|} \,. \tag{J.12}$$

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As $\|A\|$ is a number, the norm of e^{tA} is finite and therefore well defined. In particular, the exponential of a matrix is well defined for all values of t, and the linear differential equation (4.10) has a solution for all times.

J.3 Trace class and Hilbert-Schmidt class

This section is mainly an extract from ref. [J.9]. Refs. [J.7, J.10, J.11, J.14] should be consulted for more details and proofs. The trace class and Hilbert-Schmidt property will be defined here for linear, in general non-hermitian operators $\mathbf{A} \in \mathcal{L}(\mathcal{H})$: $\mathcal{H} \to \mathcal{H}$ (where $\mathcal{H}$ is a separable Hilbert space). The transcription to matrix elements (used in the prior chapters) is simply $a_{ij} = \langle \phi_i, \mathbf{A}\phi_j \rangle$ where $\{\phi_n\}$ is an orthonormal basis of $\mathcal{H}$ and $\langle \, , \, \rangle$ is the inner product in $\mathcal{H}$ (see sect. J.5 where the theory of *von Koch matrices* of ref. [J.12] is discussed). So, the trace is the generalization of the usual notion of the sum of the diagonal elements of a matrix; but because infinite sums are involved, not all operators will have a trace:

Definition:

(a) An operator $\mathbf{A}$ is called **trace class**, $\mathbf{A} \in \mathcal{J}_1$, if and only if, for every orthonormal basis, $\{\phi_n\}$:

$$\sum_n |\langle \phi_n, \mathbf{A}\phi_n \rangle| < \infty. \tag{J.13}$$

The family of all trace class operators is denoted by $\mathcal{J}_1$.

(b) An operator $\mathbf{A}$ is called **Hilbert-Schmidt**, $\mathbf{A} \in \mathcal{J}_2$, if and only if, for every orthonormal basis, $\{\phi_n\}$:

$$\sum_n \|\mathbf{A}\phi_n\|^2 < \infty. \tag{J.14}$$

The family of all Hilbert-Schmidt operators is denoted by $\mathcal{J}_2$.

Bounded operators are dual to trace class operators. They satisfy the the following condition: $|\langle\psi, B\phi\rangle| \leq C\|\psi\|\|\phi\|$ with $C < \infty$ and $\psi, \phi \in \mathcal{H}$. If they have eigenvalues, these are bounded too. The family of bounded operators is denoted by $\mathcal{B}(\mathcal{H})$ with the norm $\|B\| = \sup_{\phi\neq 0} \frac{\|\mathbf{B}\phi\|}{\|\phi\|}$ for $\phi \in \mathcal{H}$. Examples for bounded operators are unitary operators and especially the unit matrix. In fact, every bounded operator can be written as linear combination of four unitary operators.

A bounded operator $\mathbf{C}$ is *compact*, if it is the norm limit of finite rank operators.

An operator $\mathbf{A}$ is called *positive*, $\mathbf{A} \geq 0$, if $\langle \mathbf{A}\phi, \phi\rangle \geq 0 \;\; \forall \phi \in \mathcal{H}$. Notice that $\mathbf{A}^\dagger\mathbf{A} \geq 0$. We define $|\mathbf{A}| = \sqrt{\mathbf{A}^\dagger\mathbf{A}}$.

The most important properties of the trace and Hilbert-Schmidt classes are summarized in (see refs. [J.7, J.9]):

(a) $\mathcal{J}_1$ and $\mathcal{J}_2$ are $*$ideals., i.e., they are vector spaces closed under scalar multiplication, sums, adjoints, and multiplication with bounded operators.

(b) $\mathbf{A} \in \mathcal{J}_1$ if and only if $\mathbf{A} = \mathbf{BC}$ with $\mathbf{B}, \mathbf{C} \in \mathcal{J}_2$.

(c) $\mathcal{J}_1 \subset \mathcal{J}_2 \subset$ Compact operators.

(d) For any operator $\mathbf{A}$, we have $\mathbf{A} \in \mathcal{J}_2$ if $\sum_n \|\mathbf{A}\phi_n\|^2 < \infty$ for a single basis.
For any operator $\mathbf{A} \geq 0$ we have $\mathbf{A} \in \mathcal{J}_1$ if $\sum_n |\langle\phi_n, \mathbf{A}\phi_n\rangle| < \infty$ for a single basis.

