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# Analyticity of the Partition Function for Finite Quantum Systems

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**Abstract.** The partition function $Z(\beta,\lambda)=\mathrm{Tr}\,e^{-\beta(T+\lambda V)}$ for a finite quantized system is investigated. If the interaction $V$ is a relatively bounded operator with respect to the kinetic energy $T$ with $T$-bound $b<1$, $Z(\beta,\lambda)$ is shown to be a holomorphic function of $\beta$ and $\lambda$ for

$$|\arg\beta| < \operatorname{arc\,tg}\frac{\sqrt{1-b^2|\lambda|^2}}{b|\lambda|} \quad \text{and} \quad |\lambda|<b^{-1}.$$

For $b=0$ $Z(\beta,\lambda)$ is an entire function of $\lambda$ and holomorphic in $\beta$ for $\mathrm{Re}\,\beta>0$.

## 1. Introduction

The partition function for a canonical ensemble is defined to be $\mathrm{Tr}\,e^{-\beta H}$, where $H$ is the Hamiltonian of the system under consideration. We are dealing in this work with finite systems only (i.e., a finite number of particles in a box of finite volume), for which $H$ can be decomposed into the kinetic energy $T$ and the interaction energy $\lambda V$ ($\lambda$ = coupling constant). In the Schrödinger representation $T$ is given by the $3n$-dimensional Laplace operator $T=-\Delta_{3n}$ ($n$ = number of particles) with suitable boundary conditions to make it self-adjoint; $V$ is usually represented by a set $\{V_m(\underline{x}_1,\ldots,\underline{x}_m)\}$ of $m$-body potentials. In the definition of the partition function $Z(\beta,\lambda)=\mathrm{Tr}\,e^{-\beta(T+\lambda V)}$ we encounter immediately two mathematical problems:

i) find conditions on $V$ under which it is possible to define a semi-bounded self-adjoint Hamiltonian $H=T+\lambda V$;

ii) show that $\mathrm{Tr}\,e^{-\beta H}$ exists for $\beta>0$.

If this has been achieved we may further ask, what are the analytical properties of $Z(\beta,\lambda)$:

a) is $Z(\beta,\lambda)$ an analytic function of $\lambda$ at $\lambda=0$, what is the radius of convergence for the perturbation series?

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b) is $Z(\beta, \lambda)$ analytic in $\beta$ for $\beta > 0$ or are there singularities?

All these questions have been answered in Ref. [1] for interactions, for which $V$ is a bounded operator. It turns out that $Z(\beta, \lambda)$ behaves as nicely as possible in this particular case: it is an analytic function both in $\beta$ and $\lambda$ for $\operatorname{Re}\beta > 0$ and all complex $\lambda$. Unfortunately, in most applications one has to do with potentials which give rise to unbounded operators, as there is the Coulomb potential or the Yukawa potential. However, though these potentials give rise to unbounded operators these are small compared to the kinetic energy $T$, even infinitely small in the sense that for any $b > 0$ we can find some $a > 0$ with $\|V\varphi\| \leqq a\|\varphi\| + b\|T\varphi\|$ for all $\varphi$ in the domain of $T$ [2]. In this case, it is known that $T + \lambda V$ can be uniquely defined as a semi-bounded self-adjoint operator for all real $\lambda$. Furthermore $T + \lambda V$ has a discrete spectrum which is not too different from that of $T$. From that we may infer that $Z(\beta, \lambda)$ has the same nice analyticity properties as for bounded operators $V$. In the following, we shall aim at proving this. Let us first provide some mathematical tools.