(e) If $\mathbf{A} \in \mathcal{J}_1$, $\mathrm{Tr}(\mathbf{A}) = \sum\langle\phi_n, \mathbf{A}\phi_n\rangle$ is independent of the basis used.

(f) Tr is linear and obeys $\mathrm{Tr}(\mathbf{A}^\dagger) = \overline{\mathrm{Tr}(\mathbf{A})}$; $\mathrm{Tr}(\mathbf{AB}) = \mathrm{Tr}(\mathbf{BA})$ if either $\mathbf{A} \in \mathcal{J}_1$ and $\mathbf{B}$ bounded, $\mathbf{A}$ bounded and $\mathbf{B} \in \mathcal{J}_1$ or both $\mathbf{A}, \mathbf{B} \in \mathcal{J}_2$.

(g) $\mathcal{J}_2$ endowed with the inner product $\langle\mathbf{A}, \mathbf{B}\rangle_2 = \mathrm{Tr}(\mathbf{A}^\dagger\mathbf{B})$ is a Hilbert space. If $\|\mathbf{A}\|_2 = [\,\mathrm{Tr}(\mathbf{A}^\dagger\mathbf{A})\,]^{\frac{1}{2}}$, then $\|\mathbf{A}\|_2 \geq \|\mathbf{A}\|$ and $\mathcal{J}_2$ is the $\| \, \|_2$-closure of the *finite* rank operators.

(h) $\mathcal{J}_1$ endowed with the norm $\|\mathbf{A}\|_1 = \mathrm{Tr}(\sqrt{\mathbf{A}^\dagger\mathbf{A}})$ is a Banach space. $\|\mathbf{A}\|_1 \geq \|\mathbf{A}\|_2 \geq \|\mathbf{A}\|$ and $\mathcal{J}_1$ is the $\| \, \|_1$-norm closure of the *finite* rank operators. The dual space of $\mathcal{J}_1$ is $\mathcal{B}(\mathcal{H})$, the family of bounded operators with the duality $\langle\mathbf{B}, \mathbf{A}\rangle = \mathrm{Tr}(\mathbf{BA})$.

(i) If $\mathbf{A}, \mathbf{B} \in \mathcal{J}_2$, then $\|\mathbf{AB}\|_1 \leq \|\mathbf{A}\|_2\|\mathbf{B}\|_2$. If $\mathbf{A} \in \mathcal{J}_2$ and $\mathbf{B} \in \mathcal{B}(\mathcal{H})$, then $\|\mathbf{AB}\|_2 \leq \|\mathbf{A}\|_2\|\mathbf{B}\|$. If $\mathbf{A} \in \mathcal{J}_1$ and $\mathbf{B} \in \mathcal{B}(\mathcal{H})$, then $\|\mathbf{AB}\|_1 \leq \|\mathbf{A}\|_1\|\mathbf{B}\|$.

Note the most important property for proving that an operator is trace class is the decomposition **(b)** into two Hilbert-Schmidt ones, as the Hilbert-Schmidt property can easily be verified in one single orthonormal basis (see

(d)). Property **(e)** ensures then that the trace is the same in any basis. Properties **(a)** and **(f)** show that trace class operators behave in complete analogy to finite rank operators. The proof whether a matrix is trace-class (or Hilbert-Schmidt) or not simplifies enormously for diagonal matrices, as then the second part of property **(d)** is directly applicable: just the moduli of the eigenvalues (or – in case of Hilbert-Schmidt – the squares of the eigenvalues) have to be summed up in order to answer that question. A good strategy in checking the trace-class character of a general matrix **A** is therefore the decomposition of that matrix into two matrices **B** and **C** where one, say **C**, should be chosen to be diagonal and either just barely of Hilbert-Schmidt character leaving enough freedom for its partner **B** or of trace-class character such that one only has to show the boundedness for **B**.

J.4 Determinants of trace class operators

This section is mainly based on refs. [J.8, J.10] which should be consulted for more details and proofs. See also refs. [J.11, J.14].

Pre-definitions (Alternating algebra and Fock spaces):
Given a Hilbert space $\mathcal{H}$, $\otimes^n\mathcal{H}$ is defined as the vector space of multi-linear functionals on $\mathcal{H}$ with $\phi_1 \otimes \cdots \otimes \phi_n \in \otimes^n\mathcal{H}$ in case $\phi_1, \ldots, \phi_n \in \mathcal{H}$. $\bigwedge^n(\mathcal{H})$ is defined as the subspace of $\otimes^n\mathcal{H}$ spanned by the wedge-product

$$\phi_1 \wedge \cdots \wedge \phi_n = \frac{1}{\sqrt{n!}} \sum_{\pi \in \mathcal{P}_n} \epsilon(\pi)[\phi_{\pi(1)} \otimes \cdots \otimes \phi_{\pi(n)}] \tag{J.15}$$

where $\mathcal{P}_n$ is the group of all permutations of n letters and $\epsilon(\pi) = \pm 1$ depending on whether π is an even or odd permutation, respectively. The inner product in $\bigwedge^n(\mathcal{H})$ is given by

$$(\phi_1 \wedge \cdots \wedge \phi_n, \eta_1 \wedge \cdots \wedge \eta_n) = \det\{(\phi_i, \eta_j)\} \tag{J.16}$$

where $\det\{a_{ij}\} = \sum_{\pi \in \mathcal{P}_n} \epsilon(\pi) a_{1\pi(1)} \cdots a_{n\pi(n)}$. $\bigwedge^n(\mathbf{A})$ is defined as functor (a functor satisfies $\bigwedge^n(\mathbf{AB}) = \bigwedge^n(\mathbf{A}) \bigwedge^n(\mathbf{B})$) on $\bigwedge^n(\mathcal{H})$ with

$$\bigwedge^n(\mathbf{A})\,(\phi_1 \wedge \cdots \wedge \phi_n) = \mathbf{A}\phi_1 \wedge \cdots \wedge \mathbf{A}\phi_n\ . \tag{J.17}$$

When $n = 0$, $\bigwedge^n(\mathcal{H})$ is defined to be C and $\bigwedge^n(\mathbf{A})$ as 1: $C \to C$.

Properties: If **A** trace class, i.e., $\mathbf{A} \in \mathcal{J}_1$, then for any k, $\bigwedge^k(\mathbf{A})$ is trace class, and for any orthonormal basis $\{\phi_n\}$ the cumulant

$$\mathrm{Tr}\left(\bigwedge^k(\mathbf{A})\right) = \sum_{i_1 < \cdots < i_k} ((\phi_{i_1} \wedge \cdots \wedge \phi_{i_k}), (\mathbf{A}\phi_{i_1} \wedge \cdots \wedge \mathbf{A}\phi_{i_k})) < \infty \tag{J.18}$$

is independent of the basis (with the understanding that $\mathrm{Tr}\bigwedge^0(\mathbf{A}) \equiv 1$).

Definition: Let $\mathbf{A} \in \mathcal{J}_1$, then $\mathbf{det(1{+}A)}$ is defined as

$$\det(\mathbf{1}+\mathbf{A}) = \sum_{k=0}^{\infty} \mathrm{Tr}\left(\bigwedge^k(\mathbf{A})\right) \qquad (J.19)$$

Properties:

Let $\mathbf{A}$ be a linear operator on a separable Hilbert space $\mathcal{H}$ and $\{\phi_j\}_1^\infty$ an orthonormal basis.

(a) $\sum_{k=0}^{\infty} \mathrm{Tr}\left(\bigwedge^k(\mathbf{A})\right)$ converges for each $\mathbf{A} \in \mathcal{J}_1$.

(b) $|\det(\mathbf{1}{+}\mathbf{A})| \leq \prod_{j=1}^{\infty}(1+\mu_j(\mathbf{A}))$ where $\mu_j(\mathbf{A})$ are the *singular* values of $\mathbf{A}$, i.e., the eigenvalues of $|\mathbf{A}| = \sqrt{\mathbf{A}^\dagger\mathbf{A}}$.

(c) $|\det(\mathbf{1}+\mathbf{A})| \leq \exp(\|\mathbf{A}\|_1)$.