## 2. Mathematical Preliminary

Let $\mathscr{H}$ denote a Hilbert space, $\mathfrak{B}(\mathscr{H})$ the Banach space of bounded linear operators on $\mathscr{H}$ equipped with the usual operator norm $\|T\| = \sup \|T\varphi\|/\|\varphi\|$. In addition, we introduce the Banach spaces $\mathfrak{B}_p(\mathscr{H})$ of operators $T \in \mathfrak{B}(\mathscr{H})$ with $\operatorname{Tr}(T^* T)^{p/2} < \infty (p \geqq 1)$ with the norm $\|T\|_p = (\operatorname{Tr}(T^* T)^{p/2})^{1/p}$. They satisfy the remarkable inclusion property

$$\mathfrak{B}_1(\mathscr{H}) \subset \mathfrak{B}_p(\mathscr{H}) \subset \mathfrak{B}_q(\mathscr{H}) \subset \mathfrak{B}(\mathscr{H})$$

for $q \geqq p \geqq 1$, such that the injection of $\mathfrak{B}_p(\mathscr{H}) \to \mathfrak{B}_q(\mathscr{H})$ is a continuous map. Furthermore, the norms $\|.\|_p$ have the following properties [2, 3]:

i) $\|ATB\|_p \leqq \|A\| \; \|B\| \; \|T\|_p$ for $A, B \in \mathfrak{B}(\mathscr{H})$, $T \in \mathfrak{B}_p(\mathscr{H})$;
ii) $\|TS\|_1 \leqq \|T\|_2 \; \|S\|_2$ for $T, S \in \mathfrak{B}_2(\mathscr{H})$;
iii) $|\operatorname{Tr} T| \leqq \|T\|_1$ for $T \in \mathfrak{B}_1(\mathscr{H})$;
iv) $\|T\| \leqq \|T\|_p \leqq \|T\|_q \leqq \|T\|_1$ for $p \geqq q$;
v) $T_1 \geqq T_2 \geqq 0 \Rightarrow \|T_1\|_p \geqq \|T_2\|_p$ for $T_1, T_2 \in \mathfrak{B}_p(\mathscr{H})$;
vi) For $T, S \in \mathfrak{B}(\mathscr{H})$ with $T = T^* \geqq 0$, $S = S^* \geqq 0$, one has, $\operatorname{Tr}(TS)^{2^r} \leqq \operatorname{Tr}(T^{2^q} S^{2^q})^{2^{r-q}}$ for $r \geqq q \geqq 0$, entire, whenever the right-hand side exists [4][1].

From Ref. [2], IV (1.1), we take over the following

*Definition.* If $T$ is some operator with a domain $\mathscr{D}_T$, we call $V$ a $T$-bounded operator if it is defined on $\mathscr{D}_T$ and we can find $a > 0$ and

[1] I am grateful to Professor W. Thirring for pointing out this inequality to me.

$b>0$, such that

$$\|V\varphi\| \leqq a\|\varphi\| + b\|T\varphi\| \quad \text{for all} \quad \varphi \in \mathscr{D}_T. \tag{1}$$

The infimum of all possible $b$'s for which Eq. (1) is true with some $a>0$ is called the $T$-bound of $V$.

### 3. The Analyticity Properties of $e^{-\beta(T+\lambda V)}$ and $Z(\beta, \lambda)$

The analyticity properties of the partition function $Z(\beta, \lambda)$ may be inferred from the following

**Theorem.** *Let $T$ be a non-negative self-adjoint operator with $\|(T-z_0)^{-1}\|_{2^r} < \infty$ for some $z_0 < 0$ and $r \geqq 0$, entire, and $V$ be T-bounded with T-bound $b<1$, then $\mathscr{U}(\beta, \lambda) = e^{-\beta(T+\lambda V)}$ can uniquely be continued to a holomorphic map of the domain*

$$G_b = \left\{(\beta, \lambda) \in \mathbb{C}^2; |\arg \beta| < \operatorname{arc\,tg} \frac{\sqrt{1-b^2|\lambda|^2}}{b|\lambda|}, \ |\lambda| < b^{-1}\right\}$$