(d) For any $\mathbf{A}_1, \ldots, \mathbf{A}_n \in \mathcal{J}_1$, $\langle z_1, \ldots, z_n\rangle \mapsto \det\left(\mathbf{1} + \sum_{i=1}^{n} z_i\mathbf{A}_i\right)$ is an entire analytic function.

(e) If $\mathbf{A}, \mathbf{B} \in \mathcal{J}_1$, then

$$\begin{aligned}
\det(\mathbf{1}+\mathbf{A})\det(\mathbf{1}+\mathbf{B}) &= \det\left(\mathbf{1}+\mathbf{A}+\mathbf{B}+\mathbf{AB}\right) \\
&= \det\left((\mathbf{1}+\mathbf{A})(\mathbf{1}+\mathbf{B})\right) \\
&= \det\left((\mathbf{1}+\mathbf{B})(\mathbf{1}+\mathbf{A})\right) \; . \qquad (J.20)
\end{aligned}$$

If $\mathbf{A} \in \mathcal{J}_1$ and $\mathbf{U}$ unitary, then

$$\det\left(\mathbf{U}^{-1}(\mathbf{1}+\mathbf{A})\mathbf{U}\right) = \det\left(\mathbf{1}+\mathbf{U}^{-1}\mathbf{A}\mathbf{U}\right) = \det(\mathbf{1}+\mathbf{A}) \; . \qquad (J.21)$$

(f) If $\mathbf{A} \in \mathcal{J}_1$, then $(\mathbf{1}+\mathbf{A})$ is invertible if and only if $\det(\mathbf{1}+\mathbf{A}) \neq 0$.

(g) If $\lambda \neq 0$ is an n-times degenerate eigenvalue of $\mathbf{A} \in \mathcal{J}_1$, then $\det(\mathbf{1}+z\mathbf{A})$ has a zero of order n at $z = -1/\lambda$.

(h) For any ϵ, there is a $C_\epsilon(\mathbf{A})$, depending on $\mathbf{A} \in \mathcal{J}_1$, so that $|\det(\mathbf{1}+z\mathbf{A})| \leq C_\epsilon(\mathbf{A})\exp(\epsilon|z|)$.

(i) For any $\mathbf{A} \in \mathcal{J}_1$,

$$\det(\mathbf{1}+\mathbf{A}) = \prod_{j=1}^{N(\mathbf{A})}(1+\lambda_j(\mathbf{A})) \qquad (J.22)$$

where here and in the following $\{\lambda_j(\mathbf{A})\}_{j=1}^{N(\mathbf{A})}$ are the eigenvalues of $\mathbf{A}$ counted with algebraic multiplicity .

(j) *Lidskii's theorem:* For any $\mathbf{A} \in \mathcal{J}_1$,

$$\mathrm{Tr}(\mathbf{A}) = \sum_{j=1}^{N(\mathbf{A})} \lambda_j(\mathbf{A}) < \infty \ . \tag{J.23}$$

(k) If $\mathbf{A} \in \mathcal{J}_1$, then

$$\begin{aligned} \mathrm{Tr}\left(\bigwedge^k(\mathbf{A})\right) &= \sum_{j=1}^{N(\bigwedge^k(\mathbf{A}))} \lambda_j\left(\bigwedge^k(\mathbf{A})\right) \\ &= \sum_{1\le j_1<\cdots<j_k\le N(\mathbf{A})} \lambda_{j_1}(\mathbf{A})\cdots\lambda_{j_k}(\mathbf{A}) < \infty. \end{aligned}$$

(l) If $\mathbf{A} \in \mathcal{J}_1$, then

$$\det(1+z\mathbf{A}) = \sum_{k=0}^{\infty} z^k \sum_{1\le j_1<\cdots<j_k\le N(\mathbf{A})} \lambda_{j_1}(\mathbf{A})\cdots\lambda_{j_k}(\mathbf{A}) < \infty \tag{J.24}$$

(m) If $\mathbf{A} \in \mathcal{J}_1$, then for $|z|$ small (i.e., $|z|\max|\lambda_j(\mathbf{A})| < 1$) the series $\sum_{k=1}^{\infty} z^k \mathrm{Tr}\left((-\mathbf{A})^k\right)/k$ converges and

$$\begin{aligned} \det(1+z\mathbf{A}) &= \exp\left(-\sum_{k=1}^{\infty}\frac{z^k}{k}\mathrm{Tr}\left((-\mathbf{A})^k\right)\right) \\ &= \exp\left(\mathrm{Tr}\ln(\mathbf{1}+z\mathbf{A})\right) \ . \end{aligned} \tag{J.25}$$

(n) *The Plemelj-Smithies formula:* Define $\alpha_m(\mathbf{A})$ for $\mathbf{A} \in \mathcal{J}_1$ by

$$\det(\mathbf{1}+z\mathbf{A}) = \sum_{m=0}^{\infty} z^m \frac{\alpha_m(\mathbf{A})}{m!} \ . \tag{J.26}$$

Then $\alpha_m(\mathbf{A})$ is given by the $m \times m$ determinant:

$$\alpha_m(\mathbf{A}) = \begin{vmatrix} \mathrm{Tr}(\mathbf{A}) & m-1 & 0 & \cdots & 0 \\ \mathrm{Tr}(\mathbf{A}^2) & \mathrm{Tr}(\mathbf{A}) & m-2 & \cdots & 0 \\ \mathrm{Tr}(\mathbf{A}^3) & \mathrm{Tr}(\mathbf{A}^2) & \mathrm{Tr}(\mathbf{A}) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & & 1 \\ \mathrm{Tr}(\mathbf{A}^m) & \mathrm{Tr}(\mathbf{A}^{(m-1)}) & \mathrm{Tr}(\mathbf{A}^{(m-2)}) & \cdots & \mathrm{Tr}(\mathbf{A}) \end{vmatrix} \tag{J.27}$$

with the understanding that $\alpha_0(\mathbf{A}) \equiv 1$ and $\alpha_1(\mathbf{A}) \equiv \mathrm{Tr}(\mathbf{A})$. Thus the cumulants $c_m(\mathbf{A}) \equiv \alpha_m(\mathbf{A})/m!$ satisfy the following recursion relation

$$\begin{aligned} c_m(\mathbf{A}) &= \frac{1}{m}\sum_{k=1}^{m}(-1)^{k+1}c_{m-k}(\mathbf{A})\,\mathrm{Tr}(\mathbf{A}^k) \quad \text{for } m \ge 1 \\ c_0(\mathbf{A}) &\equiv 1 \ . \end{aligned} \tag{J.28}$$

Note that in the context of quantum mechanics formula (J.26) is the quantum analog to the curvature expansion of the semiclassical zeta function with $\mathrm{Tr}(\mathbf{A}^m)$ corresponding to the sum of all periodic orbits (prime and also repeated ones) of *total* topological length m, i.e., let $c_m(\text{s.c.})$ denote the m^{th} curvature term, then the curvature expansion of the semiclassical zeta function is given by the recursion relation

$$\begin{aligned} c_m(\text{s.c.}) &= \frac{1}{m}\sum_{k=1}^{m}(-1)^{k+m+1}c_{m-k}(\text{s.c.})\sum_{\substack{p;r>0\\ \text{with } [p]r=k}}[p]\,\frac{t_p(k)^r}{1-\left(\frac{1}{\Lambda_p}\right)^r} \qquad \text{for } m\geq 1 \\ c_0(\text{s.c.}) &\equiv 1\,. \end{aligned} \tag{J.29}$$

In fact, in the cumulant expansion (J.26) as well as in the curvature expansion there are large cancelations involved. Let us order – without lost of generality – the eigenvalues of the operator $\mathbf{A}\in\mathcal{J}_1$ as follows:

$$|\lambda_1|\geq|\lambda_2|\geq\cdots\geq|\lambda_{i-1}|\geq|\lambda_i|\geq|\lambda_{i+1}|\geq\cdots$$