*into $\mathfrak{B}_1(\mathscr{H})$. Furthermore, $Z(\beta, \lambda) = \operatorname{Tr} \mathscr{U}(\beta, \lambda)$ is holomorphic on the same domain and has the perturbation expansion $Z(\beta, \lambda) = \sum_{n=0}^{\infty} \lambda^n Z_n(\beta)$ with*

$$\begin{aligned} Z_n(\beta) = (-\beta)^n \int_{B_n} du_1 \dots du_n \operatorname{Tr}(e^{-\beta(1-u_1)T} \\ \cdot V e^{-\beta(u_1-u_2)T} V \dots V e^{-\beta(u_{n-1}-u_n)T} V e^{-\beta u_n T}), \end{aligned} \tag{2}$$

*where $B_n = \{(u_1, \dots, u_n) \in \mathbb{R}^n : 0 \leqq u_1 \leqq 1, 0 \leqq u_i \leqq u_{i-1}, i = 2, \dots, n\}$.*

**Corollary.** *If $V$ has T-bound zero, then the domain of holomorphy of $Z(\beta, \lambda)$ is $\{\operatorname{Re} \beta > 0\} \times \mathbb{C}$.*

*Remark.* It is easily recognized that the kinetic energy operator $T = -\Delta_{3n}$ in a finite box meets the conditions made above, if we take $z_0 < 0$ and $2^r \geqq 3n$.

*Proof of the Theorem.* 1. $\mathscr{U}(\beta, \lambda)$ as a map from $G_b$ to $\mathfrak{B}(\mathscr{H})$.

Self-adjointness and semi-boundedness of $T + \lambda V$ for all $\lambda \in \boldsymbol{R}$ follow from Th.V.4.11 in Ref. [2]. Th.IX.2.6 in Ref. [2] shows that $\mathscr{U}(\beta, \lambda)$ is a holomorphic map from some domain of the form

$$\{|\arg \beta| < \varepsilon\} \times \{|\lambda| < \delta\} \quad \text{to} \quad \mathfrak{B}(\mathscr{H}).$$

Closer inspection of the proof of Th. 2.6 shows that this domain is, in fact, equal to $G_b$ defined above[2]. The definition of $\mathscr{U}(\beta, \lambda)$ for complex

[2] Compare Section 3 of the proof below.

arguments is, by the way, given by formula IX. 1.50 in Ref. [2]

$$\mathcal{U}(\beta, \lambda) = \frac{1}{2\pi i} \int_{\Gamma_{b,\lambda}} e^{-z\beta}(T + \lambda V - z)^{-1} dz \tag{3}$$

We need, however, much more than holomorphy of $\mathcal{U}(\beta, \lambda)$ as a map to $\mathfrak{B}(\mathcal{H})$, since the topology of $\mathfrak{B}_1(\mathcal{H})$ is much finer than that of $\mathfrak{B}(\mathcal{H})$.

2. $\mathcal{U}(\beta, 0)$ lies in $\mathfrak{B}_1(\mathcal{H})$ for $\operatorname{Re}\beta > 0$.

Let $R(z) = (T - z)^{-1}$ be the resolvent of $T$ and $\boldsymbol{P}(T)$ its resolvent set, then we get by

$$R(z) = R(z_0) + (z - z_0) R(z) R(z_0)$$

for $z, z_0 \in \boldsymbol{P}(T)$ and by i)

$$\|R(z)\|_{2^r} \leqq \|R(z_0)\|_{2^r}(1 + |z - z_0| \, \|R(z)\|) < \infty \quad \text{for all} \quad z \in \boldsymbol{P}(T). \tag{4}$$

On the other hand, we find

$$\begin{aligned}\|e^{-\beta T}\|_1 &= \operatorname{Tr} e^{-\operatorname{Re}\beta T} = e^{-z_0 \operatorname{Re}\beta} \operatorname{Tr} e^{-\operatorname{Re}\beta(T - z_0)} \\ &\leqq \frac{e^{-z_0 \operatorname{Re}\beta} c(r)}{(\operatorname{Re}\beta)^{2^r}} \operatorname{Tr}(T - z_0)^{-2^r} < \infty\end{aligned}$$

by v) and because of

$$e^{-x} \leqq \frac{c(r)}{x^{2^r}} \quad \text{for} \quad x > 0.$$

Thus we get $\|e^{-\beta T}\|_1 < \infty$ for $\operatorname{Re}\beta > 0$.

3. The resolvent set of $T + \lambda V$.

For the resolvent $R_\lambda(z) = (T + \lambda V - z)^{-1}$ we have the perturbation expansion

$$R_\lambda(z) = R(z) \sum_{n=0}^{\infty} (\lambda V R(z))^n$$

which converges for $|\lambda| \, \|V R(z)\| < 1$. Eq. (1) gives

$$\begin{aligned}\|V R(z)\| &\leqq a \|R(z)\| + b \|T R(z)\| \\ &\leqq \begin{cases} \dfrac{a}{|\operatorname{Im} z|} + \dfrac{b|z|}{|\operatorname{Im} z|} & \text{for} \quad \operatorname{Re} z \geqq 0 \\[2ex] \dfrac{a}{|z|} + b & \text{for} \quad \operatorname{Re} z < 0. \end{cases}\end{aligned}$$

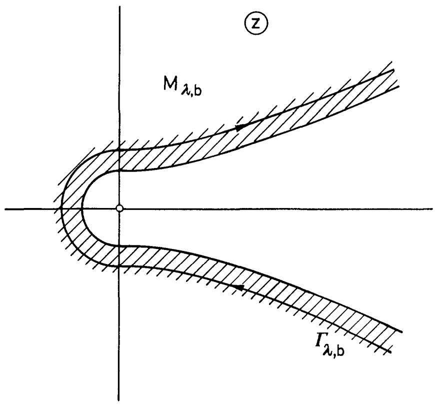


Fig. 1.

From this we conclude that the resolvent set contains the domain (Fig. 1)

$$M_{\lambda,b} = \left\{ \begin{array}{ll} |z| > \dfrac{a|\lambda|}{1-b|\lambda|} \quad \text{for} \quad \operatorname{Re} z \leqq 0 \\ |\operatorname{Im} z| > \dfrac{a|\lambda|}{1-b^2|\lambda|^2} + \dfrac{b|\lambda|}{\sqrt{1-b^2|\lambda|^2}} \sqrt{(\operatorname{Re} z)^2 + \dfrac{a^2|\lambda|^2}{1-b^2|\lambda|^2}} \end{array} \right\} \quad \text{for} \quad \operatorname{Re} z > 0.$$

We observe that for fixed $\lambda$ and $b$ the asymptotic slope of the border line of the domain $M_{\lambda,b}$ is equal to

$$\frac{b|\lambda|}{\sqrt{1-b^2|\lambda|^2}}.$$

4. $\mathscr{U}(\beta, \lambda)$ maps $G_b$ into $\mathfrak{B}_{2^r}(\mathscr{H})$.
From Eq. (3) we get

$$\mathscr{U}(\beta, \lambda) = \frac{1}{2\pi i} \int_{\Gamma_{\lambda,b}} e^{-z\beta} R_\lambda(z)\, dz$$

where $\Gamma_{\lambda,b}$ is the path drawn in Fig. 1. The integral is to be understood as a Bochner integral in $\mathfrak{B}(\mathscr{H})$.
The integral converges for

$$\operatorname{Re}\beta \cdot \operatorname{Re} z > \operatorname{Im}\beta \cdot \operatorname{Im} z \quad \text{for} \quad z \to \infty$$

on $\Gamma_{\lambda,b}$, i.e.,

$$\left| \frac{\operatorname{Im}\beta}{\operatorname{Re}\beta} \right| < \frac{\sqrt{1-b^2|\lambda|^2}}{b|\lambda|}.$$