(This is always possible because of $\sum_{i=1}^{N(\mathbf{A})}|\lambda_i|<\infty$.) Then, in the standard (Plemelj-Smithies) cumulant evaluation of the determinant, eq. (J.26), we have enormous cancellations of big numbers, e.g. at the k^{th} cumulant order ($k>3$), all the intrinsically large 'numbers' λ_1^k, $\lambda_1^{k-1}\lambda_2$, …, $\lambda_1^{k-2}\lambda_2\lambda_3$, … and many more have to cancel out exactly until only $\sum_{1\leq j_1<\cdots<j_k\leq N(\mathbf{A})}\lambda_{j_1}\cdots\lambda_{j_k}$ is finally left over. Algebraically, the fact that there are these large cancellations is of course of no importance. However, if the determinant is calculated numerically, the big cancellations might spoil the result or even the convergence. Now, the curvature expansion of the semiclassical zeta function, as it is known today, *is* the semiclassical approximation to the curvature expansion (unfortunately) in the Plemelj-Smithies form. As the exact quantum mechanical result is approximated semiclassically, the errors introduced in the approximation might lead to big effects as they are done with respect to large quantities which eventually cancel out and not – as it would be of course better – with respect to the small surviving cumulants. Thus it would be very desirable to have a semiclassical analog to the reduced cumulant expansion (J.24) or even to (J.22) directly. It might not be possible to find a direct semiclassical analog for the individual eigenvalues λ_j. Thus the direct construction of the semiclassical equivalent to (J.22) is rather unlikely. However, in order to have a semiclassical "cumulant" summation without large cancellations – see (J.24) – it would be just sufficient to find the semiclassical analog of each complete cumulant (J.24) and not of the single eigenvalues. Whether this will eventually be possible is still an open question.

J.5 Von Koch matrices

Implicitly, many of the above properties are based on the theory of von Koch matrices [J.11, J.12, J.13]: An infinite matrix $\mathbf{1}-\mathbf{A}=\|\delta_{jk}-$

$a_{jk}\|_1^\infty$, consisting of complex numbers, is called a matrix with an *absolutely convergent determinant*, if the series $\sum |a_{j_1 k_1} a_{j_2 k_2} \cdots a_{j_n, k_n}|$ converges, where the sum extends over all pairs of systems of indices $(j_1, j_2, \cdots, j_n)$ and $(k_1, k_2, \cdots, k_n)$ which differ from each other only by a permutation, and $j_1 < j_2 < \cdots j_n$ $(n = 1, 2, \cdots)$. Then the limit

$$\lim_{n\to\infty} \det\|\delta_{jk} - a_{jk}\|_1^n = \det(\mathbf{1} - \mathbf{A})$$

exists and is called the determinant of the matrix $\mathbf{1} - \mathbf{A}$. It can be represented in the form

$$\det(\mathbf{1} - \mathbf{A}) = 1 - \sum_{j=1}^{\infty} a_{jj} + \frac{1}{2!} \sum_{j,k=1}^{\infty} \begin{vmatrix} a_{jj} & a_{jk} \\ a_{kj} & a_{kk} \end{vmatrix} - \frac{1}{3!} \sum_{j,k,m=1}^{\infty} \begin{vmatrix} a_{jj} & a_{jk} & a_{jm} \\ a_{kj} & a_{kk} & a_{km} \\ a_{mj} & a_{mk} & a_{mm} \end{vmatrix} + \cdots$$

where the series on the r.h.s. will remain convergent even if the numbers a_{jk} $(j, k = 1, 2, \cdots)$ are replaced by their moduli and if all the terms obtained by expanding the determinants are taken with the plus sign. The matrix $\mathbf{1} - \mathbf{A}$ is called *von Koch matrix*, if both conditions

$$\sum_{j=1}^{\infty} |a_{jj}| \quad < \quad \infty \,, \tag{J.30}$$

$$\sum_{j,k=1}^{\infty} |a_{jk}|^2 \quad < \quad \infty \tag{J.31}$$

are fulfilled. Then the following holds (see ref. [J.11, J.13]): (1) Every von Koch matrix has an absolutely convergent determinant. If the elements of a von Koch matrix are functions of some parameter μ ($a_{jk} = a_{jk}(\mu)$, $j, k = 1, 2, \cdots$) and both series in the defining condition converge uniformly in the domain of the parameter μ, then as $n \to \infty$ the determinant $\det\|\delta_{jk} - a_{jk}(\mu)\|_1^n$ tends to the determinant $\det(\mathbf{1} + \mathbf{A}(\mu))$ uniformly with respect to μ, over the domain of μ. (2) If the matrices $\mathbf{1} - \mathbf{A}$ and $\mathbf{1} - \mathbf{B}$ are von Koch matrices, then their product $\mathbf{1} - \mathbf{C} = (\mathbf{1} - \mathbf{A})(\mathbf{1} - \mathbf{B})$ is a von Koch matrix, and

$$\det(\mathbf{1} - \mathbf{C}) = \det(\mathbf{1} - \mathbf{A}) \det(\mathbf{1} - \mathbf{B}) \,. \tag{J.32}$$