This gives

$$\|\mathscr{U}(\beta,\lambda)\|_{2^r} \leqq \frac{1}{2\pi} \int_{\Gamma_{\lambda,b}} |e^{-z\beta}| \, \|R_\lambda(z)\|_{2^r} |dz|$$

$$\overset{\text{i)}}{\leqq} \frac{1}{2\pi} \int e^{-\operatorname{Re}(z\beta)} \|R(z)\|_{2^r} (1-|\lambda| \, \|VR(z)\|)^{-1} |dz|$$

$$\overset{(4)}{\leqq} \frac{1}{2\pi} \int e^{-(\operatorname{Re}\beta\cdot\operatorname{Re}z - \operatorname{Im}\beta\cdot\operatorname{Im}z)} \|R(z_0)\|_{2^r} \frac{1+|z-z_0| \, \|R(z)\|}{1-|\lambda| \, \|VR(z)\|} |dz| < \infty$$

for $|\operatorname{Im}\beta| < \dfrac{\sqrt{1-b^2|\lambda|^2}}{b|\lambda|} |\operatorname{Re}\beta|$ since $\dfrac{1+|z-z_0| \, \|R(z)\|}{1-|\lambda| \, \|VR(z)\|}$ is bounded on $\Gamma_{\lambda,b}$. This shows that

$$\mathscr{U}(\beta,\lambda) \in \mathfrak{B}_{2^r}(\mathscr{H}) \quad \text{for} \quad (\beta,\lambda) \in G_b .$$

5. $\mathscr{U}(\beta,\lambda)$ maps $G_b$ into $\mathfrak{B}_1(\mathscr{H})$.

$$\|\mathscr{U}(\beta,\lambda)\|_1 = \|\mathscr{U}(\beta/2,\lambda)^2\|_1 \overset{\text{ii)}}{\leqq} \|\mathscr{U}(\beta/2,\lambda)\|_2^2 .$$

It is even true that

$\|\mathscr{U}(\beta,\lambda)\|_1 \leqq \|\mathscr{U}(\beta/2^k,\lambda)\|_{2^k}^{2^k}$ for $k \geqq 1$, entire, since

as we may prove by induction, using vi)

$k=1$: see above

$$\begin{aligned} k\to k+1: \|\mathscr{U}(\beta/2^k,\lambda)\|_{2^k}^{2^k} &= \operatorname{Tr}(\mathscr{U}^*(\beta/2^k,\lambda)\,\mathscr{U}(\beta/2^k,\lambda))^{2^{k-1}} \\ &= \operatorname{Tr}(\mathscr{U}^*(\beta/2^{k+1},\lambda)^2\,\mathscr{U}(\beta/2^{k+1},\lambda)^2)^{2^{k-1}} \\ &= \operatorname{Tr}(\mathscr{U}(\beta/2^{k+1},\lambda)\,\mathscr{U}^*(.,.)\,\mathscr{U}^*(.,.)\,\mathscr{U}(.,.))^{2^{k+1}} \\ &\overset{\text{vi)}}{\leqq} \operatorname{Tr}[(\mathscr{U}(\beta/2^{k+1},\lambda)\,\mathscr{U}^*(.,.))^{2^{k-1}}(\mathscr{U}^*(.,.)\,\mathscr{U}(.,.))^{2^{k-1}}] \\ &\overset{\text{ii)}}{\leqq} [\operatorname{Tr}(\mathscr{U}(\beta/2^{k+1},\lambda)\,\mathscr{U}^*(.,.))^{2^k} \cdot \operatorname{Tr}(\mathscr{U}^*(.,.)\,\mathscr{U}(.,.))^{2^k}]^{1/2} \\ &= \operatorname{Tr}(\mathscr{U}^*(\beta/2^{k+1},\lambda)\,\mathscr{U}(.,.))^{2^k} = \|\mathscr{U}(\beta/2^{k+1},\lambda)\|_{2^{k+1}}^{2^{k+1}} . \end{aligned}$$

Setting $k=r$, we find

$$\|\mathscr{U}(\beta,\lambda)\|_1 \leqq \|\mathscr{U}(\beta/2^r,\lambda)\|_{2^r}^{2^r} < \infty$$

for $(\beta,\lambda)\in G_b$.

6. Holomorphy of $\mathscr{U}(\beta,\lambda)$ in $\beta$.

For $(\beta,\lambda)\in G_b$ we estimate

$$\|1/\beta'(\mathscr{U}(\beta+\beta',\lambda)-\mathscr{U}(\beta,\lambda)) + (T+\lambda V)\,\mathscr{U}(\beta,\lambda)\|_1$$

$$\overset{\text{i)}}{\leqq} \|(1/\beta'(\mathscr{U}(\beta',\lambda)-\mathbf{1}) + (T+\lambda V))\,\mathscr{U}(\beta/2,\lambda)\| \, \|\mathscr{U}(\beta/2,\lambda)\|_1 \to 0$$

for $|\beta'|\to 0$, since

$$1/\beta'(\mathscr{U}(\beta',\lambda)-\mathbf{1})\,\mathscr{U}(\beta/2,\lambda) \xrightarrow[\beta'\to 0]{} 2\frac{\partial}{\partial\beta}\mathscr{U}(\beta/2,\lambda) = -(T+\lambda V)\,\mathscr{U}(\beta/2,\lambda)$$

in $\mathfrak{B}(\mathscr{H})$ as we deduce from Section 1 of the proof.

7. Holomorphy of $\mathcal{U}(\beta, \lambda)$ in $\lambda$.

$$\mathcal{U}(\beta, \lambda+\lambda') - \mathcal{U}(\beta, \lambda) = -\beta\lambda' \int_0^1 \mathcal{U}(\beta(1-u), \lambda+\lambda')\, V\mathcal{U}(\beta u, \lambda)\, du \tag{5}$$

according to Eq. IX. 2.3 in Ref. [2]; the integral converges even in $\mathfrak{B}_1(\mathcal{H})$, since for $0 \leqq u \leqq \frac{1}{2}$

$$\|\mathcal{U}(\beta(1-u), \lambda+\lambda')\, V\mathcal{U}(\beta u, \lambda)\|_1 \leqq \left\| \mathcal{U}\left(\frac{\beta(1-u)}{2}, \lambda+\lambda'\right)\right\|_1 \cdot \left\| \mathcal{U}\left(\frac{\beta(1-u)}{2}, \lambda+\lambda'\right) V \right\| \cdot \|\mathcal{U}(\beta u, \lambda)\| \leqq \text{const.}$$

for $\beta$, $\lambda$ and $\lambda'$ fixed, $(\beta, \lambda+\lambda') \in G_b$, analogously for $\frac{1}{2} \leqq u \leqq 1$. The constant can be chosen uniformly for $|\lambda'| \leqq \varepsilon$ as can be inferred from Section 4.

From Eq. (5) we deduce the continuity of $\mathcal{U}(\beta, \lambda)$ as a function of $\lambda$ in $\mathfrak{B}_1(\mathcal{H})$. On the other hand, we obtain from Eq. (5)

$$1/\lambda'(\mathcal{U}(\beta, \lambda+\lambda') - \mathcal{U}(\beta, \lambda)) = -\beta \int_0^1 \mathcal{U}(\beta(1-u), \lambda+\lambda')\, V\mathcal{U}(\beta u, \lambda)\, du$$

which converges to

$$-\beta \int_0^1 \mathcal{U}(\beta(1-u), \lambda)\, V\mathcal{U}(\beta u, \lambda)\, du$$

for $\lambda' \to 0$ in $\mathfrak{B}_1(\mathcal{H})$ in view of the continuity of $\mathcal{U}(\beta, \lambda)$ as a function of $\lambda$.

8. Holomorphy of $\operatorname{Tr}\mathcal{U}(\beta, \lambda)$.

Tr being a continuous linear functional on $\mathfrak{B}_1(\mathcal{H})$ [compare iii)] we find the same analyticity properties for $Z(\beta, \lambda) = \operatorname{Tr}\mathcal{U}(\beta, \lambda)$ as we found for $\mathcal{U}(\beta, \lambda)$. Iterating Eq. (5) we end up with the perturbation expansion of $Z(\beta, \lambda)$ with the coefficients given by Eq. (2).

This concludes the proof of the theorem. The Corollary is an immediate consequence of it.

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