Note that every trace-class matrix $\mathbf{A} \in \mathcal{J}_1$ is also a von Koch matrix (and that any matrix satisfying condition (J.31) is Hilbert-Schmidt and vice versa). The inverse implication, however, is not true: von Koch matrices are not automatically trace-class. The caveat is that the definition of von Koch matrices is basis-dependent, whereas the trace-class property is basis-*independent*. As the traces involve infinite sums, the basis-independence is not at all trivial. An example for an infinite matrix which is von Koch, but not trace-class is the following:

$$\mathbf{A}_{ij} = \begin{cases} 2/j & \text{for} \quad i-j=-1 \quad \text{and} \quad j \text{ even} \, , \\ 2/i & \text{for} \quad i-j=+1 \quad \text{and} \quad i \text{ even} \, , \\ 0 & \text{else} \, , \end{cases}$$

i.e.,

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 1/2 & 0 & 0 & \cdots \\ 0 & 0 & 1/2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 1/3 & \ddots \\ 0 & 0 & 0 & 0 & 1/3 & 0 & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix} . \tag{J.33}$$

Obviously, condition (J.30) is fulfilled by definition. Second, the condition (J.31) is satisfied as $\sum_{n=1}^{\infty} 2/n^2 < \infty$. However, the sum over the moduli of the eigenvalues is just twice the harmonic series $\sum_{n=1}^{\infty} 1/n$ which does not converge. The matrix (J.33) violates the trace-class definition (J.13), as in its eigenbasis the sum over the moduli of its diagonal elements is infinite. Thus the *absolute* convergence is traded for a *conditional* convergence, since the sum over the eigenvalues themselves can be arranged to still be zero, if the eigenvalues with the same modulus are summed first. Absolute convergence is of course essential, if sums have to be rearranged or exchanged. Thus, the trace-class property is indispensable for any controlled unitary transformation of an infinite determinant, as then there will be necessarily a change of basis and in general also a re-ordering of the corresponding traces. Therefore the claim that *a Hilbert-Schmidt operator with a vanishing trace is automatically trace-class* is false. In general, such an operator has to be regularized in addition (see next chapter).

J.6 Regularization

Many interesting operators are not of trace class (although they might be in some $\mathcal{J}_p$ with $p > 1$ - an operator A is in $\mathcal{J}_p$ iff $\mathrm{Tr}|A|^p < \infty$ in any orthonormal basis). In order to compute determinants of such operators, an extension of the cumulant expansion is needed which in fact corresponds to a regularization procedure [J.8, J.10]:
E.g. let $\mathbf{A} \in \mathcal{J}_p$ with $p \leq n$. Define

$$R_n(z\mathbf{A}) = (\mathbf{1} + z\mathbf{A}) \exp\left(\sum_{k=1}^{n-1} \frac{(-z)^k}{k} \mathbf{A}^k \right) - \mathbf{1} \tag{J.34}$$

as the regulated version of the operator $z\mathbf{A}$. Then the regulated operator $R_n(z\mathbf{A})$ is trace class, i.e., $R_n(z\mathbf{A}) \in \mathcal{J}_1$. Define now $\det_n(\mathbf{1}+z\mathbf{A}) = \det(\mathbf{1}+R_n(z\mathbf{A}))$. Then the regulated determinant

$$\det_n(\mathbf{1}+z\mathbf{A}) = \prod_{j=1}^{N(z\mathbf{A})} \left[(1+z\lambda_j(\mathbf{A})) \exp\left(\sum_{k=1}^{n-1} \frac{(-z\lambda_j(\mathbf{A}))^k}{k} \right) \right] < \infty \tag{J.35}$$

exists and is finite. The corresponding Plemelj-Smithies formula now reads [J.10]:

$$\det_n(\mathbf{1}+z\mathbf{A}) = \sum_{m=0}^{\infty} z^m \frac{\alpha_m^{(n)}(\mathbf{A})}{m!} \,. \tag{J.36}$$

with $\alpha_m^{(n)}(\mathbf{A})$ given by the $m \times m$ determinant:

$$\alpha_m^{(n)}(\mathbf{A}) = \begin{vmatrix} \sigma_1^{(n)} & m-1 & 0 & \cdots & 0 \\ \sigma_2^{(n)} & \sigma_1^{(n)} & m-2 & \cdots & 0 \\ \sigma_3^{(n)} & \sigma_2^{(n)} & \sigma_1^{(n)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & & 1 \\ \sigma_m^{(n)} & \sigma_{m-1}^{(n)} & \sigma_{m-2}^{(n)} & \cdots & \sigma_1^{(n)} \end{vmatrix} \tag{J.37}$$

where

$$\sigma_k^{(n)} = \begin{cases} \mathrm{Tr}(\mathbf{A}^k) & k \geq n \\ 0 & k \leq n-1 \end{cases}$$

As Simon [J.10] says simply, the beauty of (J.37) is that we get $\det_n(\mathbf{1}+\mathbf{A})$ from the standard Plemelj-Smithies formula (J.26) by simply setting $\mathrm{Tr}(\mathbf{A})$, $\mathrm{Tr}(\mathbf{A}^2)$, ..., $\mathrm{Tr}(\mathbf{A}^{n-1})$ to zero.

See also ref. [J.15] where $\{\lambda_j\}$ are the eigenvalues of an elliptic (pseudo)-differential operator $\mathbf{H}$ of order m on a compact or bounded manifold of dimension d, $0 < \lambda_0 \leq \lambda_1 \leq \cdots$ and $\lambda_k \uparrow +\infty$. and the Fredholm determinant

$$\Delta(\lambda) = \prod_{k=0}^{\infty} \left(1 - \frac{\lambda}{\lambda_k}\right) \tag{J.38}$$

is regulated in the case $\mu \equiv d/m > 1$ as Weierstrass product

$$\Delta(\lambda) = \prod_{k=0}^{\infty} \left[\left(1 - \frac{\lambda}{\lambda_k}\right) \exp\left(\frac{\lambda}{\lambda_k} + \frac{\lambda^2}{2\lambda_k^2} + \cdots + \frac{\lambda^{[\mu]}}{[\mu]\lambda_k^{[\mu]}} \right) \right] \tag{J.39}$$

where $[\mu]$ denotes the integer part of μ. This is, see ref. [J.15], the unique entire function of order μ having zeros at $\{\lambda_k\}$ and subject to the normalization conditions

$$\ln \Delta(0) = \frac{d}{d\lambda} \ln \Delta(0) = \cdots = \frac{d^{[\mu]}}{d\lambda^{[\mu]}} \ln \Delta(0) = 0 \,. \tag{J.40}$$

Clearly (J.39) is the same as (J.35); one just has to identify $z = -\lambda$, $\mathbf{A} = 1/\mathbf{H}$ and $n - 1 = [\mu]$. An example is the regularization of the spectral determinant

$$\Delta(E) = \det\left[(E - \mathbf{H})\right] \tag{J.41}$$

which – as it stands – would only make sense for a finite dimensional basis (or finite dimensional matrices). In ref. [J.16] the regulated spectral determinant for the example of the hyperbola billiard in two dimensions (thus $d = 2$, $m = 2$ and hence $\mu = 1$) is given as

$$\Delta(E) = \det\left[(E - \mathbf{H})\Omega(E, \mathbf{H})\right] \tag{J.42}$$

where

$$\Omega(E, \mathbf{H}) = -\mathbf{H}^{-1} e^{E\mathbf{H}^{-1}} \tag{J.43}$$

such that the spectral determinant in the eigenbasis of $\mathbf{H}$ (with eigenvalues $E_n \neq 0$) reads

$$\Delta(E) = \prod_n \left(1 - \frac{E}{E_n}\right) e^{E/E_n} < \infty \,. \tag{J.44}$$

Note that $\mathbf{H}^{-1}$ is for this example of Hilbert-Schmidt character.

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